

Utilizing Composite Elements for Advanced Mesh Coarsening of
Heat Flow Simulation of Laser Powder Bed Fusion



UNIVERSITY OF
BIRMINGHAM

School of Metallurgy and Material Sciences

Miles H. T. S. Fan

March 2025

Word Count: 33,479

UNIVERSITY OF
BIRMINGHAM

University of Birmingham Research Archive

e-theses repository

This unpublished thesis/dissertation is copyright of the author and/or third parties. The intellectual property rights of the author or third parties in respect of this work are as defined by The Copyright Designs and Patents Act 1988 or as modified by any successor legislation.

Any use made of information contained in this thesis/dissertation must be in accordance with that legislation and must be properly acknowledged. Further distribution or reproduction in any format is prohibited without the permission of the copyright holder.

Abstract

Laser Powder Bed Fusion (LPBF) Additive Manufacturing (AM) is a layer-by-layer method of manufacturing netshape parts from metallic powder. This geometric freedom of manufacture allows new and complex geometries to be realised in many industries. However, due to the potential complex geometries and sequential application of the laser heat source this leads to complex thermal distribution. This can cause issues when there is a dramatic change in cross sectional area in part geometry, as the same parameters that produce 100% density in large bulk can cause manufacturing defects in thin sections. In order to overcome this issue, industry is adopting thermal simulation to predict possible problem areas of the build. However, current part sized thermal solutions are computationally expensive, taking many hours to compute, oftentimes comparable to the build time itself.

In this work, simulation techniques are proposed to overcome some of the limitations of the current thermal simulations and reduce the time of simulation of full build size parts. The first of these techniques establishes a benchmark simulation that leverages the power of parallel computing on modern consumer graphics cards, resulting in a seven-fold increase in simulation speed. The model is validated through comparison to physical experiments. The results suggest that the method of solution of the heat equation can predict meltpool geometries for given parameters. However, the accuracy of the meltpool geometries is heavily dependent on the volumetric source term for the laser. The heat source used here was most accurate for prediction of conduction mode meltpools.

The novel technique shown in Chapter 7 proposes a way to overcome the current limitation of mesh coarsening within a single material phase of a volume of mixed material

types. The method developed herein calculates the hybrid properties of a powder/solid volume to be established on creation of the element on coarsening. Suggestions are also made to how this calculation can be performed with minimal impact on the overall simulation time.

The techniques outlined herein show a marked improvement in macroscopic heatflow simulation speed over the standard techniques discussed in literature. It is speculated that through a combination of these techniques, developments in machine learning, and software development techniques, faster-than-real time heat flow simulation of AM is achievable.

Dedication

To my father, who always said I should be a doctor.

Who also taught me that it is through our actions, not our words, that a human soul is
measured.

Acknowledgements

This work has been carried out using financial support provided by the Engineering and Physical Sciences Research Council (EPSRC) via an iCase award. I would also like to thank the industrial sponsor of this iCase awarded project, Renishaw Plc., for providing additional funds and expertise.

Any Views or opinions expressed herein are that of myself alone, and do not necessarily reflect those of the funding partners (EPSRC and Renishaw Plc.).

I would like to extend my thanks to my supervisor, Dr Mark Ward for his continued faith and support over the long course of this project. A project spanning the COVID-19 pandemic, and the many trials and tribulations associated. Their methodical approach, and attention to detail provided an excellent template to follow as a researcher.

I am also extremely grateful to Dr Rachel Jennings, and Dr Youssef Beshay for their continued technical support and encouragement in this endeavour, and for also providing me with the experience to see this technology in a professional, industrial context. For research without context of application is frivolity.

Finally, I would like to extend my most heartfelt gratitude to Miss Emma Young, and my family. Without whom not only this project, but my other endeavours would never see fruition.

Contents

	Page
Abstract	I
Dedication	III
Acknowledgements	IV
Contents	IX
List of Figures	XV
List of Tables	XVII
List of Symbols	XVIII
Chapter 1: Introduction	1
1.1 A Brief Introduction to LPBF	1
1.2 Thermal Simulation of LPBF	2
1.3 Research Motivation	3
Chapter 2: Background	4
2.1 Powder Bed Fusion (PBF)	4
2.1.1 Process	4
2.1.2 Thermophysical Phenomena	7
2.1.2.1 Absorptivity	7
2.1.2.2 Heat Conduction	9
2.1.2.3 Radiation	12

2.1.2.4	Convection	15
2.1.2.5	Hydrodynamics	17
2.1.2.6	Solidification	19
2.1.3	Manufacturing Defects	23
2.1.3.1	Lack of Fusion Porosity	23
2.1.3.2	Gas Porosity	27
2.1.3.3	Keyhole Porosity	28
2.1.3.4	Cracking	30
2.1.3.4.1	Solidification Cracking	31
2.1.3.4.2	Liquation Cracking	31
2.1.3.4.3	Cold Cracking	32
2.1.3.4.4	Ductility-Dip Cracking	32
2.1.3.4.5	Strain-Age Cracking	33
2.1.4	300 Series High Alloy Stainless Steels and 316L	33
2.1.4.1	Chemical Composition and Phases	33
2.1.4.2	Thermophysical Properties	37
2.1.4.2.1	Enthalpy and Specific Heat Capacity	37
2.1.4.2.2	Thermal Conductivity/Diffusivity	39
2.1.4.3	Additive Manufacturing of SS316L	44
2.2	Numerical Methods	48
2.2.1	Microscopic Scale Methods	49
2.2.1.1	Cellular Automata (a.k.a. Lattice-Boltzmann Model)	49
2.2.1.1.1	Neighbourhood Selection	50
2.2.1.1.2	Cell Transition Rules	51
2.2.1.2	Phase Field (PF) Methods	51
2.2.1.2.1	The Order Parameter	51
2.2.1.2.2	Thermodynamics	52
2.2.1.2.3	Computational Method	52
2.2.1.2.4	Phase Field Modelling of Laser Powder Bed Fusion	55

2.2.2	Mesosopic Scale Methods	59
2.2.2.1	Powder Bed Generation	60
2.2.2.1.1	“Rainfall” Method	60
2.2.2.1.2	Discrete Element Method	61
2.2.3	Macroscopic Scale Methods	64
2.2.3.1	Continuum Modelling	64
2.2.3.1.1	Melt Pool Geometry	65
2.2.3.1.2	Residual Stress and Distortion	67
2.3	Computational Hardware	68
2.3.1	Graphical Process Units	69
2.3.2	Parallel Computation	70
2.4	Concluding Remarks	72
Chapter 3:	Research Aims and Objectives	74
3.1	Research Aims	74
3.2	Research Objectives	74
Chapter 4:	Simulation Methodology	76
4.1	The Heat Equation	76
4.2	Discretization	77
4.2.1	Backwards Difference and Implicit Solvers	78
4.2.1.1	Stability Criteria of Implicit Methods	80
4.2.2	Forwards Difference and Explicit Solvers	81
4.2.2.1	Stability Criteria of Explicit Methods	81
4.3	An Enthalpy Approach of Numerical Solution of the Heat Equation	83
4.3.1	Derivation of Maximum Stable Time step for an Explicit Enthalpy Approach to Solving the Heat Diffusion Equation	86
4.3.2	Representing Laser Power Input	88
4.3.3	Losses	91
4.3.3.1	Radiative Losses	91

4.3.3.2	Convective Losses	91
4.4	Combining Multiple Materials into Hybrid Elements for Mesh Coarsening .	91
4.4.1	The Fully Fine to Coarse Element Boundary	95
Chapter 5:	Materials and Methods	97
5.1	Physical Experiments	97
5.1.1	Validation Experiment 1: Single Track Experiment	98
5.1.2	Validation Experiment 2: Island Scan Experiment	99
5.1.3	Validation Experiment 3: Parameter Matrix Experiment	101
5.2	Simulation Experiments	101
5.2.1	Single Track Simulation of Validation Experiment 1	104
5.2.2	Island Scan Simulation of Validation Experiment 2	106
5.2.3	Parameter Matrix Simulation of Validation Experiment 3	107
5.2.4	Coarsening Validation Simulation	108
5.2.5	Multiple Layer Simulation	108
5.2.6	Hybrid Element Thermophysical Property Simulation	108
5.2.7	Hybrid Element Volume Simulation	111
5.2.8	Fully Fine Unit Cell Volume Simulation	112
5.2.9	Single Track with Hybrid Element Coarsening Simulation	113
5.2.10	Single Track without Hybrid Element Coarsening Simulation	115
Chapter 6:	Heat Flow Simulation of Laser Powder Bed Fusion and Val-	
	idation	116
6.1	Results	117
6.1.1	Single Track Experiment Results	117
6.1.2	Single Track Simulation Results	117
6.1.3	Island Scan Experiment Results	119
6.1.4	Island Scan Simulation Results	119
6.1.5	Parameter Matrix Experiment Results	121
6.1.6	Parameter Matrix Simulation Results	121

6.1.7	Coarsened Fully Fine Simulation Results	122
6.1.8	Multilayer Simulation Results	122
6.2	Discussion	122
6.2.1	Computational Resources	122
6.2.2	Comparison of Simulation and Physical Results	126
6.3	Conclusions	132
Chapter 7: A Hybrid Meshing Strategy for Finite Volume Methods . .		134
7.1	Results	135
7.1.1	Properties of Hybrid Elements Results	135
7.1.2	Hybrid Element Simulation Results	136
7.1.3	Coarsening with Hybrid Elements	137
7.2	Discussion	139
7.2.1	Generation of Resistivity Curve	139
7.2.2	Comparison of Fully Fine Simulated Volume to the Hybrid Element Volume	144
7.2.3	Coarsening with Hybrid Elements	150
7.3	Conclusions	150
Chapter 8: Discussion		152
8.1	Validation	152
8.2	Hybrid Elements	154
Chapter 9: Conclusions and Further Work		158
9.1	Further Work	160
Appendix A:		162
Appendix B:		165
Appendix C:		168
References		199

List of Figures

	Page
Fig. 2.1: Example of Support Structures Used for a Hemispherical Build . . .	5
Fig. 2.2: The SLM and SEBM Manufacturing Process with some of the Melt- ing Phenomena Highlighted	6
Fig. 2.3: Adjacent Spherical Powder Particles with Point Contact	10
Fig. 2.4: Flow concepts of GE Additive Concept Laser M2 (generations prior to Series 4) machine, (a) and (b), and GE Additive Concept Laser M2 Series 4 machine, (c) and (d). Image credit: GE Additive	13
Fig. 2.5: Schematic diagram of fluid flow patterns within the melt pool for: (a) negative surface tension gradient, and (b) positive surface tension gradient	19
Fig. 2.6: The Nucleation of a Spherical Solid Cap at a Liquid-Substrate Interface	21
Fig. 2.7: Lack of fusion porosity in CM247LC	23
Fig. 2.8: Graph of Area Porosity vs Area Energy Density	25
Fig. 2.9: SEM Micrograph Showing Gaseous Porosity in Metallic Powder Pro- duced by Gas Atomisation	27
Fig. 2.10: Diagram of typical keyhole meltpool morphology	29
Fig. 2.11: Types of Cracking Found in the Additive Manufacture of Metals through Powder Bed Fusion.	31
Fig. 2.12: Iron-Chromium Binary Alloy Phase Diagram	35
Fig. 2.13: Iron-Carbon Phase Diagram above 600 degrees Celsius	35
Fig. 2.14: Diagram of Laser Flash Analysis Equipment	40

Fig. 2.15: Phase distribution EBSD of 316L sample produced by LPBF showing austenitic structure (blue), with minute fraction of retained ferritic structure (red).	46
Fig. 2.16: SEM images of 316L produced by LPBF showing the intragranular dislocation network.	47
Fig. 2.17: XRD Elemental Maps of 316L Produced by LPBF	48
Fig. 2.18: Definition of Possible 2D Cellular Neighbourhoods: (a) von Neumann, (b) Moore, (c) 7-cels-neighbourhood and (d) 25-cells-neighbourhood. (The centre cell is regarded as part of the neighbourhood, because the new state depends on its old state.)	50
Fig. 2.19: Surface Rendering of Calculated Liquid/Nucleus Interface Energies for a Range of Elements. Colormapping Corresponds to Relative Values of Interface Energies, with Blue being the Lowest and Red being the Highest.	53
Fig. 2.20: Flowchart showing the numerical implementation of the PF, FEA, and Nucleation Modules to simulate the LPBF process.	56
Fig. 2.21: Schematic of crack propagation specimens. Designed to achieve complex crack paths.	57
Fig. 2.22: Comparison of numerical and experimental results for various specimens built at various orientations relative to the build direction . .	58
Fig. 2.23: Schematic of selective laser melting of a horizontal layer of equal-sized metal powders placed on top of the substrate and surrounded by argon gas. Phase field variables ϕ_1 , ϕ_2 , and ϕ_3 indicate the volume fractions of argon gas, metal powders, and the substrate, respectively. D represents the width of the computational domain, and the Gaussian beam is featured by its irradiation intensity H and a characteristic spot radius a.	59

Fig. 2.24:	Illustration of the Rainfall Method of Powderbed Generation. (a) Schematic of the Rain Model for Random Packing with Rotations. (b) Powderbed Produced by the Rain Model. (c) Adjusting the Relative Density by Removing Some of the Particles. (d) Cross Section of a Real Powderbed (Titanium Alloy.)	60
Fig. 2.25:	Illustration of the Proportion of Melt to Evaporation in AA6061 . . .	66
Fig. 2.26:	Deformation Validation Results	68
Fig. 2.27:	Diagram of GPU Chip Layout of Latest NVIDIA Ada Lovelace Architecture.	72
Fig. 4.1:	Schematic showing two adjacent cubic elements of dimension h	84
Fig. 4.2:	Schematics and sections of an arbitrary element and its six neighbouring elements	87
Fig. 4.3:	Schematics of Commonly Utilised Volumetric Heat Sources for Modelling and Simulation of LPBF, (a) Cylindrical; (b) Semi-spherical; (c) Semi-ellipsoid; (d) Conical; (e) Radiation Transfer Method; (f) Ray-Tracing Method; (g) Linearly Decaying Method; (h) Exponentially Decaying Method.	89
Fig. 4.4:	Schematic of a 2-Dimensional Volume Consisting of Both Powder and Solid	93
Fig. 4.5:	Diagram of Boundary between Fully Fine and Coarsened Elements . .	96
Fig. 5.1:	Images of the Open Architecture Rig	98
Fig. 5.2:	Schematic of Stainless Steel Substrate Coupons	98
Fig. 5.3:	Schematic of Vector Layout of Single track Experiments	99
Fig. 5.4:	Schematic of Vector Layout of Meander Experiments	100
Fig. 5.5:	Schematic of Meander Scanning Strategy	100
Fig. 5.6:	Plot of Derivative of Coefficient of ΔH With Respect to Temperature When Calculated Using Variable Density.	105
Fig. 5.7:	Schematic of Order of Island Scans	107

Fig. 5.8:	Cross Sections of the Hybrid Elements	109
Fig. 5.9:	Schematic of the Simulation Setup for Calculating the Thermal Con- ductivity of the Hybrid Element Unit Cell	110
Fig. 5.10:	Representative Diagram of the Simulation Setup for Evaluating the Conductive Performance of the Hybrid Elements in a Large Volume.	112
Fig. 5.11:	Representative Diagram of the Simulation Setup for Evaluating the Conductive Performance of the Hybrid Elements in a Large Volume.	113
Fig. 5.12:	Representative Diagram of the Simulation Setup for Evaluating the Conductive Performance of the Hybrid Elements with Fully Fine Elements, and Laser Exposure.	114
Fig. 6.1:	Optical Micrograph Showing Cross-section of the Single Track Melt- pool.	117
Fig. 6.2:	Boxplots of Meltpool Dimensions of Single Track Samples (a) Width (b) Depth	118
Fig. 6.3:	Single Track Simulation Heat-Map Results with Solidus and Liquidus Isotherms Marked.	118
Fig. 6.4:	Optical Micrograph Showing the Cross-section of the Meander Track Meltpool.	119
Fig. 6.5:	Boxplots of Meltpool Dimensions of Meander Track Samples (a) Width (b) Depth	119
Fig. 6.6:	Island Scan Simulation Results	120
Fig. 6.7:	Surface Plots of Width and Depth of the Matrix Parameters (a) Width (b) Depth	122
Fig. 6.8:	Micrographs Showing Examples of the Observed Processing Modes	123
Fig. 6.9:	Surface Plots of Width and Depth of the Simulated Matrix Param- eters (a) Width (b) Depth	125
Fig. 6.10:	Coarsened Simulation Results	125
Fig. 6.11:	Boxplots of Meander Meltpool Geometries with Reference Lines of the Simulation Results for Comparison (a) Width (b) Depth	126

Fig. 6.12:	Boxplots of Single Track Meltpool Geometries with Reference Lines of the Simulation Results for Comparison (a) Width (b) Depth . . .	128
Fig. 6.13:	Surface Plots Showing the Difference Between Simulated and Measured Geometries (a) Width (b) Depth	129
Fig. 6.14:	Contour Plot Showing the Processing Mode vs the Laser Power and Scanning Speed.	131
Fig. 7.1:	Calculated Properties of the Hybrid Solid/Powder Elements	136
Fig. 7.2:	Temperature Profiles of Select Parts of Both Fully Fine and Coarse Simulation Volumes	137
Fig. 7.3:	Predicted Meltpools for Fully Fine and Hybrid Element Coarsened Simulations	138
Fig. 7.4:	Calculated Properties of the Hybrid Solid/Powder Elements with Reference Temperature Marked	140
Fig. 7.5:	Boxplot Showing the Distribution of α Values	140
Fig. 7.6:	Scatterplot Comparing the Calculated Resistivity Curves	141
Fig. 7.7:	Plot of Calculated Diffusion Time versus Temperature (a) Time in Seconds (b) Time in Simulation Steps	144
Fig. 7.8:	Comparative Plots of Results from 200 and 200,000 Time Step Steady State Simulations	145
Fig. 7.9:	Percentage Temperature Difference versus Time Between Fully Fine and Hybrid Volumes (a) Top Layer (b) Bottom Layer	146
Fig. 7.10:	Illustration of Initial Heat Flow in Fully Fine and Hybrid Element Simulations	146
Fig. 7.11:	Comparison of Temperature Profiles versus Time for both Fully Fine and Hybrid Element Simulations	147
Fig. 7.12:	Performance of Simulations Using Varied Temperature Gradients to Generate Resistivity Curves	148
Fig. 7.13:	Temperature Gradient Across Coarsening Boundary in Coarsening Simulation	149

Fig. C.1:	40 W 100 mm/s	168
Fig. C.2:	40 W 500 mm/s	168
Fig. C.3:	40 W 900 mm/s	169
Fig. C.4:	40 W 1300 mm/s	169
Fig. C.5:	40 W 1700 mm/s	169
Fig. C.6:	90 W 100 mm/s	170
Fig. C.7:	90 W 500 mm/s	170
Fig. C.8:	90 W 900 mm/s	170
Fig. C.9:	90 W 1300 mm/s	171
Fig. C.10:	90 W 1700 mm/s	171
Fig. C.11:	140 W 100 mm/s	172
Fig. C.12:	140 W 500 mm/s	172
Fig. C.13:	140 W 900 mm/s	173
Fig. C.14:	140 W 1300 mm/s	173
Fig. C.15:	140 W 1700 mm/s	173
Fig. C.16:	190 W 100 mm/s	174
Fig. C.17:	190 W 500 mm/s	174
Fig. C.18:	190 W 900 mm/s	175
Fig. C.19:	190 W 1300 mm/s	175
Fig. C.20:	190 W 1700 mm/s	175
Fig. C.21:	240 W 100 mm/s	176
Fig. C.22:	240 W 500 mm/s	176
Fig. C.23:	240 W 900 mm/s	177
Fig. C.24:	240 W 1300 mm/s	177
Fig. C.25:	240 W 1700 mm/s	177

List of Tables

	Page
Table 2.1: Composition Specification for 316L/1.4404 Austenitic Stainless Steel	37
Table 2.2: Table of values for k with corresponding n	42
Table 2.3: Summary of Mechanical Properties of AISI 316 SS, manufactured by LENS.	44
Table 5.1: Table showing the Laser Parameters used for Validation Experiments	99
Table 5.2: Table showing the Laser Parameters used for Validation Experiments	100
Table 5.3: Table showing the Parameters Matrix	102
Table 5.4: Table of Temperature Variant Thermophysical Properties used in Simulation	104
Table 5.5: Table of Static Thermophysical Properties	104
Table 5.6: Table of Simulation Domain and Element Dimensions for the Single Track Simulation	105
Table 5.7: Table of Simulation Domain and Element Dimensions for the Island Scan Simulations	106
Table 5.8: Table of Simulation Domain and Element Dimensions for the Fully Fine with Coarsening Simulation with Laser Heat Input	108
Table 5.9: Table of Simulation Domain and Element Dimensions for the Cal- culation of the Thermal Resistivity of the Hybrid Elements	110
Table 5.10: Table of Simulation Domain and Element Dimensions for the Hy- brid Element Volume Simulation	111
Table 5.11: Table of Simulation Domain and Element Dimensions for the Fully Fine, Unit Cell Volume Simulation	112

Table 5.12:	Table of Simulation Domain and Element Dimensions for the Fully Fine and Hybrid Element Coarsened Simulation with Laser Heat Input	114
Table 5.13:	Table of Simulation Domain and Element Dimensions for the Uncoarsened Simulation with Laser Heat Input	115
Table 6.1:	Table of Meltpool Measurements from the Single Track Simulation	118
Table 6.2:	Table of Computational Resources Used by the Single Track Simulation	119
Table 6.3:	Table of Meltpool Measurements from the Island Scan Simulation .	120
Table 6.4:	Table of Computational Resources Used by the Simulation Methods	120
Table 6.5:	Table of Measurements of Matrix Parameters	121
Table 6.6:	Table of Numerical Results for Matrix Parameters	124
Table 6.7:	Table of Simulation Measurements of Coarsened Volume	124
Table 6.8:	Table of Computational Resources Used by the Coarsened Simulation	125
Table 6.9:	Table Showing the Error in Simulation Results Compared to the Observed Processing Mode	130
Table 7.1:	Table of Computational Resources Used by Resistivity Curve Generation	136
Table 7.2:	Table of Computation Resources Required by Each Type of Simulation	136
Table 7.3:	Table of Meltpool Measurements and Simulation Time of Fully Fine and Coarsened Simulations	137

List of Symbols

Symbol	Usage
A	Contact area
A_{fs}	Surface area of the solid/substrate interface
A_p	Absorption of radiation polarised parallel to the plane of propagation
A_s	Absorption of radiation polarised perpendicular to the plane of propagation
A_{sl}	Surface area of the solid/liquid interface
a	Radius of contact area between two powder particles
arctan	Inverse trigonometric tangent function
B	Scaling exponent
$\mathbf{b}$	Magnetic field vector
c	Speed of light in a vacuum
c_i	Concentration of chemical species i
c_p	Specific heat capacity
c_{pp}	Specific heat capacity
c_{px}	Specific heat capacity of sample
cos	Trigonometric cosine function
D	Total dimension of simulated volume
d	Layer thickness
E	Energy emitted per unit area at given temperature
E	Linear energy density
E	Area energy density
E	Volumetric energy density

E_m	Young's modulus
$\mathbf{e}$	Electric field vector
e	Exponential function
erf	Error function
$\mathbf{F}$	Force matrix
$\mathbf{F}_i$	Matrix of forces acting on particle i
$\mathbf{F}^c$	Contact force matrix
$\mathbf{F}^{cn}$	Normal contact force matrix
$\mathbf{F}^{cs}$	Shear force matrix
F	Total free energy of the phase field
F	Heat input source term
Fo	Fourier number
f	Free energy
f_s	Volume fraction of lattice unit cell
$f(\theta)$	Ratio between volume of nucleus and sphere with identical radius
G	Gibbs free energy
G_{homo}	Gibbs free energy of homogenous nucleation
G_I	Gibbs free energy of the solid/liquid interface
G_V	Gibbs free energy of the solid and liquid phases
g	Gravitational constant
g	Shortest distance (in z axis) between the surfaces of two contacting powder particles at radius R
g	Absorption depth
H	Internal energy
H_{max}	Maximum enthalpy change
h	Heat transfer coefficient
h	Plank's constant
h	Hatch spacing

h_0	Heat transfer coefficient of the contact area between two contacting powder particles
h_s	Specific enthalpy
h_x	Spatial resolution in the x -axis
h_y	Spatial resolution in the y -axis
h_z	Spatial resolution in the z -axis
$\mathbf{I}$	Identity matrix
I	Power required to maintain the sample chamber at a given temperature
I	Moment of inertia
$I(x, y)$	Light intensity
J	Energy emitted by a black body
K	Linear conversion coefficient
Kn	Knudsen number
k	Boltzmann constant
k	Thermal conductivity
k	Powder/Solid linear scaling factor
k_n	Normal elastic modulus
k_r	Rotations stiffness modulus
k_s	Shear stiffness modulus
k_t	Torsional stiffness modulus
$\ln$	Natural logarithm
L	Sample thickness
L	Kinetic coefficient of the phase field mobility
$\mathbf{M}_i$	Matrix of momentum for particle i
m	Mass of particle
m_g	Mass coefficient of the solid phase
m_p	Mass coefficient of the liquid phase
m_x	Mass of sample
N	Coordination number

$\mathbf{n}$	Normal vector
n	Complex wave impedance
n	Harmonic coefficient
$\mathbf{O}$	Position matrix
P	Input power
P	Laser Power
p	Pressure
Q	Heat flux
Q	Heat Energy
R	Radius of powder particle
R	Thermal resistivity
R	Radius of curvature of nucleus
R_c	Critical radius of nucleus to form an embryo
$\mathbf{r}$	Orientation vector
r	Displacement from point of laser incidence
r	Radius
S	Conductive shape factor
S	Signal fr a single sample pan during DSC
s_f	Enthalpy of fusion per unit volume
sgn	Sign function
cos	Trigonometric sine function
T	Temperature
T_0	Initial temperature
T_b	Solid body temperature
T_f	Fluid temperature
$T_{x,y,z,t}$	Temperature at position x, y, z at time t
t	Time
t_θ	Layer thickness
tan	Trigonometric tangent function

$\tanh$	Hyperbolic tangent function
$\mathbf{u}$	Vector velocity field
$\dot{\mathbf{u}}_s$	Shear velocity vector
$\mathbf{u}_n$	Overlap distance
u	Scanning speed
u_{ijk}	Value of u at position i, j, k
V	Volume
V_s	Volume of the nucleus
v	laser scanning speed
v^s	Frequency of quanta type s
W	Work
$\dot{\mathbf{x}}_i$	Velocity of particle i
$\ddot{\mathbf{x}}_i$	Acceleration of particle i
x, y, z	Cartesian coordinates
z	Distance (cylindrical coordinate)
z	Depth of heat conduction

Greek Symbols

α	Absorptivity of a body
α	Thermal conductivity
α	Thermal diffusivity of irradiated material
α	Linear interpolation coefficient
$\alpha(T)$	Thermal conductivity at temperature T
γ	Adiabatic exponent
γ	Interface energy
γ	Thermal dependence of surface tension
γ_e	Effective thermal conductivity
γ_{fl}	Substrate/liquid interface energy
γ_{fs}	Solid/substrate interface energy

γ_g	Thermal conductivity of the gaseous atmosphere
γ_{sl}	Solid/liquid interface energy
ΔC	Difference in heat capacity
Δt	Maximum discrete time step
ΔT	Discrete temperature difference
Δx	Spatial resolution
ε	Emissivity of a body
ε^{el}	Elastic strain
ε^{pl}	Plastic strain
ε^{th}	Thermal strain
ε^{total}	Total strain
ζ	Liquid phase parameter
η	Absorptivity of a body
η	Absorptivity of irradiated material
θ	Angle of incidence
θ	Wetting angle
θ	Scaling coefficient
θ	Temperature
κ	Interface gradient coefficient
Λ_{sl}	Gibbs-Thompson coefficient
λ	Thermal conductivity
λ	Absorptivity
μ	Dynamic viscosity
ν	Poisson's ratio
ξ	Ratio of distance between equivalent points on contacting spheres
ξ	Distance moved by laser at time t
$\boldsymbol{\pi}^r$	Rotation Vector
$\boldsymbol{\pi}^t$	Torsion vector
π	Universal mathematical constant

ρ	Density
Σ	Summation function
Σ	Thermal resistance
σ	Stephan-Boltzmann constant
σ	Laser spot diameter
σ_x	Laser spot diameter in x -axis
σ_y	Laser spot diameter in y -axis
$d\sigma$	Change in surface tension
τ	Dimensionless temperature
τ	Ratio of material temperature to its liquidus temperature
ϕ	Order parameter
φ	Configured phase field order parameter
χ	Mean free path of a gas
$\dot{\omega}_i$	Angular velocity vector of particle i
$\ddot{\omega}_i$	Angular acceleration vector of particle i

Chapter 1

Introduction

1.1 A Brief Introduction to LPBF

Additive manufacturing is a production technique for the manufacture of netshape parts through layer-by-layer application of material. This technique began in 1988 with a patent by Charles Hull for the first Stereolithography Apparatus (SLA) [1]. This then began a decades long journey which led to the US Additive Manufacturing industry being valued at \$20.37 billion USD in 2023 [2]. In this time there have been many variations on the technology since the original. SLA being focused on production of parts in light-reactive thermoset resins, the earliest systems were focused on polymers. It wasn't until 1995 that the first metallic machine was developed by the Fraunhofer Institute [3]. This was the birth of Laser Powder Bed Fusion (LPBF). The LPBF process can be broken down into a number of steps:

1. A CAD file of the part to be created is created;
2. the CAD file is sliced into a sequence of 2D layers of a predetermined thickness (hereafter referred to as the build file);
3. the LPBF machine applies a layer of powder equal to the predetermined layer thickness onto the build plate;
4. the machine then melts the powder layer as according to the instructions set in the

build file;

5. the build plate is then lowered by the predetermined layer thickness;

6. steps 3 to 5 are repeated until there are no more remaining layers.

The exact details of the physics of this process are discussed in further detail in [Sec. 2](#). An advantage of manufacture via this layer-by-layer approach is that complex geometries such as internal structures and lattice morphologies can be achieved where other methods of manufacture fail. These novel complex geometries then introduce novel challenges that must be overcome. Due to the complex geometries now possible come complex thermal histories that can cause defects and build failures. As the cost of raw material for LPBF is somewhat elevated when compared to wrought stock used in subtractive methods [4, 5]. Thus, the impact of a failed production run is higher in LPBF.

1.2 Thermal Simulation of LPBF

In order to prevent these build failures due to thermal phenomena, great effort has been put into modeling the thermal flow during LPBF. These simulations are performed prior to the build to identify problem areas of processing. Once a problem area is identified, the laser parameters of this section can be adapted to reduce the thermal load of the problem section. However, where thermal simulations of entire part sized builds reduce the cost of failed builds, they currently add huge overheads in time. Current approaches to build-sized simulation are limited to CPU based programming paradigms, and are therefore inherently limited by computational hardware. In order to attempt to overcome this speed limitation, some thermal simulation products heavily simplify the build volume. Autodesk Netfabb's simulation package, simulates a single vector of the relevant material and parameters, then from the results of this simulation attempts to infer the heat flow in the entire part [6]. Whilst this approach does reduce computational time, due to the inference from a single small simulation, this method can fall short in extremely complex geometries, such as lattice structures. In these cases, due to the reduced cross-section of the solid, the reduced thermal conductivity of the powder, and the constant transition

of solid to powder; heat conduction away from the part is greatly reduced. Hence, heat within the part is retained, and as the build progresses, fatal defects can occur in the solid due to overheating. These extremes can be difficult to predict when the simulation methodologies simplify the build to such an extent.

1.3 Research Motivation

Thus, a simulation methodology that allows a near full solution of the heat equation for the build volume and leverages hardware optimisation strategies to achieve this in time faster than that of CPU based simulations is proposed herein. By utilising this method of simulation a high accuracy prediction for heat distribution within the part can be predicted. This can also be obtained in a time faster than real-time, reducing the time limitation of the current thermal simulations whilst avoiding the fiscal cost of failed builds.

Chapter 2

Background

2.1 Powder Bed Fusion (PBF)

2.1.1 Process

Production of consolidated parts using PBF can be achieved by the use of two distinct technologies: Selective Laser Melting (SLM) [7, 8] and Selective Electron Beam Melting (SEBM) [9, 10]. Both utilize a layer-by-layer build approach but achieve the heating of the powder bed in very different ways, and thus are subject to varying phenomena in varying amounts [11]. Both manufacturing processes can be broken down into three general steps: pre-processing, manufacture, and post-processing. Pre-processing requires the manipulation of a digital representation of the final component (usually a stereolithography file produced by a CAD software). The CAD representation of the part is broken down into constituent layers that are to be produced during manufacturing. This is often performed by software specific to the AM machine being used, and contains the production parameters that are to be used throughout the build. It is this ‘sliced’ file that is passed into the machine for manufacture. Depending on the geometry of the part being produced, it is sometimes required to add ‘support structures’ to the CAD file, prior to slicing. Due to the nature of manufacturing parts layer by layer, there are limits to the length and angle of any overhanging structure. If these limits are exceeded, then supporting structures must be added and built to prevent geometric inaccuracy in the finished part, an example

of support structures is given in [Fig. 2.1](#). The manufacturing process for both SLM and SEBM are shown in [Figure 2.2](#).

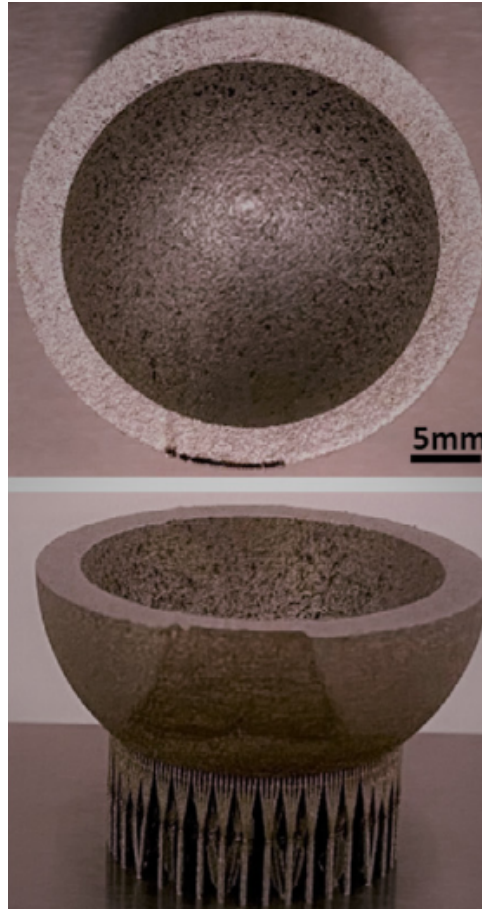


Figure 2.1: Example of Support Structures Used for a Hemispherical Build. Taken from [12].

Both processes involve the component to be built layer-by-layer on a substrate plate (usually, but not limited to, the same material as the powder being used). A fine layer of powder is mechanically spread across the substrate, and is melted by the heat source beam as per the instruction embedded in the pre-processed digital file. In order to ensure the integrity of the component, melting must be induced in previous layers in order for the layers to consolidate upon solidification [14]. After a single layer is complete, the substrate is lowered by the layer thickness and another layer of powder is spread on top and the component is built up layer-by-layer. Some processes utilize a “preheat” step in which a heater or the heat source beam is used to raise the temperature of the powder bed before melting occurs. The benefit of doing so is discussed in [Section 2.1.2](#). Once manufacturing is completed, the component must be separated from the substrate plate, and

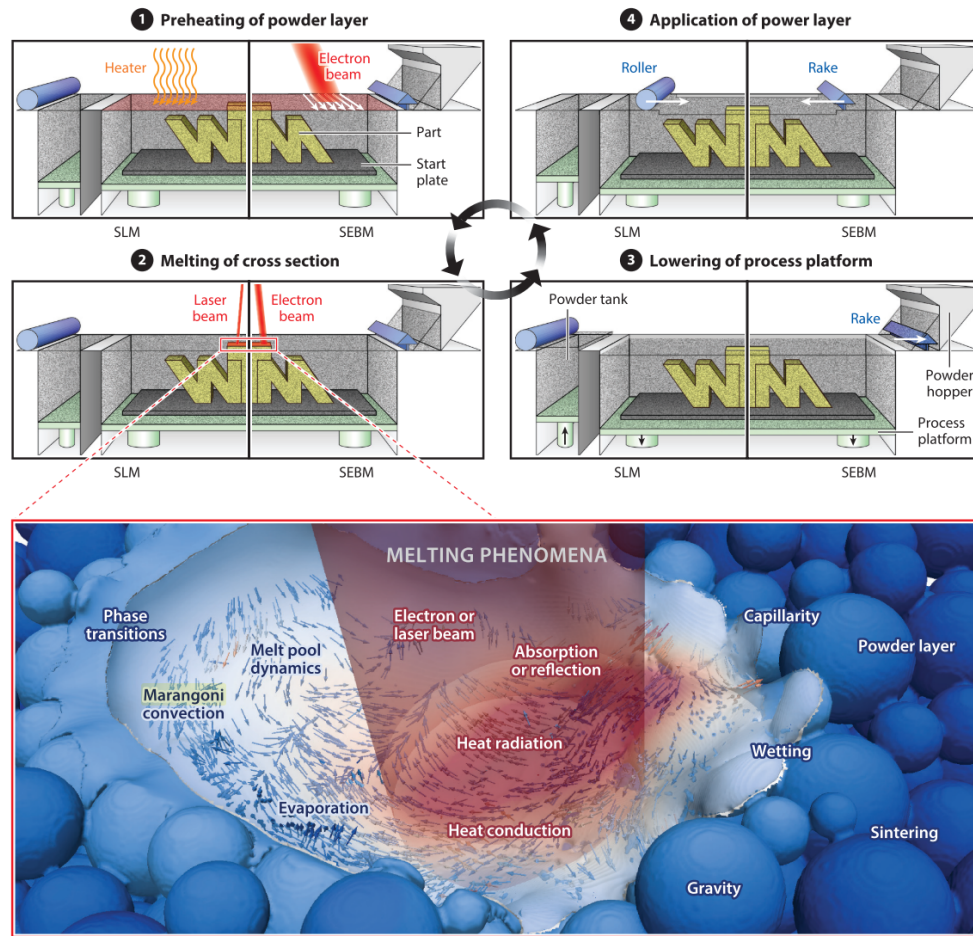


Figure 2.2: The SLM and SEBM Manufacturing Process with some of the Melting Phenomena Highlighted [13]

any support structure that was needed for manufacture. This, plus any heat-treatment required, is performed in the post-processing step. Due to the requirement of a full layer of powder to be applied across the build plate every layer, any build that utilizes the full build height of the build volume of a PBF machine must require an entire build volumes' amount of metal powder. The volumes of powder required to do so, quickly raises the cost of manufacturing substantially [15]. Thus, the recyclability of the powder becomes a large factor in the reduction of the costs of PBF manufacturing.

Due to the differences in the technologies required for SLM and SEBM, the solutions to this problem will likely differ just as much. SLM, as the name suggests, utilizes a high power laser to melt the powder bed [7,8]. The control of the laser beam beam is performed using a system of actuated mirrors and lenses. Due to the utilization of a photon beam, SLM manufacturing can be conducted under an inert gas atmosphere, such as Argon.

Whereas, SEBM utilizes an electron beam in order to melt the powder bed; and due to the short mean free path of electrons in gaseous environments, the build chamber must be held at high vacuum [16]. However, recent commercially available SEBM systems, utilize a very low pressure gaseous environment, that may be used to help prevent undesirable events, such as powder smoke. It is due to the variations in the manufacturing technologies of these two processes that the many thermophysical phenomena present have varying impact on the manufacturing when compared.

2.1.2 Thermophysical Phenomena

Figure 2.2 (bottom) shows that there are many physical phenomena that are present in the melt region during the manufacture of PBF manufactured parts. Each of these phenomena contribute to the stability of the manufacturing process and the final component integrity.

2.1.2.1 Absorptivity

Both SLM and SEBM utilize high energy beams to heat the powder, and thus the first thermophysical phenomenon involved in the manufacturing process is the energy transfer mechanic due to beam/powder interaction. The laser used in SLM, relies on photon/powder interaction for the energy transfer of the manufacturing process. Thus, the amount of power transferred from the beam to the powder bed is reliant on the absorptivity of the powder [17].

The relationship between the absorption of energy of an incident beam of light, at angle θ and S or P polarisation and a flat surface is given generally by the Fresnel equations [18]:

$$\begin{aligned} A_s &= 1 - \left| \frac{\cos\theta - (n^2 - \sin^2\theta)^{1/2}}{\cos\theta + (n^2 - \sin^2\theta)^{1/2}} \right|^2, \\ A_p &= 1 - \left| \frac{n^2\cos\theta - (n^2 - \sin^2\theta)^{1/2}}{n^2\cos\theta + (n^2 - \sin^2\theta)^{1/2}} \right|^2. \end{aligned} \quad (2.1)$$

Where n is the complex wave impedance of the flat surface in question. The equations (Eqn. 2.1) were used to formulate ray-tracing experiments performed by the Lawrence

Livermore National Laboratory (LLNL) of the US. It was found that using this methodology, the effective absorptivity of a metal powder is higher than that of a flat opaque surface of the same material [19]. As the inhomogeneous surface of the powder causes incident light to be reflected from the uneven surface of the powder bed, resulting in some of the photons being reflected further into the open-pore system of the powder. Thus, the laser penetration into the powder bed can be comparable to the powder layer thickness [20]. This results in a higher fraction of the incident energy being absorbed by the powder bed when compared to a flat surface of equal area. This is also confirmed by Gusarov and Kruth [21]. The implication of laser penetration into the bed means that the laser must be represented as a volumetric heat source in the powder bed, instead of a surface heat source.

However, in both these experiments, powder particles are assumed to be perfectly spherical, which is not always the case for metallic powders. Whilst perfectly spherical powders are ideal to maximize the flowability of the powder for equivalent powder size distributions, current manufacturing methods cannot guarantee purely spherical powder particles without spheroidal particles and satellite particles [22]. Also, the results from both these studies are dependent on a specific particle size distribution, therefore implying that two metallic powders of identical elemental composition, but with different particle size distributions can have differing absorptivity values. Furthermore, the formulation of a ray-tracing methodology disregards wave phenomena, simplifying the ray as a constant beam of energy [18]. Therefore, Eqn. 2.1 can be considered an average that does not account for individual photon behaviour. This is not a method of solving the Maxwell equations [23]:

$$\nabla \mathbf{b} = 0, \quad (2.2)$$

$$\nabla \times \mathbf{e} = -\frac{1}{c} \cdot \frac{\partial \mathbf{b}}{\partial t}, \quad (2.3)$$

and as such, photonic interactions such as destructive interference and diffraction are not taken into account.

Direct measurement of the absorptivity of powder samples can be performed, but requires

specialist equipment to do so, as demonstrated by Trapp *et al.* [24]. Thus, the data for specific alloys and powder distributions is not well known. As a result, absorptivity remains one of the greatest sources of uncertainty in the simulation of LPBF process. Trapp *et al.* measured the temperature rise of a sample of powder compared to the measured input energy of a laser, using thermocouples in a thermally isolated environment. In these experiments, the powder layer thickness was taken to be nominally 100 μm , which is much larger than those utilised in the LPBF of full density parts. Gusarov and Kuth [21] showed that the absorbtivity of a powder layer is dependent on layer thickness, therefore the measured absorptivities of Trapp *et al.* should be considered an upper bound value for stainless steel of that specific composition, for that specific size distribution, for that specific wavelength of laser being utilized.

2.1.2.2 Heat Conduction

The absorbance of the of photons by the powder particles occurs within the first few nanometers of the powder particle, energy is then distributed into the the particle, and to other powder particles in powder bed through conduction mechanisms [17]. If two powder particles are to be considered spheres of radius R_1 and R_2 , with temperatures and thermal conductivities T_1 , T_2 , λ_1 , and λ_2 respectively, then the adjacent powder particles can be considered to have a circular contact area in the x - y plane (illustrated in [Figure 2.3](#)).

Heat conduction due to the solid-solid contact is governed by the Laplace equation (in cylindrical coordinates) [20]:

$$\frac{\partial^2 \tau}{\partial z^2} + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \tau}{\partial r} \right) = 0. \quad (2.4)$$

Where τ is dimensionless temperature:

$$\tau = \begin{cases} (T(\lambda_1 + \lambda_2) - (\lambda_1 T_1 + \lambda_2 T_2)) / \lambda_2 (T_2 - T_1), & z < 0 \\ (T(\lambda_1 + \lambda_2) - (\lambda_1 T_1 + \lambda_2 T_2)) / \lambda_1 (T_2 - T_1), & z > 0 \end{cases}, \quad (2.5)$$

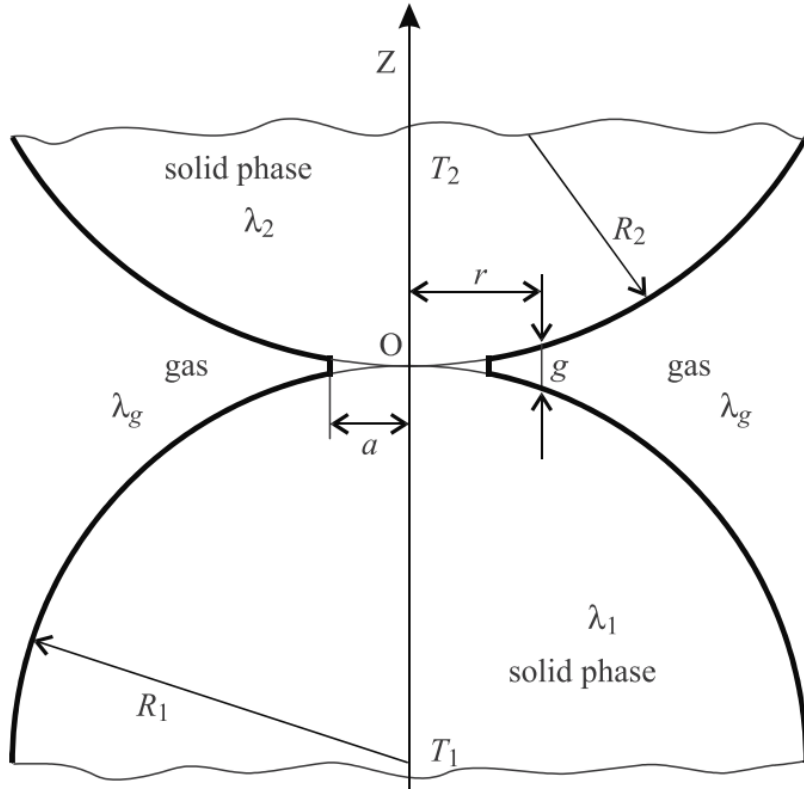


Figure 2.3: Adjacent Spherical Powder Particles with Point Contact [20]

thus the thermal resistance, Σ , of the solid-solid contact can be evaluated as [20]:

$$\frac{1}{\Sigma} = \frac{2\pi\lambda_1\lambda_2}{\lambda_1 + \lambda_2} \int_0^\infty \frac{\partial\tau}{\partial z} \Big|_{z=0} r dr. \quad (2.6)$$

However, there remains a space adjacent to the solid-solid contact area, (in which the surrounding gaseous atmosphere occupies) where the distance between the two sphere surfaces is shorter than the mean free path of the gas. Therefore, conduction of heat between the two spheres due to the gas must also be considered. This was investigated by Gusarov *et al.* in 2009 [20] and is shown below. For any pair of points on the two contacting spheres with equivalent x and y coordinates, the distance, between them is given by:

$$g = \frac{r^2(R_1 + R_2)}{2R_1R_2}. \quad (2.7)$$

Thus, the heat transfer coefficient at distance $r > a$ from the z axis is defined as:

$$\frac{h}{h_0} = \frac{1}{2} \frac{1}{1 + \xi/\chi} + \frac{1}{2} \frac{1}{[1 + (\xi/\chi)^{1/2}]^2}. \quad (2.8)$$

Where ξ/χ is the ratio between the the distance between equivalent points on the surface on the spheres and the mean free path of the gas:

$$\xi = \frac{pR_1R_2(9\gamma - 5)}{3\gamma_p(R_1 + R_2)(\gamma - 1)} \left(\frac{2k}{mT} \right)^{1/2}, \quad \text{and} \quad (2.9)$$

$$\chi = \frac{2\sqrt{\pi}(9\gamma - 5)}{3(\gamma - 1)}. \quad (2.10)$$

Thus the conductivity of the powder bed depends on the packing density of the powder and the gaseous environment of the processing chamber, by utilizing Eqn. 2.6 and Eqn. 2.8, and integrating across the powder bed an explicit expression for the effective thermal conductivity of the bed:

$$\frac{\lambda_e}{\lambda_g} = \frac{f_s N}{2} \left[\frac{1}{2} \ln(1 + L) + \ln(1 + \sqrt{L}) + \frac{1}{1 + \sqrt{L}} - 1 \right], \quad (2.11)$$

where

$$L = \frac{3(\gamma + 1)}{4\sqrt{\pi}(9\gamma - 5)Kn} \quad (2.12)$$

and $Kn = l/D$ is the Knudsen number [20].

This is corroborated by Chin *et al.* [25] who showed that the measured conductivity of the powder was tightly correlated with the gaseous properties of the atmosphere, and only loosely correlated with the metal powder properties. Although, the applicability to the LPBF process of the effective thermal conductivity of a powder measured in a steady gaseous environment must be questioned. Firstly, the work by Chin *et al.* was performed to a maximum temperature of 473 K. This is incredibly limited in scope, especially when compared to the temperatures the powder bed is exposed to during LPBF. At higher temperatures new phenomena become more dominant. For example, at elevated temperatures, the contact area between powder particles can become increased due to partial sintering. Therefore, the dominant transport of heat between particles could shift to direct solid/solid conduction rather than through the gas medium as assumed by Chin *et al.*. This then limits the applicability and generalizability of the conclusions they have drawn. Secondly, Chen, Vastolaz, and Zhang [26] showed that non-uniformity in the gas

flow throughout a build chamber directly impacted the defect density and build quality of parts manufactured in the same build, and gas flow across the powder bed varies from machine to machine. Therefore, when considering the thermal properties of the powder for SLM are to be considered, it must be considered that they will vary from machine to machine, due to the varied design in inert gas flow management in the build chamber. It must also be considered that during the laser processing of the material, metal vapour accumulates immediately above the melt [27]. The rate of vapour build-up is dependent on the energy deposited into the powder bed, and the ability of the gaseous flow in the chamber to advect the vapour away. The accumulated vapour is able to disrupt the gaseous cross-flow of the chamber, therefore the thermal conductivity of the powder would not be so closely correlated with the conductivity of the gaseous atmosphere as shown by Chin *et al.* [25].

Furthermore, if a heated bed is being utilized, the powder bed is held at an above-ambient temperature, thus reducing the required laser power to melt the powder. If the heated bed is above the powder sintering temperature but below the solidus temperature, partial sintering occurs in the powder bed. This increases the contact area between the powder particles, increasing the thermal conductivity of the powder bed [28]. Also, during the LPBF of many metallic alloys, low boiling temperature elements are volatilized and form a plume that interacts with the gas flow in the process chamber [29]. This causes fluctuations in the gaseous atmosphere, which could induce localised variations in the thermal conductivity of the powder, as per the results of Chin *et al.* [25]. The gaseous flow within the build chamber can even vary wildly between machines produced by the same manufacturer, as demonstrated by [Figure 2.4](#). Thus, showing that the properties observed in one machine will not be the same as those observed in another.

2.1.2.3 Radiation

The reality of additive manufacture means that a consolidated part cannot energetically be considered a closed volume: the part will lose heat to the machine chassis via conduction, and radiation; and to the gaseous atmosphere through convection. Once heat

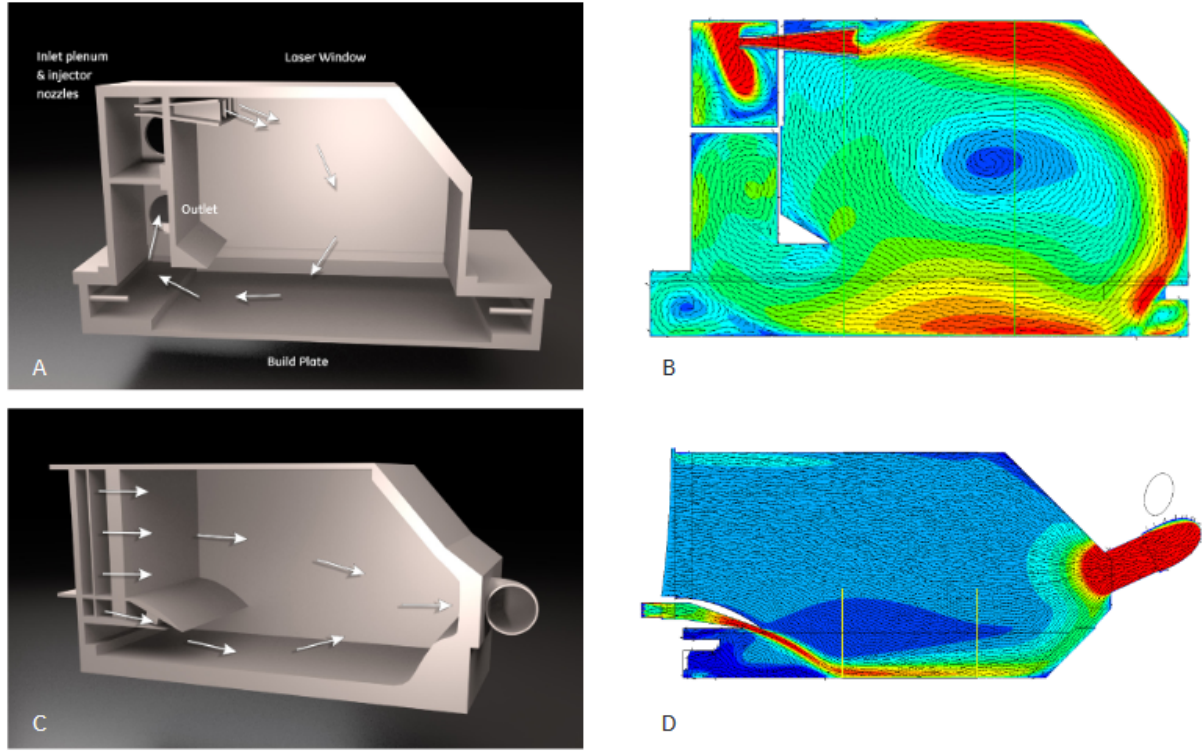


Figure 2.4: Flow concepts of GE Additive Concept Laser M2 (generations prior to Series 4) machine, (a) and (b), and GE Additive Concept Laser M2 Series 4 machine, (c) and (d). Image credit: GE Additive taken from [30]

has been input into the powder bed, the raise in temperature of the heat affected zone (HAZ) causes heat loss by radiation. The radiation loss from a heated body (across all wavelengths), in Watts per unit area, is given by the Stefan-Boltzmann Law [1]:

$$J(T) = \varepsilon \sigma T^4. \quad (2.13)$$

Where ε is the emissivity of the body, for a perfect “black-body” $\varepsilon = 1$, whereas for a “grey-body” $0 < \varepsilon < 1$; and σ is the Stefan-Boltzmann constant:

$$\sigma = \frac{2\pi^5 k^4}{15c^2 h^3} = 5.670373 \times 10^{-8} \text{ Wm}^{-2}\text{K}^{-4}. \quad (2.14)$$

The value of the Stefan-Boltzmann constant comes from the derivation of the Stefan-Boltzmann Law from Plank’s Law, thus the derivation of both laws is intrinsically linked. The derivation of Planck’s Law was first proposed by Bose in 1924 [31]. Planck’s Law, calculates the energy emitted per unit area of a given body at temperature T , and is as

follows:

$$E(v, T) = \sum_s \frac{8\pi h v^3}{c^3} V \frac{1}{e^{hv^s/kT} - 1} dv^s, \quad (2.15)$$

where h is Plank's constant, c is the speed of light in a vacuum, v is the frequency of the quanta of type s , enclosed by volume V , k is the Boltzmann constant, and T is the temperature of the volume. The form presented by Bose presents Planck's Law applied at an atomic level. When considering the macroscopic application of Planck's Law, a shape factor must be applied, as a body can only radiate energy from its surface, and any energy radiated into the body is irrelevant. The shape factor is one of a hemisphere, and gives Planck's Law in an alternative form [32]:

$$E(v, T) = \frac{2hv^3}{c^2} \frac{1}{e^{hv^s/kT} - 1}, \quad (2.16)$$

Thus, the Stephan-Boltzmann Law (2.13) is a solution to the definite integral of Plank's Law (2.16) over all frequencies of quanta, for a given temperature [33]:

$$J(T) = \int_0^\infty E(v, T) dv = \int_0^\infty \left(\frac{2hv^3}{c^2} \frac{1}{e^{hv^s/kT} - 1} \right) dv. \quad (2.17)$$

Materials used in PBF do not act as perfect "black-bodies" ($\varepsilon \neq 1$), thus the emissivity of the materials must be ascertained. The emissivity of a "grey body" (ε_{gb}) is related to the emissivity of a black body (ε_{bb}) via the absorptivity:

$$\varepsilon_{gb} = \alpha \varepsilon_{bb}. \quad (2.18)$$

The absorptivity of a material and how it is measured is discussed in Sec. 2.1.2.1.

ASTM C835-06 [34], specifies a standardized method for measuring the hemispherical emissivity of materials. However, the standard is only valid to 1400 °C. Temperatures greater than this are used in the manufacture of parts, such as Tungsten, with a liquidus in excess of 3000 °C [35,36]. Thus, using values obtained through the methods outlined in the standard to predict radiative losses during PBF should be deemed as extrapolation, and treated with due apprehension.

In addition, the emissivity of metal alloys have been shown to be a function of temperature [37], which would imply that there would be a variation in heat loss due to radiation as the build time increases during LPBF. However, this also does not take into consideration, that at the elevated temperatures oxide layer formation occurs on many alloys [38, 39]. Oxide layers change a materials ability to radiate photons, especially at lower wavelengths in both steels and aluminium alloys [40, 41], thus the measured photon release of these materials at higher temperatures, may be higher than expected. Thus the use of virgin or reused powder in the LPBF process will effect the thermal behaviour of the build.

Furthermore, as shown in the work by Bidare *et al.*, during SLM, laser interaction with the powder bed produces a “shielding plasma” which interacts with the laser beam [42]. The interaction of the laser and the plasma, proves that the plasma has a “lensing” effect on electromagnetic radiation [43]. Thus, any radiation produced by the heated material would equally interact with the plasma. This would cause any surface temperature readings from pyrometry to be attenuated through this plasma, and affect the accuracy of the readings.

2.1.2.4 Convection

Heat loss due to radiation occurs in both SLM and SEBM; however, in SLM heat loss due to convection of the of the inert gas atmosphere used in the manufacturing process dominates the heat loss from the top surface [44]. Due to SEBM being performed under a high vacuum, this effect is not considered to be present.

Natural convection is caused by the buoyancy induced by variation in temperature throughout a fluid. The governing relationship for heat losses for a heated body in a cool fluid was first proposed in an anonymous letter from Sir Isaac Newton to Philosophical Transactions in 1701 [45]. Whilst no formal equations were presented, it stated that the rate at which heat was lost from the body was directly proportional to the magnitude of the difference in temperatures of the body and the fluid. Mathematically this is represented

thus:

$$Q = hA(T_f - T_b), \quad (2.19)$$

where Q is the heat flux, h is the heat transfer coefficient, A is the area of the heat transfer surface, T_f is the fluid temperature, and T_b is the temperature of the body's surface. This was corroborated by others following its publication [46, 47]. However, it wasn't until 1817 in which Dulong and Petit showed that this was not valid for large temperature differences, and that an exponent factor should be incorporated [48]. Thus a renewed relation was proposed:

$$Q = hA(T_f - T_b)^B. \quad (2.20)$$

As a characteristic property of SLM is the presence of large thermal gradients [49] Eqn. 2.20 should be utilized, over the original Newtonian form. Both the heat transfer coefficient h and the scaling exponent B are dependent on the physical set-up of the system, thus must be derived from experimental data. Thus, the work of Li *et al.* [50] in deriving experimental values for h for common SLM alloys; this was based on the work of Gouge *et al.*, who devised a multi-scale Finite Element (FE) thermal model with powder layer deposition [51]. Li *et al.* used this model to derive equivalent h values for the various sides of part-sized builds of various sizes. However, the governing equation used for the multi-scale FE:

$$T = T_\infty + \frac{\eta P}{\rho C_p h_s t_{\theta v}}, \quad (2.21)$$

does not recognise that the values for ρ and C_p are temperature variant, therefore validating numerical results against numerical data, without physical data should be called into question. Thus, the accuracy of the h values obtained by Gouge *et al.* [51] is not without doubt. The temperature values should be compared to real build temperature values for further validation.

Eqn. 2.20 is used to describe the loss of heat due to naturally induced convection. However, as Figure 2.4 (of Section 2.1.2.2) and Bitharas *et al.* [29] the gas in the process chamber does not begin as a static 'Brownian' environment, but is a dynamic, forced flow. Therefore, convection is not induced naturally due to the thermal gradients of the

process. As a result, h values should be calculated on an *ad hoc* basis, for each material and machine.

2.1.2.5 Hydrodynamics

Once the powder bed is exposed to the laser or electron beam, localized melting occurs, and as such this melt pool is subject to its own set of hydrodynamic and thermal phenomena. The geometry of the melt pool is subject to many phenomena, convection is effected by the viscosity of the fluid. It is also influenced by other such phenomena such as gravity, buoyancy, surface tension, capillary, Marangoni effects, and evaporation pressure [52]. Whilst there are numerous physical phenomena within the liquidus region, it has been shown in studies of Laser Beam Welding, that Marangoni effects dominate the mass transfer within melt pool [53].

The Marangoni Effect is the name given to the mass transfer phenomenon in which a fluid flow is induced by a surface tension gradient mass flows from areas of low surface tension to high surface tension. This phenomenon was studied in detail by Carlo Marangoni in his doctoral thesis, published in 1865, from which the effect was given its name [54].

The surface tension of a fluid is dependent on the temperature and composition of the fluid [55]. Thus, the change in surface tension of a fluid ($d\sigma$) is given as:

$$d\sigma = \frac{\partial\sigma}{\partial T}dT + \sum_i \left(\frac{\partial\sigma}{\partial c_i} dc_i \right), \quad (2.22)$$

where T is temperature in Kelvin, and c_i is the concentration of a single chemical species present in the fluid's surface. This gives rise to the thermal dependence of surface tension, denoted by γ :

$$\gamma = \left| \frac{d\sigma}{dT} \right|. \quad (2.23)$$

The absolute value is used in order to maintain the positive domain of the Marangoni number. From Eqn. 2.23 a boundary condition for the free surface of a liquid/gas interface can be derived:

$$[\mu(\nabla \mathbf{u} + \nabla \mathbf{u}^T)] \cdot \mathbf{n} = \gamma \nabla_t T, \quad (2.24)$$

where μ is the dynamic viscosity of the fluid, $\mathbf{u}$ is the fluid velocity, and $\mathbf{n}$ is the normal vector to the free surface. This boundary condition can then be used in conjunction with the Navier-Stokes Equations [56]:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot (\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} + \mathbf{F}, \quad (2.25)$$

to derive a solution to fluid flow induced by surface tension gradients. Here, ρ is the fluid density, $\mathbf{u}$ is the fluid velocity, p is the fluid pressure, and F is any external force acting on the fluid. In PBF the laser heat source induces thermal and compositional gradients at the point of impact, driving the Marangoni Effect in the melt pool, as shown by Eqn. 2.22. When applied to the problem of Laser PBF, the surface Marangoni flows cause convection currents in the melt pool, accommodating further heat transfer throughout the melt pool and into the solid part. Due to its dependence on the concentration of all chemical species present, Eqn. 2.22 also shows that not only the alloying elements can contribute to the formation of such fluid flows, but also alloy impurities must also be considered [57].

The non-trivial contribution of these impurity elements to the overall Marangoni flow is well documented in its effects on the welding of metal alloys [53,57–59]. Here, it shows that it is possible for sufficient concentrations of sulphur can cause a reversal in the Marangoni flows within a melt pool, which in turn, affects the melt pool geometry:

Le *et al.* showed that in 316 stainless steel, the transition from a positive to a negative surface tension gradient occurred from 13 ppm of sulphur to 156 ppm [57]. This implies the existence of a meta-stable point where a specific concentration of sulphur, could cause there to be no surface tension gradient. Thus, there would be no Marangoni flow at all and heat transfer through the melt pool would be dominated by conduction and buoyancy effects. The effect of sulphur concentration on the surface tension gradient is well documented in steel systems [60,61], and in Inconel718 [62]; but whether a similar observation can be made in other alloy systems is a topic for further investigation.

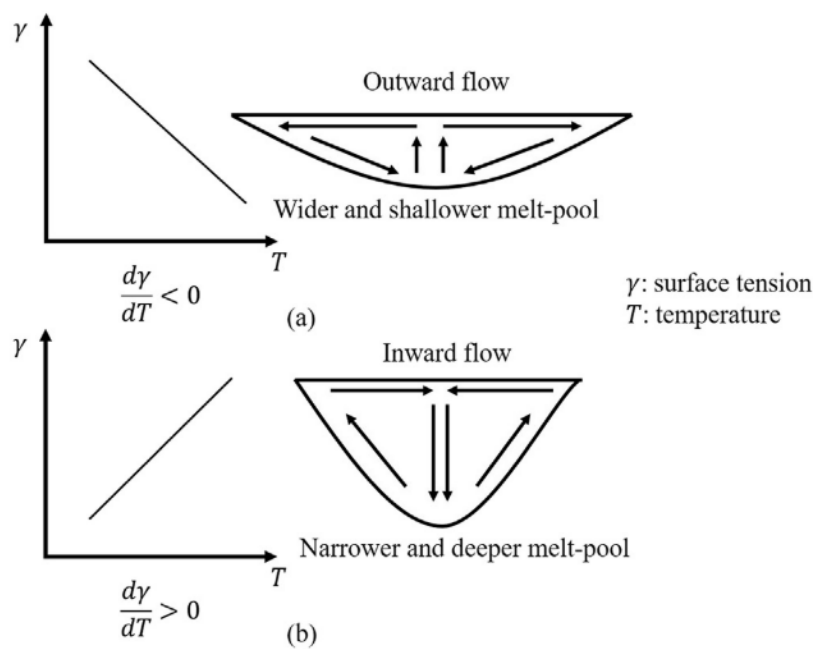


Figure 2.5: Schematic diagram of fluid flow patterns within the melt pool for: (a) negative surface tension gradient, and (b) positive surface tension gradient [57]

2.1.2.6 Solidification

Once there is no more heat input from the laser, heat transfer away from the melt pool occurs due to conduction, convection, and radiation. Whilst Marangoni convection helps to reduce the magnitude of the temperature gradients within the liquidus region; the melt pool still loses heat to the gaseous environment, the bulk of the component, the substrate plate, and even the surrounding powder through the mechanisms described in [Sections 2.1.2.2 - 2.1.2.3](#). These temperature gradients serve as the driving force for the transformation process of liquid to solid.

The start of this process begins with nucleation. Nucleation occurs when the free energy of a solid phase is lower than that of the liquid phase. The transformation from solid to liquid does not occur instantly, thus a liquid has the potential to hold a state of undercooling or supersaturation.

The formation of nuclei in the body of a melt without any influence from outside material is referred to as homogeneous nucleation [63]. Not all nuclei go on to form grains during solidification in the melt there are clusters of atoms which could go on to form embryos but this only occurs if they are energetically preferable. If the clusters of nuclei are assumed to

be spherical the associated change in free energy associated with the solid/liquid interface is given [64]:

$$\Delta G = \Delta G_I + \Delta G_V = 4\pi r^2 \gamma - \frac{4\pi r^3}{3} \Delta s_f \Delta T. \quad (2.26)$$

Here the equation is the sum of two terms: ΔG_I is the associated interface energy of the solid/liquid interface formed; and ΔG_V is the difference in free energy associated between the solid and liquid phases. The free energy associated with the solid/liquid interface is defined by its shape and the interface energy, in this case the atom clusters are assumed to be spherical, thus the shape of the interface is given as $4\pi r^2$, where r is the radius of the sphere. This is then multiplied by γ , which is the interface energy. The difference in free energy between the solid and liquid phases is given by the term ΔG_V , again, assuming the cluster is spherical in shape the volume of the cluster is given as $4\pi r^3/3$; this is then multiplied by Δs_f (the entropy of fusion per unit volume), and ΔT (the variation in temperature from liquidus). For any temperature above liquidus, ΔG_V is always positive, therefore it is always energetically favourable to remain in a liquid state. Once temperature decreases below liquidus, ΔG_V becomes negative and transformation to solid state is supported. On further inspection of 2.26, it can be seen that the left term has an r^2 dependency, and the right term has an r^3 dependency; therefore this results in a function with a turning point of maximum ΔG . The value for both the maximum ΔG and the corresponding radius at which this occurs can be calculated via the use of calculus, which yields:

$$\Delta G_{homo} = \frac{16\pi}{3} \frac{\gamma_{sl}^3}{(\Delta s_f)^2 \Delta T^2}, \quad (2.27)$$

and

$$R_c = \frac{2\gamma_{sl}}{\Delta s_f \Delta T} = \frac{2\Gamma_{sl}}{\Delta T}. \quad (2.28)$$

Here, Γ_{sl} is known as the Gibbs-Thompson coefficient, and is equal to $\gamma_{sl}/(\Delta s_f)$. Equation (2.27) is known as the required activation energy for homogeneous nucleation, and equation (2.28) is known as the critical radius of nucleus required to form an embryo.

It is often the case that there are foreign bodies interacting with the melt, whether this be solid particulate suspended in the melt, or the wall of a mould or crucible. In the case

of LPBF it is the edge of the meltpool itself, that acts as a foreign substrate for the melt. These foreign bodies can act to facilitate the nucleation of embryos for solidification, and is known as heterogeneous nucleation [65]. The outline of the process of heterogeneous nucleation is shown in Fig 2.6.

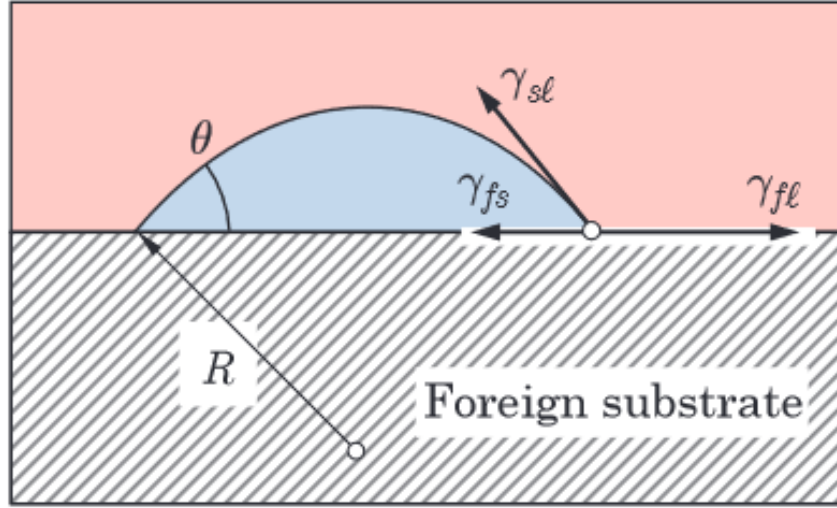


Figure 2.6: The Nucleation of a Spherical Solid Cap at a Liquid-Substrate Interface [65]

Resolving the forces parallel to the substrate surface, a relationship between the surface energies and the wetting angle, θ , is obtained:

$$\gamma_{fl} = \gamma_{fs} + \gamma_{sl} \cos \theta. \quad (2.29)$$

This is known as the Young-Laplace Equation [66]. If θ is such that $\gamma_{fl} > \gamma_{fs} + \gamma_{sl}$, the preferable state is for the solid cap to form a thin layer across the surface of the substrate, separating the substrate from the liquid. Whilst this does not prevent nucleation, it is not the orthodox schema and must be treated separately. If θ is such that $\gamma_{fs} > \gamma_{fl} + \gamma_{sl}$ then the preference is for the solid cap to separate from the foreign substrate to form a spherical particle in the melt, no longer contributing to heterogeneous nucleation, but homogeneous nucleation. The final case is for θ that satisfies:

$$\left| \frac{\gamma_{fl} + \gamma_{fs}}{\gamma_{sl}} \right| < 1. \quad (2.30)$$

In this case, when $0 \leq \theta \leq \frac{\pi}{2}$ the surface is considered to be “wetted” and the change in volumetric Gibbs Free Energy is given by:

$$\Delta G = V_s(G_s - G_l) + A_{sl}\gamma_{sl} + A_{fs}(\gamma_{fs} - \gamma_{fl}), \quad (2.31)$$

where V_s is the volume of the solid nucleus; and A_{sl} and A_{fs} are the surface areas of the nucleus-liquid and the nucleus-substrate interfaces, respectively. Using trigonometry, and substituting $g_s - g_l = -\Delta s_f \Delta T$ an expression for the change in Gibbs Free Energy for heterogeneous nucleation for undercooling ΔT :

$$\Delta G = \left(4\pi r^2 \gamma_{sl} - \frac{4\pi r^3}{3} \Delta s_f \Delta T \right) f(\theta). \quad (2.32)$$

Here, $f(\theta) \in [0, 1]$, where $f(\theta)$ is a ratio between the volume of the nucleus and the volume of a sphere with identical radius of curvature, in terms of θ :

$$f(\theta) = \frac{V_s}{4\pi r^3/3} = \frac{(2 + \cos \theta)(1 - \cos \theta)^2}{4}. \quad (2.33)$$

If the expressions for homogeneous (2.26) and heterogeneous (2.32) nucleation are to be compared, it can be seen that the Gibbs Free Energy of heterogeneous nucleation is a factor of $f(\theta)$. As with homogeneous nucleation, calculus is applied to find the required activation energy, and critical radius for heterogeneous nucleation. This yields:

$$\Delta G_{heter} = \Delta G_{homo} f(\theta) = \frac{16\pi}{3} \frac{\gamma_{sl}^3}{(\Delta s_f)^2 \Delta T^2} f(\theta), \quad (2.34)$$

and

$$R_c = \frac{2\gamma_{sl}}{\Delta s_f \Delta T} = \frac{2\Gamma_{sl}}{\Delta T}. \quad (2.35)$$

As can be seen, the critical radius is independent of θ and is therefore the same as with homogeneous nucleation; and the activation energy is less than the homogeneous activation energy by a factor of $f(\theta)$. Therefore, it is always the case that it requires less

energy to induce nucleation heterogeneously. Thus, in the context of LPBF, the grain growth is much more likely to begin at the melt pool boundary and proceed into the center of the melt pool.

Further, solid-state changes of this microstructure can be achieved through previous layers being exposed to the HAZ of the current layer [67, 68]. This can often result in the recrystallisation of the meltpool grain structure so that overall columnar grain growth is observed, with the column aligned with the build direction (z axis) as was observed by Carter *et al.* [69], and is considered characteristic of PBF manufacturing.

2.1.3 Manufacturing Defects

There are a number of defects that can occur during the LPBF of metallic alloys; namely Lack of Fusion (LoF) porosity, Gas Porosity, Keyhole Porosity, and Cracking.

2.1.3.1 Lack of Fusion Porosity

LoF porosity occurs when insufficient melting occurs in the powderbed to form a continuous melt pool, thus unmelted powder particles can be observed in the part's cross-section, as is shown in [fig. 2.7](#).

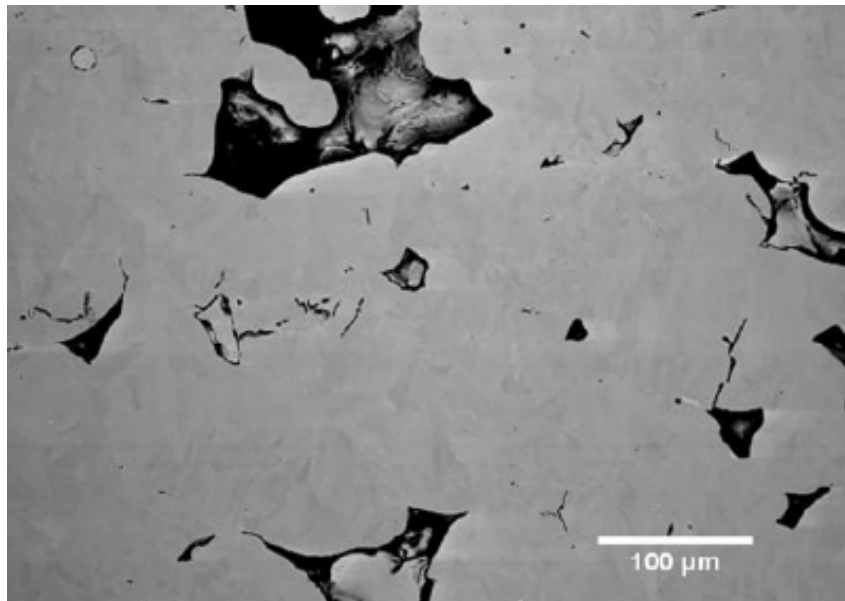


Figure 2.7: Lack of fusion porosity in CM247LC, taken from [70]

LoF porosity can occur for a number of reasons; insufficient energy deposition of the

beam in the powderbed, discrepancies in the powder packing density of the powderbed, or surface chemistry of the powderbed.

There have been numerous studies on the minimum threshold for energy deposition during LPBF to achieve maximum density parts [71–73]. However, there lies a challenge in quantifying a universal index for the energy deposition into a powderbed, due to the high number of machine and process parameters that change from manufacturer to manufacturer; and the numerous different alloy systems employed in LPBF. The common indices utilized for energy deposition in PBF are the series of expressions for Energy Density (E). There are three energy densities in common use, linear, area, and volumetric; each one incorporates different process parameters:

$$E = \frac{P}{u}, \quad (2.36)$$

$$E = \frac{P}{hu}, \quad (2.37)$$

$$E = \frac{P}{hud}. \quad (2.38)$$

Here, P is the laser power in watts, u is the laser scanning speed in $mm s^{-1}$, h is the laser hatch spacing in mm , and d is the layer thickness in mm . It is this reason that each Energy Density is referred to as linear, area, and volumetric; as each one has units of Jmm^{-1} , Jmm^{-2} , and Jmm^{-3} respectively. Carter *et al.* used area energy density to empirically derive an optimised processing parameters for a number of Nickel-based Superalloys the threshold for maximum density parts can be seen in [fig. 2.8](#).

Carter *et al.* were able to propose a threshold for minimising porosity in a number of Nickel-based Superalloy systems. However, due to the lack of material information utilised in the expression of energy density there is little applicability to alloy systems beyond the Nickel-based Superalloys of the study. The same limitations apply to Tan *et al.* [72], Letenneur *et al.* [73] and any other attempt to use energy density as a universal measure to transfer alloy systems between different LPBF machines. As the downfalls of the Energy Density criteria are well known [74–77], others have attempted to derive other indices to fulfill its intended purpose that incorporates more information about the

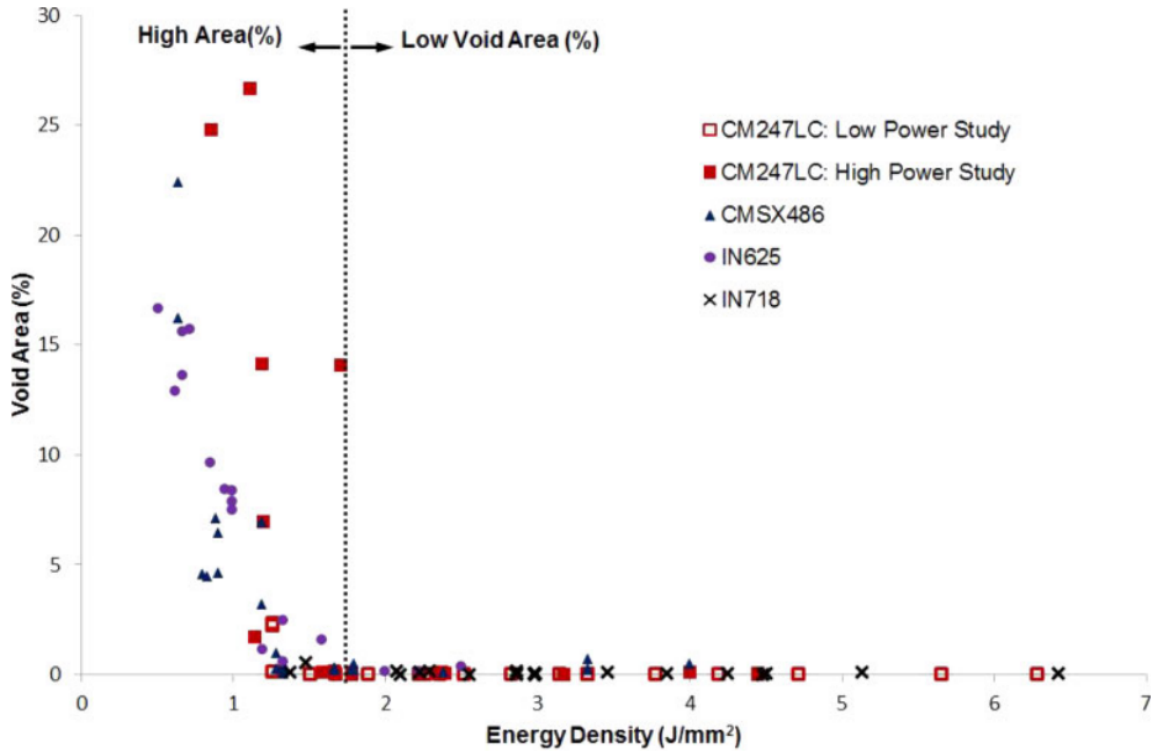


Figure 2.8: Graph of Area Porosity vs Area Energy Density, taken from [70]

alloy system, and the machine system. Specific Enthalpy ($\Delta H/\Delta h_s$) was developed for Laser Beam Welding, and incorporates thermophysical properties, such as thermal conductivity; and machine properties such as laser spot size. Hann *et al.* [78] provide a derivation of the Specific Enthalpy expression. The formula for Specific Enthalpy is a solution to the energy balance equation:

$$\begin{aligned}
 (\Delta x \Delta y) \Delta z \Delta H_{max} &= \int_{-\infty}^{\infty} \frac{\eta 2P e^{2(ut)^2/\sigma^2}}{\pi \sigma^2} (\Delta x \Delta y) dt \\
 &- \int_{-\infty}^{\infty} S \alpha \rho \Delta H_{max} dt.
 \end{aligned} \tag{2.39}$$

Here, the first term of Eqn. 2.39 is the energy input into the volume, and the second term is the heat lost through conduction. As can be seen in Eqn. 2.39 the first term incorporates more machine information in the form of the laser spot size (σ), and more material information in the form of the material's absorptivity (η). The second term also incorporates further material information in the form of the material's thermal conduc-

tivity (α) and the density (ρ). There is also incorporation of the term S , the ‘Conductive Shape Factor’. The conductive shape factor is well known in the study of solutions to the heat flow problem, and is a ratio between the surface area of the isotherms between two isothermal surfaces and the distance between the two isothermal surfaces, and is dependent on the geometry of the problem. In the case of simple geometries, the shape factor is trivial, and can be derived through inspection; for more complex geometries, the shape factor must be calculated through numerical methods [79]. Hann *et al.* relate the depth of heat conduction during the time of heating via the relationship defined for ‘early regime’ heating given by Bejan [79]:

$$\Delta z \approx \sqrt{\alpha \times \frac{2\sigma}{u}}. \quad (2.40)$$

Here, α is the thermal conductivity of the material, σ is the spot diameter, and u is the scanning speed; by making this substitution and solving for $\Delta H/h_s$, Eqn. 2.39 becomes:

$$\frac{\Delta H}{h_s} = \frac{1}{1 + S'\sqrt{Fo}} \frac{\eta P}{\rho h_s \sqrt{\pi \alpha \sigma^3 u}}, \quad (2.41)$$

where S' is the ‘average shape factor’, and Fo is the Fourier Number. However, Hann *et al.* provide no explanation as to the expected value or derivation for S' , nor how the shape factor has been averaged. Due to the integrals of Eqn. 2.39 being with respect to time, one can only assume it is the time averaged shape factor. This still leaves the problem of selecting a reasonable approximation for the shape factor.

If a “best estimate” for the shape factor is attempted, then according to the work conducted into the absorptivity of metallic powder beds [19, 20], it would be most suitable to model the laser heat source as an isothermal volume embedded into the surface of a semi-infinite medium. However, none of the common expressions for such shape factors are bound over the domain of the time integral. Therefore, a lack of expansion on the selection of a conductive shape factor, and the accompanying method of averaging, renders this index for predicting material behaviour during AM not fit for purpose.

Due to the pitfalls of the energy density criteria, and the lack of suitable replacement, extensive design of experiment (DOEs) are required per material prior to part produc-

tion. During which, many different processing parameters are trialed to produce simple geometry parts. These are then sectioned and examined for defects to establish which processing parameters are optimum for part density. As the range of parameters is so varied, these DOEs may need to be repeated several times. Each one consuming material and time, adding to the overall expense of part production. Once, parameters have been established for a single material, on a single machine, then a DOE need not be performed again. However, as shown earlier, factors such as gas flow, vary between upgrades, therefore, theoretically, DOE must be performed after any machine changes also. Consuming more material, and time.

2.1.3.2 Gas Porosity

Another form of porosity defect is referred to as gas porosity. Gas porosity is characteristically smaller than LoF porosity, and has a spherical morphology. In LPBF, gas porosity can be introduced to the part prior to processing (via powder manufacturing) [80] or during the build process. Inert gas atomisation, is a popular method for producing stock powder for the AM process. During inert gas atomisation, a droplet or stream of molten material is exposed to a jet of high pressure inert gas. The surface tension causes the stream to break into spherical particles that solidify, and can be collected. By altering the pressure of the gas jet, one can modify the size distribution range of the powder particles that are formed [81].

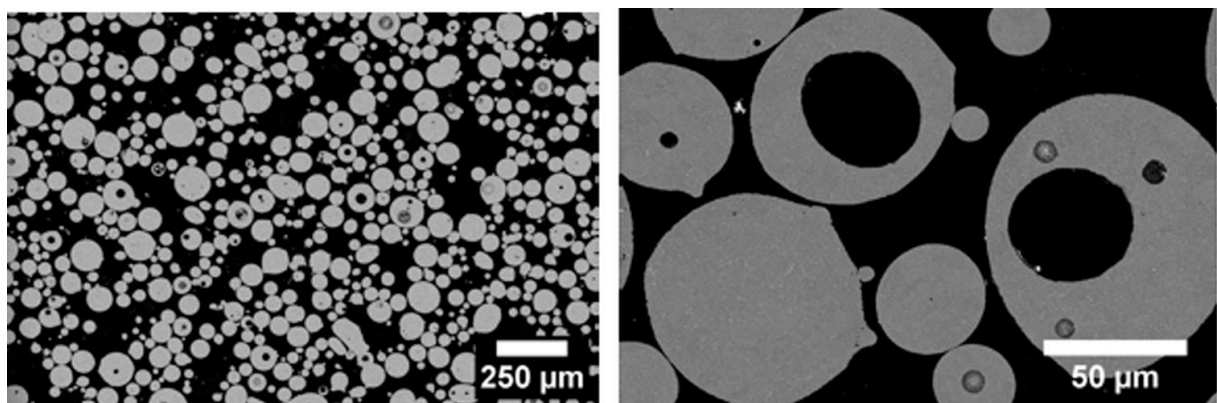


Figure 2.9: SEM Micrograph Showing Gaseous Porosity in Metallic Powder Produced by Gas Atomisation [82]

There are two accepted methods for gas pore formation in metallic powders: entrapment,

and dissolution. Gas entrapment occurs when the inert gas forms a bubble within the molten metal, the molten metal then solidifies around the gas. An example of such a pore can be seen in [Fig. 2.9](#). Gas porosity can also form when the inert gas used for atomisation is dissolved in the molten metal by the high pressure of the jet, then during solidification, the gas is forced out of the metallic matrix and into the inter-dendritic space, forming a pore. While gas pores formed via both mechanisms are spherical in shape, those formed via dissolution tend to be of smaller diameters than those formed via entrapment.

Both entrapment and dissolution porosity is possible during LPBF due to the inert atmosphere required for processing. In order to predict the level of gaseous porosity present in the final part would require prior knowledge of the gas porosity content of the feedstock powder, an exact knowledge of the fluid flow dynamics of both the inert atmosphere and the molten metal, and the thermal history of the build. Such calculations would require high fidelity, high-capacity, large-throughput, multi-physics simulations, and as such are innately incompatible with industrially relevant timescales, with the current technology available (explored in [Sec. 2.3](#)).

2.1.3.3 Keyhole Porosity

The purpose of the heat source in EB and LPBF is to, of course, melt selected areas of powder in the powder bed. A side-effect of the elevated temperatures of these areas is the evaporation of low boiling-point elements present in the alloy system. There are those which are there by design, for example, aluminium, and those that are unavoidable, such as sulphur and phosphorous impurities. When these species are evaporated from the melt, the momentum carried by the vaporised atoms result in a recoil pressure exerted normal to the molten surface [83]. The greater the rate of evaporation, the greater the recoil pressure exerted onto the surface of the melt. This can cause the surface of the liquid phase to bow inward, causing a gas cavity. The size and shape of the gas cavity is determined by the recoil pressure of the evaporated elements, the hydrostatic pressure and the surface tension of the liquid phase [27]. Should a sufficient amount of evaporation be maintained then the dominant process for heat transfer into the material transitions

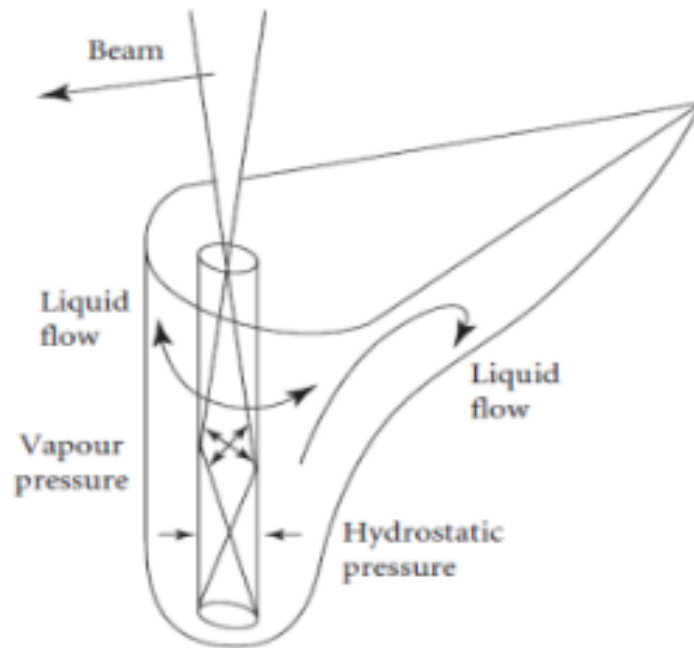


Figure 2.10: Diagram of typical keyhole meltpool morphology. Taken from [83]

from conduction dominant, to fluid flow dominated; these modes of heating are referred to as Conduction-mode and Keyhole-mode respectively.

During keyhole-mode processing, the melt pool takes on a very distinct shape, as shown in Fig. 2.10, after which keyhole-mode is named. As shown in Sec. 2.1.2.5, the motion of the liquid region is heavy dependent on the chemical species present. Thus, as the beam travels across the surface of the powder-bed the chemical species will vary, and as shown by [57–59], even small variations in ppm concentration of species such as sulphur can have large effects on the fluid flow of the melt. Thus, it can be difficult maintaining a stable keyhole. Should instability cause the keyhole to collapse, it is easy for the gas within the cavity to become trapped as the molten metal encloses around the gas of the cavity, and the solidifies. Defects caused in this way are referred to as keyhole porosity, and are characteristically orders of magnitude larger than gas porosity.

Prediction of the transition of processing mode from Conduction-mode to Keyhole-mode has been the subject of extensive investigation [78, 83–85], using a multitude of indices from Energy Density (eqns. 2.36, 2.37, 2.38), to Specific Enthalpy (eqn. 2.41). The range of values that processing mode transitions has proved to be dependent on many factors, including both material properties, and processing properties [84]. However, it can also

be shown that in a simplified case, where the thermal field of a volume is represented by the Rosenthal’s Solution adapted for a moving heat source [86]:

$$T = T_0 + \frac{\lambda P}{2\pi k r} e^{-\frac{V(r+\xi)}{2\alpha}} \quad (2.42)$$

the temperature of any point can be represented as a summation over time of the previous Rosenthal solutions. it can be deduced that the starting temperature (T_0) of the subsequent laser vectors is a summation of the starting temperature of the volume and the contribution from previous laser exposures. Thus, each subsequent laser exposure is subject to a “preheating” effect. This means that for constant laser parameters, the processing mode may transition from conduction to keyhole due to geometry and build strategy. Alternatively, when keyhole mode is desired, the keyhole may grow unstable and lead to build defects due to the preheating phenomena. This is shown by the work of Zhao *et al.* of Virginia Tech. University geometric accuracy of constant processing parameters decreased as laser vector length became shorter due to the reduced time between subsequent laser vectors due to the increased preheating experienced [87]. Thus, any in order to calculate the processing mode beforehand, not only should material properties and laser parameters be considered, but also geometry and scanning strategy. In this case, it may be more desirable to simulate the thermal field of the build in order to identify areas where overheating may occur.

2.1.3.4 Cracking

One of the many characteristic parts of the PBF process is the formation of incredibly high thermal gradients, and cooling rates in the produced part. Due to these intense gradients, PBF produces parts with exceptionally high levels of residual stress. Depending on the material used in production, unless these residual stresses are mitigated, or relaxed, they may cause the part to warp/distort or crack. Types of cracking can be seen in Fig. 2.11.

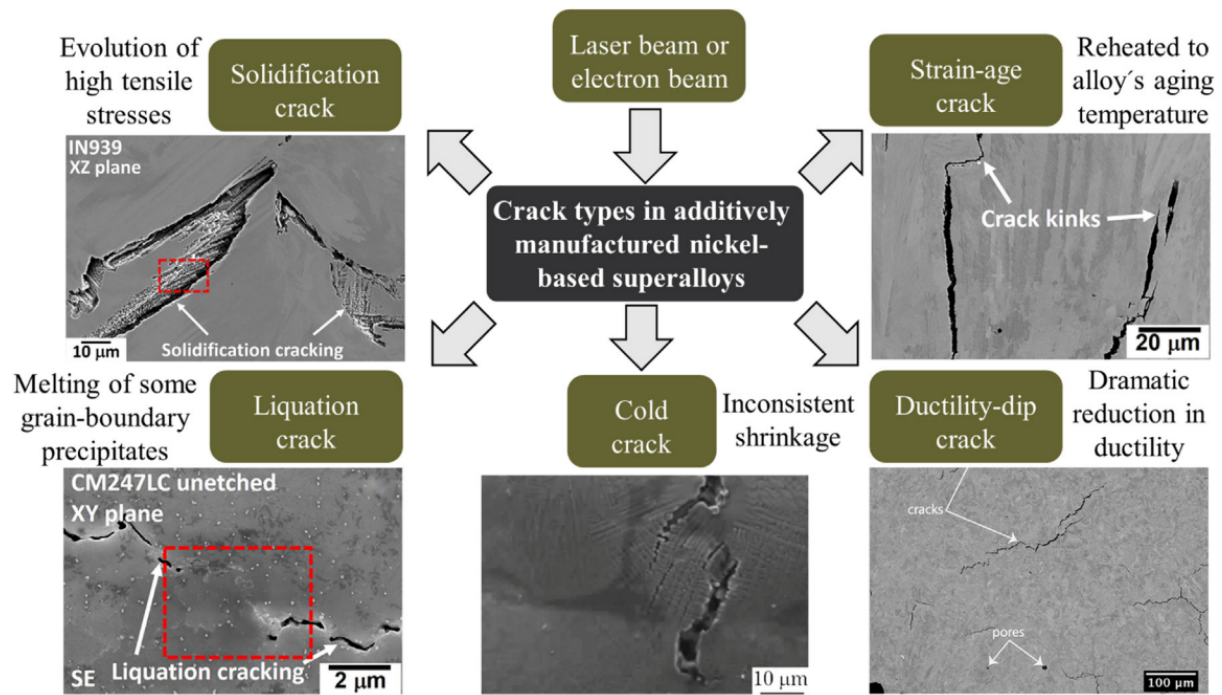


Figure 2.11: Types of Cracking Found in the Additive Manufacture of Metals through Powder Bed Fusion. Taken from [88].

2.1.3.4.1 Solidification Cracking Solidification cracking occurs during the liquid to solid transformation of the alloy system during processing. As the solidification front propagates into the liquid meltpool, the change in density from liquid to solid produces a negative hydrostatic pressure that is exerted on the molten metal. If sufficient pressure is exerted, cavitation can occur in the molten metal, causing multiple microscopic voids to nucleate. These pores then act as initiation sites for microcracks which then propagate and interconnect, forming one large defect in the bulk upon cooling [89].

2.1.3.4.2 Liquation Cracking Liquation cracking occurs in the HAZ surrounding the heat source/material interaction. The elevated temperature in the HAZ causes localized melting along grain boundaries (or areas of lower interface energy). The hydrostatic pressure generated by the introduction of liquid at the boundary causes stress in the boundary. If this hydrostatic pressure overcomes the yield stress of the material, then deformation occurs and the crack propagates along the boundary [90].

The presence of certain chemical species can increase the probability of localised melting. Such chemical species include low melting point oxides, sulphur, phosphorous, and boron.

As mentioned previously, LPBF is commonly performed under an inert gas shielding atmosphere, and EPBF under vacuum, however, due to powder production technologies, and the increased surface area to volume ratio of the metallic powders, each powder particle usually possesses a stable oxide layer. Some alloy systems such as 300 series stainless steels and aluminium alloys are designed to possess a stable oxide layer in order to improve the corrosion resistance of the alloy. Any oxide present in the powder before processing acts as a source of oxygen for reaction during processing. Thus, even in a perfect atmosphere, processing via PBF can produce low melting point oxides, which will encourage liquation cracking.

2.1.3.4.3 Cold Cracking Another mechanism for cracking that is driven by the highly anisotropic heat distribution in LPBF is cold-cracking [91]. Due to the anisotropic heat distribution within the processed part high levels of residual stress is induced within the solidified metal. Upon cooling the geometry drives non-uniform shrinkage and distortion within the part. If the stresses induced exceed the ultimate tensile stress of the alloy then to relieve the residual stresses cracking ensues. This mechanism of cracking can be somewhat overcome through the selection of processing parameters. However, aggregation of the build geometry to identify problematic areas is either left to the experience of the engineer or requires lengthy, iterative simulations to be performed to find the correct parameters.

2.1.3.4.4 Ductility-Dip Cracking Ductility-Dip cracking is a mechanism that is only observed in the additive manufacture of nickel-base super alloys [92]. The mechanics of ductile-dip cracking is not very well understood. However, it has been described as “creep-like”, and occurs at a temperature range that increases intragranular motion but too low to induce dynamic recrystallisation [92]. Therefore, this temperature range is usually 0.5 to 0.7 times the solidus temperature of the alloy, at which there is usually a sharp drop-off in ductility [93].

2.1.3.4.5 Strain-Age Cracking Due to the point-wise application of energy and the layer-by-layer production method of parts with PBF AM, a single point within the part will undergo a repeated cycle of heating and cooling. Once solidified, it is possible that a point within the part will be raised above the aging temperature of the alloy system. Precipitation-strengthening alloys such as some nickel-base super alloys are particularly susceptible to a type of cracking called “Strain-Age Cracking” when this occurs [90]. Precipitation-strengthening alloys develop precipitates above the aging temperature which aid with dislocation pinning, which increases strength. However, this increase in strength comes at the cost of the ductility of the material. Hence, without initially relieving the high residual stress, also characteristic with PBF AM, a reduction in the ductility may cause cracking to occur in the solid state during the build process if the residual stresses were to exceed the ductility of the alloy. Carter *et al.* showed that these cracks are most likely along grain boundaries that align with the build direction [94].

2.1.4 300 Series High Alloy Stainless Steels and 316L

Stainless Steels are a staple material in all industries, with the stainless steel industry itself expected to exceed a net worth of \$182 Billion USD by 2027 [95]. While most of this growth is expected to be due to the infrastructure/construction industries due to rapid urban expansion worldwide, a considerable part of the growth is due to the petro-chemical industry [96]. The petro-chemical industry has utilized stainless steels for many years due to its excellent corrosion resistance in the chemically extreme environments caused by the caustic substances used. Due to rising pressure globally, i.e. The Paris Agreement [97], on industries to increase energy efficiency and reduce carbon emissions, fossil fuel companies have turned to additive manufacturing to optimise burn rates and tooling production in order to meet these goals [98].

2.1.4.1 Chemical Composition and Phases

Stainless steels, via the addition of Chromium, were discovered in 1913 by Harry Brearley whilst investigating novel steels for rifle barrels. Whilst Iron/Chromium alloys

had been commonplace throughout the previous century, it was the discovery that at 0.3wt.% Carbon and 13wt.% Chromium the resultant alloy was resistant to etching and corrosion at ambient conditions. This alloy became the basis for the 400 series stainless steels which are still in wide use today.

Concurrently, in Germany, Iron/Nickel alloys were in circulation as tarnish-resistant, but lacked the required corrosion resistance. It was at this time that a patent was filed for an Iron/Nickel/Chromium alloy with improved corrosion resistance over the standard Iron/Nickel alloys. These alloys became the basis for the 300 series of austenitic stainless steels.

In the Iron/Chromium binary system, the introduction of increasing amounts of Chromium leads to increased corrosion resistance. At the 12wt.% Chromium a threshold is met where the alloy is able to sustain a thin, passive, protective layer of Cr_2O_3 Chromium Oxide at room temperature. This oxide layer prevents any potential corrosive species from coming into contact with the bulk. Hence, the excellent corrosion resistance that is characteristic of stainless steels.

Between 42-50wt.% Cr the alloy system forms an intermetallic tetragonal sigma phase that is hard and brittle, and is detrimental to the corrosion resistance of the system. The phase diagram for the Iron/Chromium system can be seen in [Fig. 2.12](#). Commercially, the range of weight percent Chromium that is of interest on the phase diagram is between 12wt.% and 25wt.%. However, due to the ability of Chromium to encourage the formation of inter-granular carbides, it is also desirable for any Iron/Chromium system to possess very low Carbon levels (of the order of <0.2wt.%) as these carbides would reduce the corrosion resistance. The Iron/Carbon phase diagram is shown in [Fig. 2.13](#).

From [Fig. 2.12](#) and [2.13](#) it can be seen that a low-Carbon, Iron/Chromium alloy would present as an alpha, body centered cubic (BCC), ferritic alloy at room temperature. However, due to the properties of ferritic steel when used in fabrication processes such as welding, they are susceptible to microstructural changes in the HAZ. This can lead to compromised corrosion resistance and embrittlement post fabrication. Therefore, in order to overcome these shortcomings, a way to retain the gamma, face centered cubic (FCC),

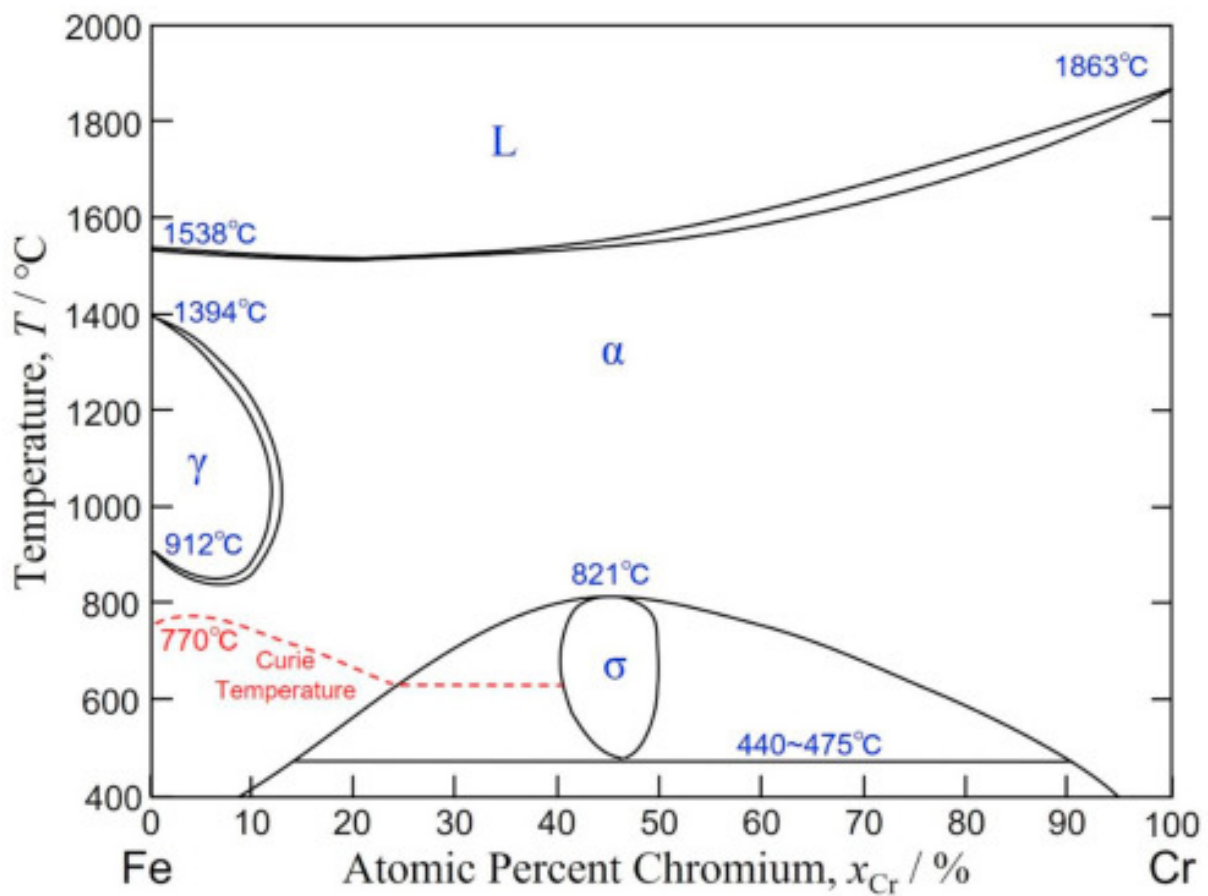


Figure 2.12: Iron-Chromium Binary Alloy Phase Diagram. Taken from [99].

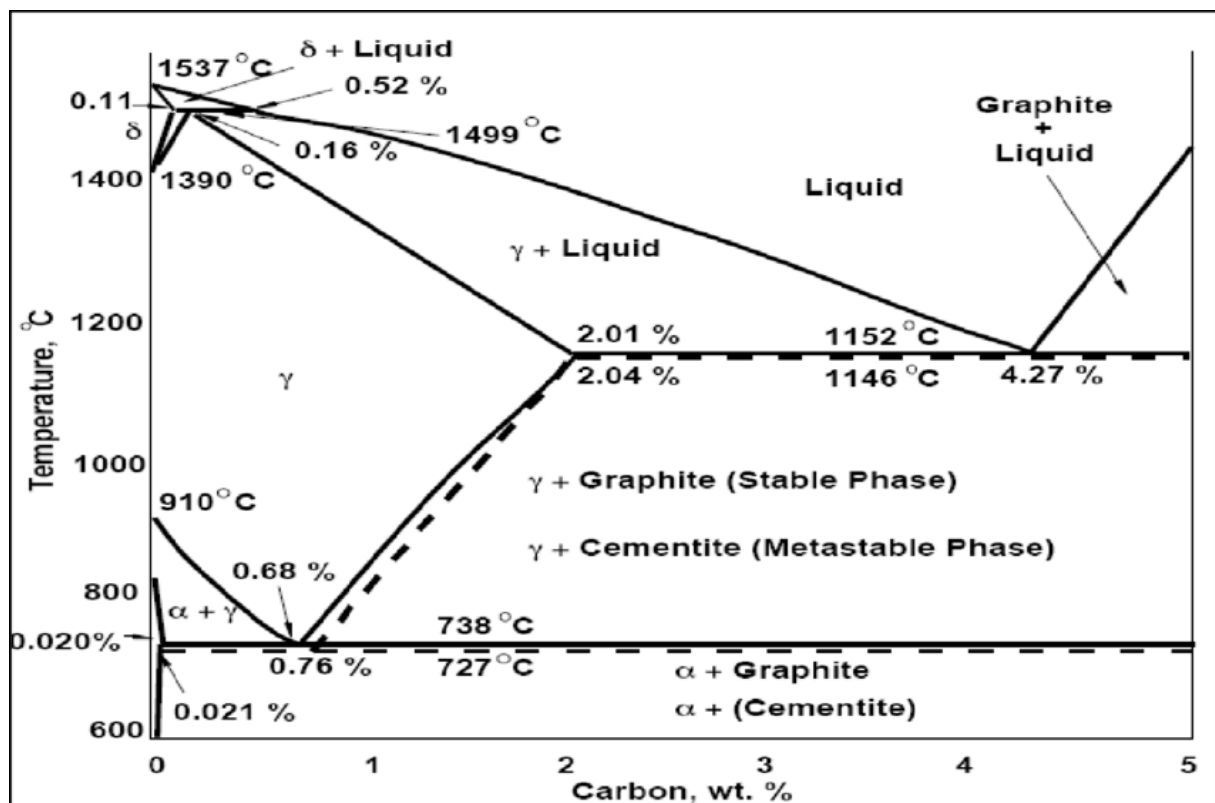


Figure 2.13: Iron-Carbon Phase Diagram above 600 degrees Celsius. Taken from [100]

austenitic structure at room temperature is required.

As mentioned earlier, in the 1910s a patent was filed for an Iron/Chromium/Nickel alloy with excellent corrosion resistance. The addition of Nickel to the Iron/Chromium binary suppresses the austenite to ferrite transformation to sub-zero temperatures. Allowing the system to retain a stable fully-austenitic microstructure. The AISI dubbed “300 series” of stainless steels is based on this quaternary system of Iron, 0.02-0.2wt.% Carbon, 17-20wt.% Chromium, and 8-12wt.% Nickel.

The AISI 316L is also referred to as 1.4404 in the UK, the specification of which is given by BS EN 10088-3:2005. The composition specification is given in [Table 2.1](#). As can be seen from this specification, there are additional elements added beyond the base quaternary system. The 300 series were designed to be fully austenitic stainless steels preferable for any application that required fabrication via welding. Therefore the additional elements added to the base quaternary system are to improve weldability and discourage phase changes due to the elevated temperatures and fast cooling rates of welding. Molybdenum’s inclusion into the system increases resistance to pitting corrosion, especially in chloride and sulphurous environments. Silicon is added to reduce the surface tension and increase the fluidity of the molten alloy, however, is a ferrite forming element and can preferentially oxidize to form “slag spots” during processing, therefore many stainless steels limit inclusion of Silicon to 0.75 wt.%. Sulphur and Phosphorous are included to improve weld penetration during processing, they do this by encouraging greater marangoni flow in the liquid region, increasing heat transfer into the bulk. However, high Sulphur and Phosphorous content steels are prone to the precipitation of Sulphide and Phosphide type inclusions upon welding, thus the need for Manganese. Manganese is added to increase strength, toughness, and hot working properties of the alloy by reacting with the Sulphur to create Manganese Sulphide inclusions. It is also an austenitic promoter to increase the stability of the alloy across all working temperatures, it is even used as a replacement for Nickel in the AISI 200 series steels. Finally, Nitrogen, like Nickel, is an austenite forming element. It also increases yield strength, and increases pitting resistance.

Table 2.1: Composition Specification for 316l/1.4404 Austenitic Stainless Steel. Taken from [101]

Element	wt.% Present
Carbon (C)	0.0 - 0.03
Chromium (Cr)	16.50 - 18.50
Molybdenum (Mo)	2.00 - 2.50
Silicon (Si)	0.0 - 1.00
Phosphorous (P)	0.0 - 0.05
Sulphur (S)	0.0 - 0.03
Nickel (N)	10.00 - 13.00
Manganese (Mn)	0.0 - 2.00
Nitrogen (N)	0.0 - 0.11
Iron (Fe)	Balance

2.1.4.2 Thermophysical Properties

2.1.4.2.1 Enthalpy and Specific Heat Capacity The values for enthalpy were measured via Power-compensation Differential Scanning Calorimetry (PDSC). The full method for measurement can be found in the work of Mills and Richardson [102].

Due to the complexity of the measurement apparatus, and the need for controlled heat input and measurement, it is not recommended that homemade apparatus is not used. Provided that the correct method of operation is used according to the manual provided by the machine manufacturer, the error in values should be within 1%. Sources of error in this process are introduced by unsuitable samples, incorrect machine calibration, or inadequate data processing [103].

In PDSC two pans of the exact same composition and dimensions are prepared. Pans are usually made of platinum, however other materials such as alumina and yttria are also used. A sample of the material to be measured is placed in one of the two pans. PDSC requires two pans, as both pans are thermally isolated, and the temperature of each is raised at a constant predefined regime (usually between 5 to 40 $Kmin^{-1}$). The powers required to raise the temperature of each pan are compared, revealing the thermophysical properties of the sample. The captured signal can be described:

$$S = I + K\Delta C \quad (2.43)$$

$$S = I + K(\Delta C_e + m_x c_{px}). \quad (2.44)$$

Where I is the power required to maintain the chamber at a given temperature, i.e. the isothermal losses of the machine chamber. The exact value of I is unimportant due to measurements being a difference between the two chambers as the temperature changes. What is of note is that the value of I is temperature dependent and therefore must be calibrated across the entire temperature range. The remainder of Eqn. 2.43 shows that the majority of the signal comes from ΔC the difference in specific heat capacities of each chamber, multiplied by K , the linear conversion coefficient. Eqn. 2.44 expands to show that the difference between the specific heat capacities of the chambers is a sum of the differences in specific heat capacities of the empty pans (ΔC_e), the mass of the sample or calibrant (m_x , where $x = s$ or $x = c$), and the specific heat capacity of the sample or calibrant (c_{px} , where $x = s$ or $x = c$). Thus:

$$S_e = I + K\Delta C_e, \quad (2.45)$$

$$S_s = I + K(\Delta C_e + m_s c_{ps}) \quad \text{and} \quad (2.46)$$

$$S_c = I + K(\Delta C_e + m_c c_{pc}). \quad (2.47)$$

Ideally, the sample pans should be of the exact same mass in order to reduce the effect on the signal. Modern manufacturing practices can assure mass variation on sample pans be no greater than $\pm 0.01g$. Therefore, the value of K can be easily measured by the use of the calibrant signal. The calibrant being a sample of material of known mass and known specific heat capacity, is compared to the signal of the empty pan:

$$\begin{aligned} S_c - S_e &= K m_c c_{pc} \\ K &= \frac{S_c - S_e}{m_c c_{pc}}. \end{aligned} \quad (2.48)$$

Common materials used for calibration of DSC machines are pure Nickel or Gold. Whilst the value of K is temperature independent, it is somewhat effected by rate of change of temperature, and is sometimes represented as $K_x \dot{T}$. Calibration of the DSC machine should be done frequently to ensure the accuracy of the conversion signal.

Comparing the signals from the empty pan and the unknown sample ($x = s$) yields and

expression for the unknown specific heat capacity:

$$c_{ps} = \frac{S_s - S_e}{Km_s}. \quad (2.49)$$

Combining this with Eqn. 2.48, an expression for the specific heat capacity of the sample is finally obtained:

$$c_{ps} = \frac{S_s - S_e}{S_c - S_e} \frac{m_c}{m_s} c_{pc}. \quad (2.50)$$

Therefore, the Enthalpy vs Temperature curve for the sample material can be trivially obtained via the numerical integration of the specific heat capacity vs temperature curve obtained via the DSC method.

$$\begin{aligned} c_{ps} &= \frac{dH_s}{dT} \quad \text{therefore} \\ H_s(T) &= \int c_{ps} dT \\ &= \int \frac{S_s - S_e}{S_c - S_e} \frac{m_c}{m_s} c_{pc} dT. \end{aligned} \quad (2.51)$$

2.1.4.2.2 Thermal Conductivity/Diffusivity The standard method for measurement of the thermal diffusivity of metals is via Laser Flash Analysis (LFA) and the procedure is outlined in ASTM standard E1461-13 [104]. The equipment setup used for measurement is shown in Figure 2.14.

LFA is based on calculating the thermal conductivity of a homogeneous sample of known dimensions, by increasing the temperature of one side of the sample, and measuring the time required for the opposing side of the sample to increase in temperature. The sample is encased in a furnace, so that the thermal conductivity can be measured over a range of temperatures, typically room temperature to 1650 degrees Celsius. The temperature increase is applied through a short pulsed laser, and the temperature rise is measured via infrared optical sensor.

The calculation for the thermal diffusivity of a material by LFA is based on the solution to the diffusion equation for a thermally insulated solid of uniform thickness, L , first

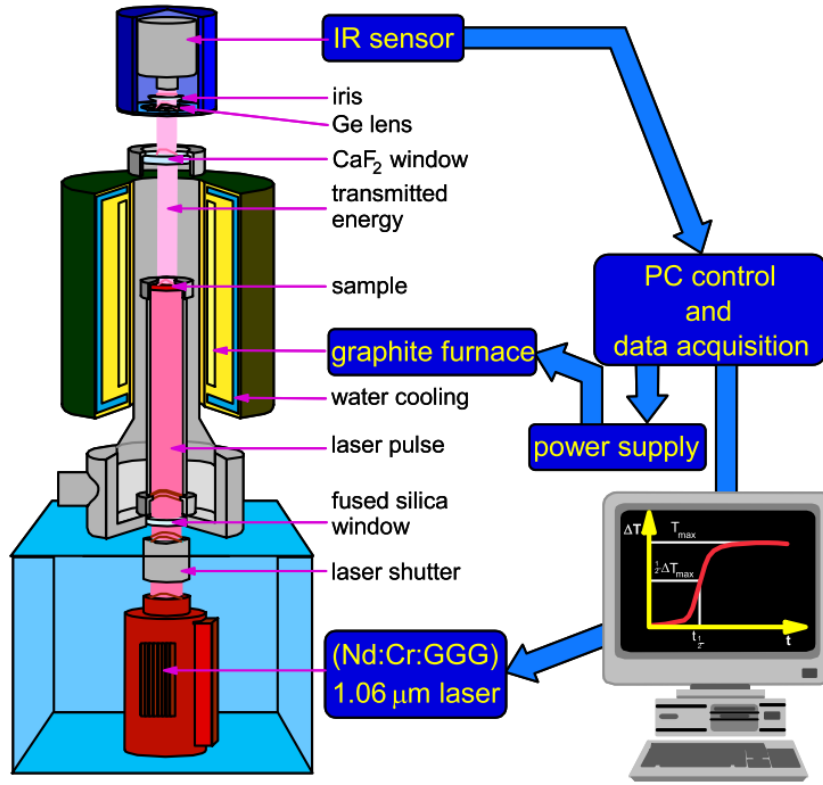


Figure 2.14: Diagram of Laser Flash Analysis Equipment. Taken from [105]

published by Carslaw and Jaeger in 1959 [106]:

$$T(x, t) = \frac{1}{L} \int_0^L T(x, 0) dx + \frac{2}{L} \sum_{n=1}^{\infty} \left(\exp \frac{-n^2 \pi^2 \alpha t}{L^2} \cos \frac{n \pi x}{L} \int_0^L T(x, 0) \cos \frac{n \pi x}{L} dx \right), \quad (2.52)$$

where α is the thermal diffusivity of the sample. Parker *et al.* [107] proposed the flash method to overcome the downfalls of previous methods:

1. Contact methods of heating and measurement introduces sources of error due to the thermal mass of the heat source and measurement probes altering the temperature distribution of the sample.
2. The short timescale between heating and measurement would minimise the error introduced to the results due to the cooling of the sample.
3. The method of heating could occur in a vacuum instead of an inert atmosphere which removes any heat loss due to atmosphere.

They also showed that for the initial conditions proposed in the LFA method Eqn. 2.52 can be used to calculate α .

Considering a laser pulse of intensity $P \text{ W/m}^2$ incident on the front surface ($x = 0$) of the sample (with absorptivity η), is instantaneously absorbed uniformly by depth g of material (where $g < L$). Then the temperature distribution at time $t = 0$ of the sample can be represented:

$$T(x, 0) = \begin{cases} \frac{\eta P}{\rho c_p g}, & 0 < x < g \\ 0, & g < x < L \end{cases} \quad (2.53)$$

where ρ is the sample density, and c_p is the sample heat capacity. Substituting this initial condition into Eqn. 2.52 yields:

$$T(x, t) = \frac{\eta P}{\rho c_p L} \left[1 + 2 \sum_{n=1}^{\infty} \left(\frac{\sin(n\pi g/L)}{n\pi g/L} \cos \frac{n\pi x}{L} \exp \frac{-n^2 \pi^2 \alpha t}{L^2} \right) \right]. \quad (2.54)$$

For opaque materials $g \ll L$, the ratio g/L is of the order of magnitude $\approx 10^6$ as discussed in 2.1.2.1, then a small angle approximation can be made for the sinusoidal term, thus the temperature measured at the reverse side of the sample $x = L$ against time, is given as:

$$T(L, t) = \frac{\eta P}{\rho c_p L} \left[1 + 2 \sum_{n=1}^{\infty} \left((-1)^n \exp \frac{-n^2 \pi^2 \alpha t}{L^2} \right) \right]. \quad (2.55)$$

This result can be expressed dimensionlessly, via two parameters:

$$V(L, t) = \frac{T(L, t)}{T_M}, \quad \text{and} \quad (2.56)$$

$$\omega = \frac{\pi^2 \alpha t}{L^2}, \quad (2.57)$$

where T_M is the maximum temperature expressed at the rear side of the sample. Combining Eqns. 2.55, 2.56 and 2.57, and solving for α , the expression for the thermal diffusivity of the sample:

$$\alpha = \frac{k_n L^2}{t_n}, \quad (2.58)$$

where t_n is the time taken for the rear surface of the sample to reach n percent of its maximum temperature; k_n is a coefficient that is dependant on the percentage n at which the thermal diffusivity is calculated for. Typically, n is 50 %, thus k_n is taken to be 1.3879, as was first proposed by Parker *et al.* [107]:

$$\alpha = 1.3879 \frac{L^2}{t_{50}}. \quad (2.59)$$

However, in order to confirm the validity of any measured LFA result, ASTM E1461-13 recommends confirming α over a range of values of n from the recorded temperature vs time curve; and as such, provides a table of the calculated values for k_n for a range of n :

Table 2.2: Table of values for k with corresponding n . Taken from [104].

$n(\%)$	k_n	$n(\%)$	k_n
10	0.066108	60	0.162236
20	0.084251	66.67	0.181067
25	0.092725	70	0.191874
30	0.101213	75	0.210493
33.33	0.106976	80	0.233200
40	0.118960	90	0.303520
50	0.13879	...	...

As outlined earlier, the use of an infrared thermometer (IRT) is desirable in LFA as due to the sensor not requiring to be in contact with the specimen, the thermal mass of the sample is not altered by the process. IRTs measure temperature by the variation in radiation of a heated body in accordance with the Stefan-Boltzman Law discussed in [Section 2.1.2.3](#). However, as shown in [Eqn. 2.13](#), the radiation of a body due to it's temperature is dependent on the emissivity (ϵ) of the surface. Therefore, the IRT must be calibrated to accommodate the emissivity in measurement, thus can be a source of error in such calculations [108]. Especially in the case of AISI 316L where the alloy system is designed to naturally produce an oxide layer for corrosion resistance, but this will alter the emissivity of the surface.

ASTM E1461-13 states that samples should typically be 10 to 12.5 mm in diameter, but a range of 6 to 30 mm are reported to also produce reliable measurements [104]. Regulation of sample thickness is less stringent, due to the required compromise between limiting

error:

- Too thin a sample results in the sample not being representative of bulk material, and the resulting value of thermal conductivity being of low accuracy.
- Too thick a sample increases the time taken for the opposing side of the sample to reach the desired temperature rise, thus lowering the accuracy of the measured time.
- Too thick a sample results in the length of laser pulse required for the desired temperature rise to increase, thus increasing temperature losses.

Therefore the standard suggests that samples to be of 1 to 6 mm thickness, with the maximum allowable variation in thickness of the sample being within 1%.

Error due to the analogue to digital conversion, and by baud rate of data capture is considered to be negligible in this process, as the sampling rate is minuscule in comparison to the target rise time outlined by ASTM E1461-13 (10 to 1000 ms) [104].

The largest source of error incurred by LFA is due to the thermal diffusivity of the material itself. As the method of measurement relies on a temperature differential between the two sides of the sample, the sample itself is never at a homogeneous temperature once the laser pulse is fired. This means that the thermal conductivity distribution throughout the sample matches that of the thermal distribution, and thus the thermal conductivity measured is that of a sample of indeterminate average temperature. In order to overcome this issue, the procedure for LFA is set so that the sample thickness should result in as near a homogeneous temperature distribution as possible upon measurement. Also, that the desired temperature rise seen at the opposing side of the sample is no more than 4 degrees Celsius. This means that the gradient of thermal conductivity with temperature is minimal, whilst the radiative emission measured from the sample is of significant signal to noise ratio. The results of Chapman *et al.* showed that when taken into consideration, the uncertainty of the LFA process is no more than 1.4% [105].

2.1.4.3 Additive Manufacturing of SS316L

Due to the development of AISI 316L stainless steel for weldability, there was a natural progression for early adoption following the advent of Direct Metal Laser Sintering (DMLS) by EOS, who filed a patent for this process in 1995 [109]. This process was validated using Cobalt-Chrome, and Titanium due to the difficulty in processing these materials using traditional processing techniques. However, less than a year later Fraunhofer Institute for Laser Technology, presented work in which a full part was produced from AISI 316L via laser processing, without the need for a polymer binder [110]. Thus began a two and a half decade journey into the microstructural, and mechanical property optimization of AISI 316L via direct laser fabrication.

In 1998, Keicher showed the comparative mechanical properties of AISI 316L manufactured via Laser Engineered Netshaping (LENS), their results are summarised in [Table 2.3](#) [111]. This showed from very early in the process development that the properties of AISI 316L could match, or even exceed that of wrought material. However, Keicher makes no mention of quantifying the density/porosity of the produced samples, thus it is unknown what dependent variables the processing parameters were optimised for, if any.

Table 2.3: Summary of Mechanical Properties of AISI 316 SS, manufactured by LENS. Taken from [111]

Plane Orientation wrt Tensile Direction	Ultimate Tensile Stress (MPa)	Yield Stress (MPa)	Elongation (% in 2.54 cm)
316 SS Perpendicular	793	448	66
316 SS Perpendicular	793	448	51
316 SS Parallel	807	593	33
316 SS Anneal bar	586	241	50

In 2004, Kuth *et al.* published a paper regarding the Selective Laser Melting (SLM) of iron-based powders and the effect of varying laser powers and scan speeds on the resultant part quality [112]. This is regarded as being the pioneering work on the processing of steels, such as AISI 316L, in what would become LPBF. These results were corroborated over the next half decade by numerous authors [113, 114], however, the expanse of academic work on this area did not exceed 200 W laser power. Whilst parts of >99 % density

could be produced, due to the limited power of the machines available in the academic sector, build rates were incredibly slow and throughput could not match traditional manufacturing technologies in most industrial sectors. It is also worth noting that due to the powder atomisation methods in use, the stock powder in use during the LPBF of metals, contains innate porosity, discussed earlier (2.1.3.2), and the use of ambient/slightly positive pressures in the LPBF process, it is difficult to produce parts of 100 % density without adopting post-treatment processes.

Following the work of Kuth in proving the processability of AISI 316L stainless steel powder without need for a binder material, academic focus shifted to the microstructural characterisation of part produced in this way, the relationship to the initial processing parameters, and the resultant mechanical properties. It was during this paradigm shift, that academia discovered and accepted the “characteristic”, columnar microstructure that is produced by the layer-wise heat application to LPBF parts [69]. The presence of these columnar grains, aligned with the build direction were confirmed in AISI 316L [115], there were also two findings of the work of Saeidi *et al.* that were also worthy of note:

1. That there was a proportion of retained delta ferrite found in grain boundaries of the as-built parts ([Figure 2.15](#)).
2. That within grain boundaries is an intragranular network of dislocations that result in a markedly higher microhardness value than wrought, or annealed AISI 316L ([Figure 2.16](#)).

The presence of the delta ferrite phase in the as-built AISI 316L parts was confirmed by Sun *et al.*, and is believed to be due to the phase transition of 316L from delta ferrite to gamma austenite upon cooling. The fast cooling rates characteristic of LPBF prevent the complete transformation of the delta phase to gamma phase and a minute fraction (less than 0.4 % by area) is retained [116].

Saeidi *et al.*, later the same year, further elucidated the characteristics of the intra-granular cellular network observed in [Figure 2.16.c](#). Through XRD analysis, it was shown that the intra-granular cell boundaries observed in the previous work, had a higher concentration of Chromium and Molybdenum than the centers of the cells [117]. The results of this analysis

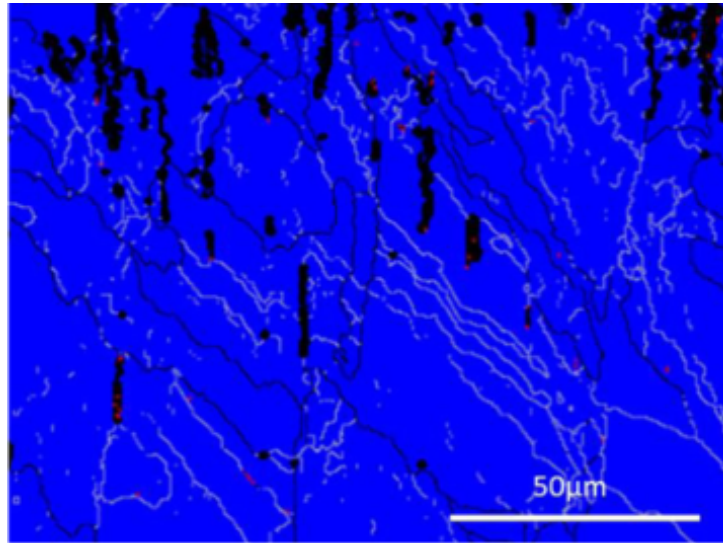


Figure 2.15: Phase distribution EBSD of 316L sample produced by LPBF showing austenitic structure (blue), with minute fraction of retained ferritic structure (red). Taken from [115]

can be seen in [Figure 2.17](#). However, due to the limitations of XRD analysis, the full range of alloying elements in the 316L system could not be quantified, and there may also be varying concentration of the lighter/trace elements of the alloy system in these regions also. In the same work, Saeidi *et al.* also show that the crystallographic orientation of these intra-granular cells did not differ significantly enough from each other to constitute separate grains, hence the lack of resolution of the cellular structure in the EBSD analysis performed in the prior work. This was corroborated by Liu *et al.* who also confirmed the presence of a higher concentration of Manganese at the cell boundaries [49]. Thus, it was believed that due to the incredibly high cooling rates of consolidated parts during LPBF, grains solidify according to the “cellular” regime [65], this causes microsegregation of Chromium, Manganese, and Molybdenum at cell boundaries with minimal angular offset between adjacent cells. This results in a network of dislocation tangling within the as-built part that raises yield stress with minimal effect on ductility [49]. The sTEM work performed by Liu *et al.* showed that the dislocation network of the intra-granular structure in the as-built parts, possessed a high concentration of twin boundaries that had previously not been observed in 316L that had not been deformed via cold-rolling or hot-torsion worked [118,119], thus the existence of such twin boundaries in 316L produced by LPBF without deformation is unique to this manufacturing process [49,117].

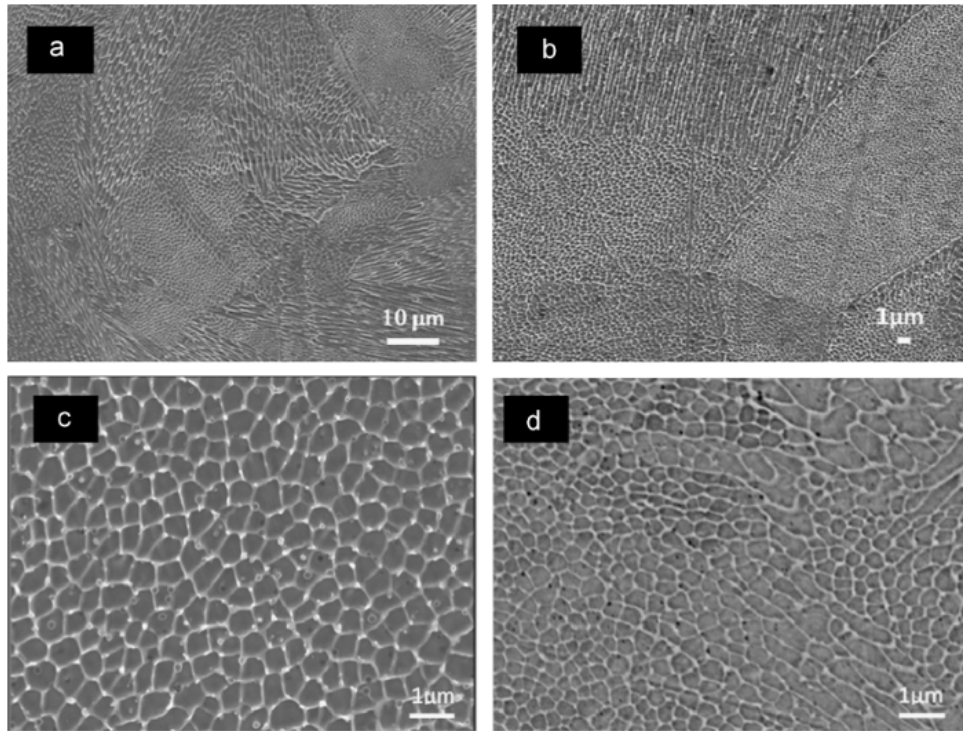


Figure 2.16: SEM images of 316L produced by LPBF showing the intragranular dislocation network. Taken from [115]

It wasn't until 2020, when Bertsch *et al.* elucidated the formation mechanisms of the high dislocation concentrations observed by the previous works of Saeidi *et al.* and Liu *et al.*. Bertsch *et al.* found that the primary formation of the dislocation network was in fact due to the thermal expansion and shrinkage that occurs by the successive application of laser heat input across the surface of the part; the microsegregation observed by Saeidi *et al.* and Liu *et al.* effects the scale, orientation, and structure of the dislocation network, but is not itself a method of dislocation formation; finally, it was found that by altering the thermal history of select areas of the build area through manipulation of the processing parameters and geometry, the dislocation network could be manipulated and gradiented microstructures could be achieved [120].

Thus, from these results, it is evident that the ability to predict, design, and optimise the microstructures within a part manufactured in AISI 316L via LPBF would be of immense value to academia and industry, and that this is possible with thermal field simulation of sufficient accuracy.

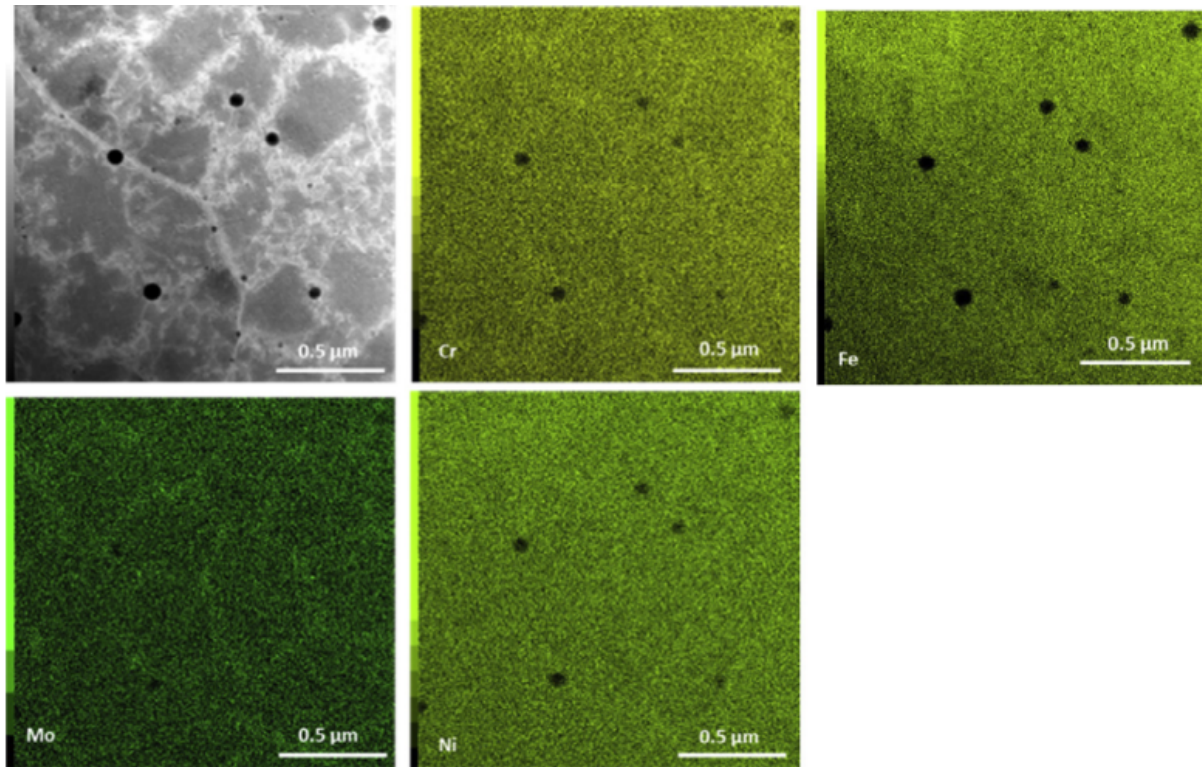


Figure 2.17: XRD Elemental Maps of 316L Produced by LPBF. Taken from [117]

2.2 Numerical Methods

The various thermophysical phenomena discussed in the previous sections (2.1.2) occur over a range of spacial and temporal scales. It is for this reason that a single method of numerical simulation will not suffice for all phenomena. Numerical methods utilized for LPBF are normally categorised into three classes based on length scale [11]:

- Microscopic,
- Mesoscopic,
- Macroscopic.

Whilst there are no firm rules on the exact length scale that defines each of these, it is accepted that: microscopic scale refers to simulation where resolution less than a tenth of the radius of a single powder particle is required; mesoscopic scale refers to simulations where resolution of individual powder particles are required; and macroscopic scale refers to simulations concerned with scales greater than that [11].

2.2.1 Microscopic Scale Methods

Microscopic methods are best utilised for microstructural prediction, due to the scale of dendrite formation and concentration fronts. There are two methods of simulation at this scale:

- Cellular Automata
- Phase Field Method

This section will briefly introduce these methods and how they have been applied to the problem of simulating LPBF.

2.2.1.1 Cellular Automata (a.k.a. Lattice-Boltzmann Model)

In 1963, Neumann and Ulam put forward the model of “cellular spaces” as a way of predicting cellular reproduction in biology [121,122]. In 1991, Hesselbarth and Göbel introduced an alternative to the JMAK method of simulation, utilizing a version of this biological model of recrystallization that marked a significant step forward in modelling theory [123]. A step that is still in use to this day. This innovation was the Cellular Automation (CA) or Cellular Automata Method. This method is easily applied in both two and three dimensions. For brevity, it shall be explained in two and the extrapolation into three should be trivial. The simulated area is spatially discretized into “cells” of shape that are able to be tessellated (commonly squares or hexagons). Nucleation sites are distributed according to the thermophysical system of the volume, e.g. randomly distributed according to the thermal field, or the fluid flow of the volume. The cells immediately surrounding the nucleation sites are defined as the “neighbourhood”, there are multiple accepted neighbourhood shapes that are used. The shape of the neighbourhood is considered a variable that is to be selected based on the known solidification behaviour of the material in question, and shall be discussed in further detail later. At each timestep, the state of each cell is defined by the states of all the cells in its neighbourhood in the previous time step. In this way, cellular automata can show the solidification of the molten metal, and the microstructural evolution of the matrix during LPBF.

2.2.1.1.1 Neighbourhood Selection There are two major considerations to be made when configuring a CA simulation, the first being the neighbourhood geometry. Selection of the neighbourhood has a profound impact on the grain shape and growth rate [123]. Possible neighbourhoods are shown in Fig. 2.18.

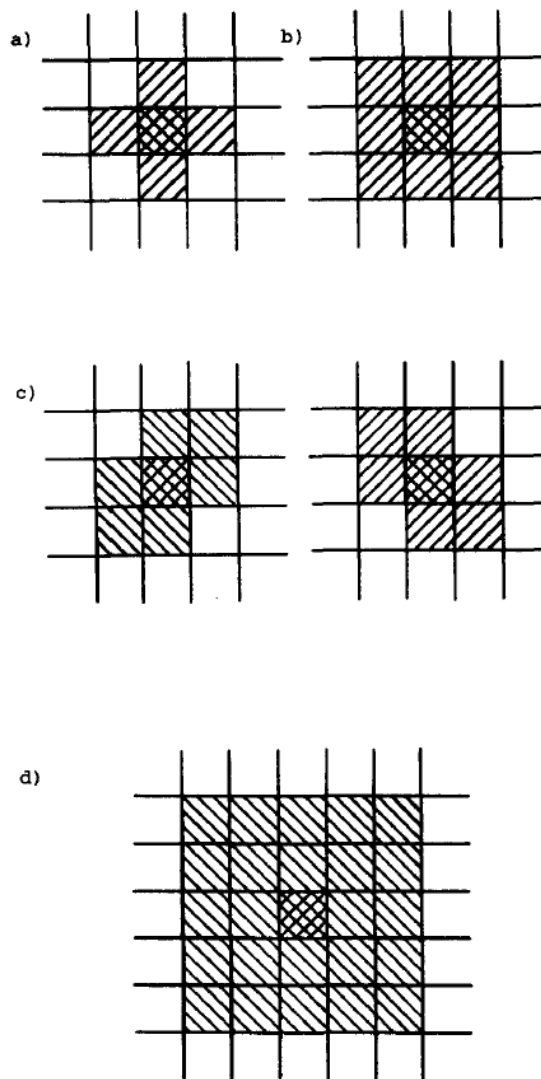


Figure 2.18: Definition of Possible 2D Cellular Neighbourhoods: (a) von Neumann, (b) Moore, (c) 7-cells-neighbourhood and (d) 25-cells-neighbourhood. (The centre cell is regarded as part of the neighbourhood, because the new state depends on its old state.) Taken from [123].

There is no standard protocol for selection of the correct neighbourhood for CA modelling. However, in the majority of cases the simplicity of the von Neumann or Moore neighbourhoods are sufficient. The von Neumann neighbourhood also converges with the spatial discretization of the solutions of the diffusion equation for isotherms (), which is com-

monly the predominant driving force for recrystallization behaviour in metallic systems. Hence, an excellent starting point.

2.2.1.1.2 Cell Transition Rules Beyond the selection of cell geometry and cell neighbourhood organisation, the other major proportion of CA modelling is defining the behaviour of the cells themselves. This is categorised in two parts:

- the number and kind of states each cell can take, and
- the rules that define the transition of a cell from one time step to the next

2.2.1.2 Phase Field (PF) Methods

Phase field methods explicitly describe the state of a material through an “order parameter” (ϕ). The basis of these methods are very well described in the review published by Qin and Bhadeshia in 2010 [124]:

Consider a precipitate forming within a matrix of an alloy system, the states of matter can be categorised into three parts: the precipitate, the matrix, and the interface that separates the two. The order parameter (ϕ) is used to define the state at each point of the system through time. In this example, $\phi = 1$ represents the precipitate, $\phi = 0$ represents the matrix, and $0 < \phi < 1$ represents the interface. The interface is therefore located by the range values at which the order parameter lies within this range within the volume, the spatial range of this range defines the width of the interface. The “phase field”, from which the method derives its name, is the set of values of the order parameter across the entire volume. Thus, the total free energy of the volume, G , can be described purely in terms of ϕ . The driving force for the evolution of the structure of the volume are the thermodynamic forces, thus the phase field methods rely on high fidelity thermal data in order to produce high fidelity results.

2.2.1.2.1 The Order Parameter In the example above, ϕ has a clear macroscopic physical meaning, which is not always the case. In two phase systems it is easy to imagine that ϕ represents the precipitate/matrix/interface or the liquid/solid/interface. However,

in general N phased systems, where ϕ_i represents the order parameter for each phase. Where $\phi_N = 1$ represents where the N^{th} phase exists and $\phi_N = 0$ represents where it does not, rather than a specific state of matter. In this generalised example, if ϕ_0 is the matrix then at any given location:

$$\sum_{i=0}^N \phi_i = 1 \quad (2.60)$$

The order parameter can also be represented in vector form, Hoffman and Cahn express the order parameter as the variation of interfacial energy as a function of interface orientation [125]. Such approaches can allow for the prediction of crystal shape formation over time [126, 127]. An example of this is shown in [Fig. 2.19](#).

2.2.1.2.2 Thermodynamics The order parameter must be coupled to a thermodynamic functional, and it is this functional that is the driving force for any phase change in the system. Traditionally, if the volume is non-isothermal, then an entropy functional should be used, Gibbs Free Energy or Helmholtz Free Energy should be used for isothermal volumes [124]. However, Penrose and Fife showed that due to the energy flow associated with temperature variation, energy density and order parameter can be consistently defined for non-isothermal volumes [128]. Combining this with the work of Wheeler *et al.* (that showed that in the non-isothermal case the gradient energy coefficient can be approximated as a non-constant [129]), allows free energy approach to be used for the non-isothermal problem. This is the most definitely the case for LPBF.

2.2.1.2.3 Computational Method The governing equations for Phase Field Methods are commonly taken to be the time-dependent Ginzburg-Landau Equations [130]. In the use case of LPBF where liquid phases and solid grains are both explicitly tracked, two order parameters must be considered. One to track the liquid phase (ζ), and one to

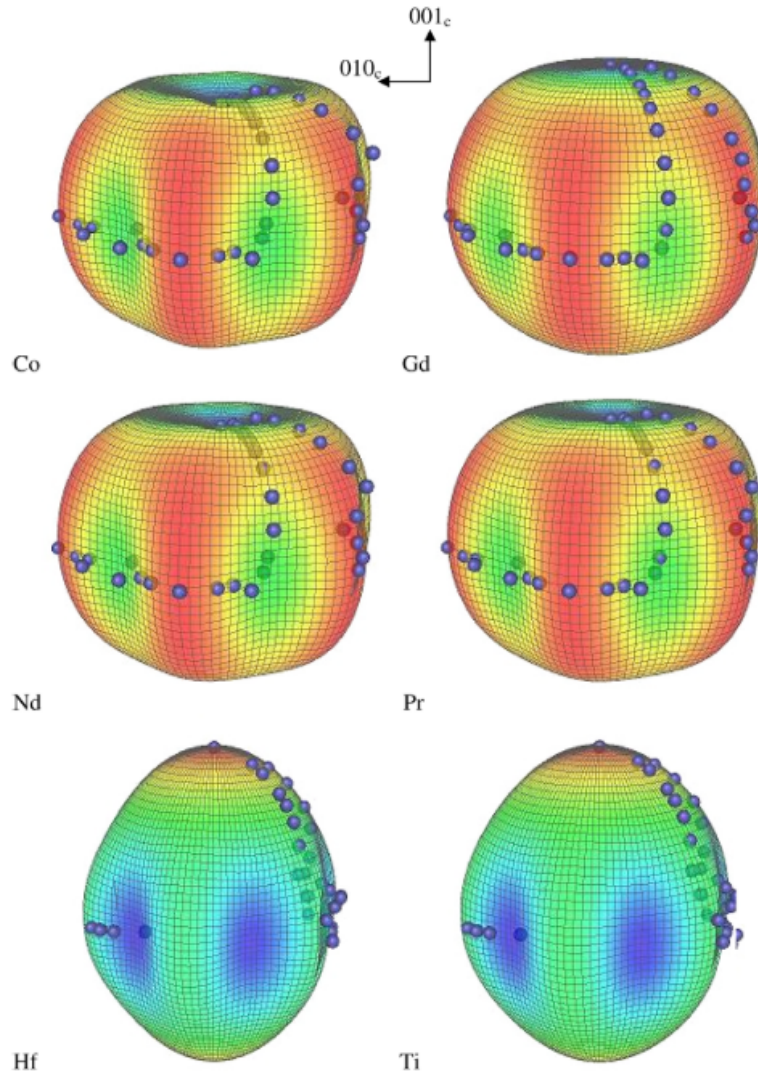


Figure 2.19: Surface Rendering of Calculated Liquid/Nucleus Interface Energies for a Range of Elements. Colormapping Corresponds to Relative Values of Interface Energies, with Blue being the Lowest and Red being the Highest. Taken from [127].

track solid grains of varying orientations (ϕ_i):

$$\frac{\partial \phi_i(\mathbf{r}, t)}{\partial t} = -L_g \left[\frac{\delta F(\zeta, \phi_i, T)}{\delta \phi_i(\mathbf{r}, t)} \right] \quad (2.61)$$

$$\frac{\partial \zeta(\mathbf{r}, t)}{\partial t} = -L_p \left[\frac{\delta F(\zeta, \phi_i, T)}{\delta \zeta(\mathbf{r}, t)} \right] \quad (2.62)$$

These equations relate the gradients of the N present field variables (where $i = 0, \dots, N$) of orientation, $\mathbf{r}$, and time, t , to the gradient between the total free energy, F , of the field variable at temperature, T . L is a kinetic coefficient of the phase interface mobility. The total free energy at temperature T is given:

$$F = \int_V (f_{\text{local}} + f_{\text{grad}}) dV \quad (2.63)$$

$$f_{\text{local}} = f_{\text{phase}} + f_{\text{grain}} \quad (2.64)$$

$$f_{\text{phase}} = m_p \{ (1 - \zeta)^2 \varphi(\tau) + \zeta^2 [1 - \varphi(\tau)] \} \quad (2.65)$$

$$\varphi(\tau) = \frac{1}{2} \{ 1 - \tanh [\theta(\tau - 1)] \} \quad (2.66)$$

$$f_{\text{grain}} = m_g \left[\sum_{i=1}^n \left(\frac{(\phi_i)^4}{4} - \frac{(\phi_i)^2}{2} \right) + \gamma \sum_{j=1}^n \sum_{i=1}^n (\phi_i)^2 (\phi_j)^2 + \frac{1}{4} + (1 - \zeta)^2 \sum_{i=1}^n (\phi_i)^2 \right] \quad (2.67)$$

$$f_{\text{grad}} = \frac{\kappa_p}{2} (\nabla \zeta)^2 + \frac{\kappa_g}{2} (\nabla \phi_i)^2 \quad (2.68)$$

Here, τ is the ratio of temperature (T) to liquidus temperature (T_l); θ is a constant that ensures φ is 0 when τ is greater than 1. κ_p and κ_g are L/S and grain interface gradient coefficients respectively; while m_p and m_g are functional coefficients of the mass of the liquid and solid phases respectively.

In the case of non-isothermal volumes, such as LPBF, these governing equations must also be coupled to a thermodynamic model in order to feed the phase field model with the required information, such as temperature or fluid flow. Both thermal field and phase field models can be handled with finite difference or finite element methods.

If handled explicitly, the maximum time-step that can be taken by the phase field model is:

$$\Delta t < \frac{1}{2} \frac{(\Delta x)^2}{D} \quad (2.69)$$

Here, Δx is the smallest spatial resolution of the phase field model, and D is the total dimension on the volume of the phase field simulation [127]. This equation shows that in order to resolve the spatial detail required for microstructural visualisation Δx needs to be in the range of $1 - 10 \mu m$. In the example of a commercially available system such as the Renishaw RenAM 500Q[®], which has a build volume of 250 x 250 x 350 mm, D would therefore be 350 mm. Therefore, if attempting to simulate a full build, Δt would be of the range of approximately 1.4 picoseconds; when compared to the approximate build time

for a full height build upwards of 72 hours, this leads to the number of full loops of the phase field algorithm to be 1.8144×10^{17} . Even if a single loop were to take only a single millisecond, this means that this total number of loops would take approximately 5.75 billion years. Obviously this is not realistic.

In order to reduce the number of calculations the spatial resolution could be increased, however doing this reduces the information that can be gleaned from the phase field model. Also, due to the coupling of the phase field model to the thermal field model, even if the computation speed of the phase field model were to be highly optimised, it would still be limited by the speed of the thermal field model it was coupled to. So would therefore benefit from techniques to increase the speed of computation of a thermal field model.

2.2.1.2.4 Phase Field Modelling of Laser Powder Bed Fusion PFM have been used to tackle numerous problems within the LPBF process, from microstructural evolution, to in-situ alloying [131–134].

Recently, in 2012, Li *et al.* of McMaster University in Canada used PFM coupled with a conduction only thermal FEM simulation to investigate the in-situ alloying process of β -Titanium alloy Ti-185. the flowchart of the methodology can be seen in [Fig. 2.20](#). In-situ alloying is the process of producing parts from blended elemental powders, the aim being that the process will alloy the constituent elements into the desired composition on processing [135]. Li *et al.* were able to show using PFM that by simulations of identical geometries produced via pre-alloyed powder versus in-situ alloying do not achieve similar microstructures due to elemental powders causing higher concentrations of dendrite inhibiting elements such as Iron, Aluminium, and Vanadium. However, it must be noted that by utilising a “conduction only” thermal model for this PFM seems counter-intuitive to the aim of the experiment. If the final goal of the work was to track concentrations of the alloying elements a process, which at its core, is a mass flow problem, then the omission of fluid-flow (bulk mass flow) from the thermal model is naive. Especially, considering in [Sec. 2.1.2.5](#), it was discussed that even a part per million change in concentrations of impurity elements such as Sulphur or Phosphorous can lead to complete reversal of

Marangoni effects in the melt pool. An effect which would have profound impact on the mixing of the molten elements and thus the final concentrations of each element.

Another application for the order parameter in PFM is to represent alternate states of

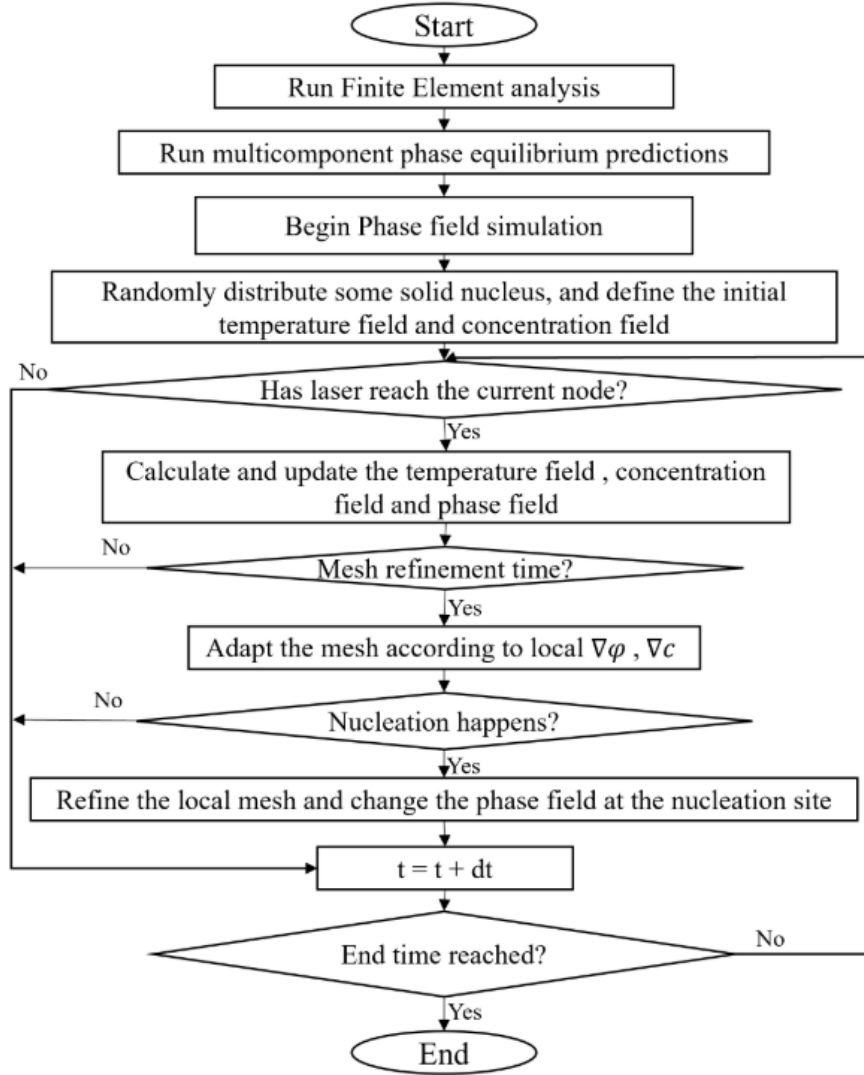


Figure 2.20: Flowchart showing the numerical implementation of the PF, FEA, and Nucleation Modules to simulate the LPBF process. Taken from [131].

matter, instead of solid/liquid, instead Phase Field Damage models (PFDMs) use the order parameter to represent fully intact material and fully damaged material. Thus, PFM can be used to predict fracture mechanics [136]. Li *et al.* of the University of Sydney applied PFDMs to the LPBF problem due to the highly columnar and anisotropic microstructure of as-built parts produced [134]. PFDM was applied in order to predict both the stress/displacement curves and crack propagation for a number of various failure sce-

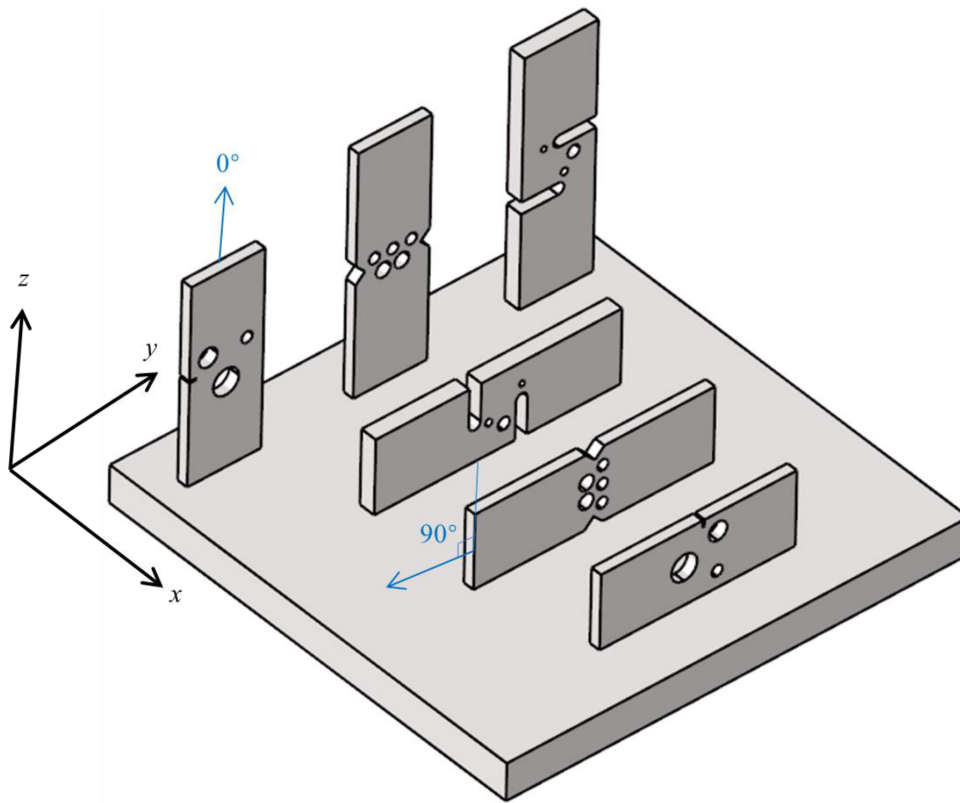


Figure 2.21: Schematic of crack propagation specimens. Designed to achieve complex crack paths. Taken from [134]

narios, as shown in [Fig. 2.21](#). Li *et al.* were able to achieve reasonable agreement between numerical and experimental results in both stress/displacement and crack path prediction ([Fig. 2.22](#)), even resolving the correct order of failure of each section of geometry. It should be noted, that Li does discuss that further work is required in the investigation into the uncertainty of this approach. It is possible that some of the discrepancy between the numerical and experimental results is due to the effect of any post-processing undergone by the physical test specimens, as Li *et al.* expand very little on this. The as-built surface will have stress amplifiers such as surface porosity, that are not taken into account by the numerical model. There will also be stochastic factors in the production method that are not accounted for also, such as powder spreading inconsistencies, and the effect on energy input of the laser by spatter produced during the processing of adjacent parts disrupting the powder bed. These effects should be quantified, and/or handled through the introduction of the appropriate noise into the PFDM in order to bring the physical results more into line with the numerical results.

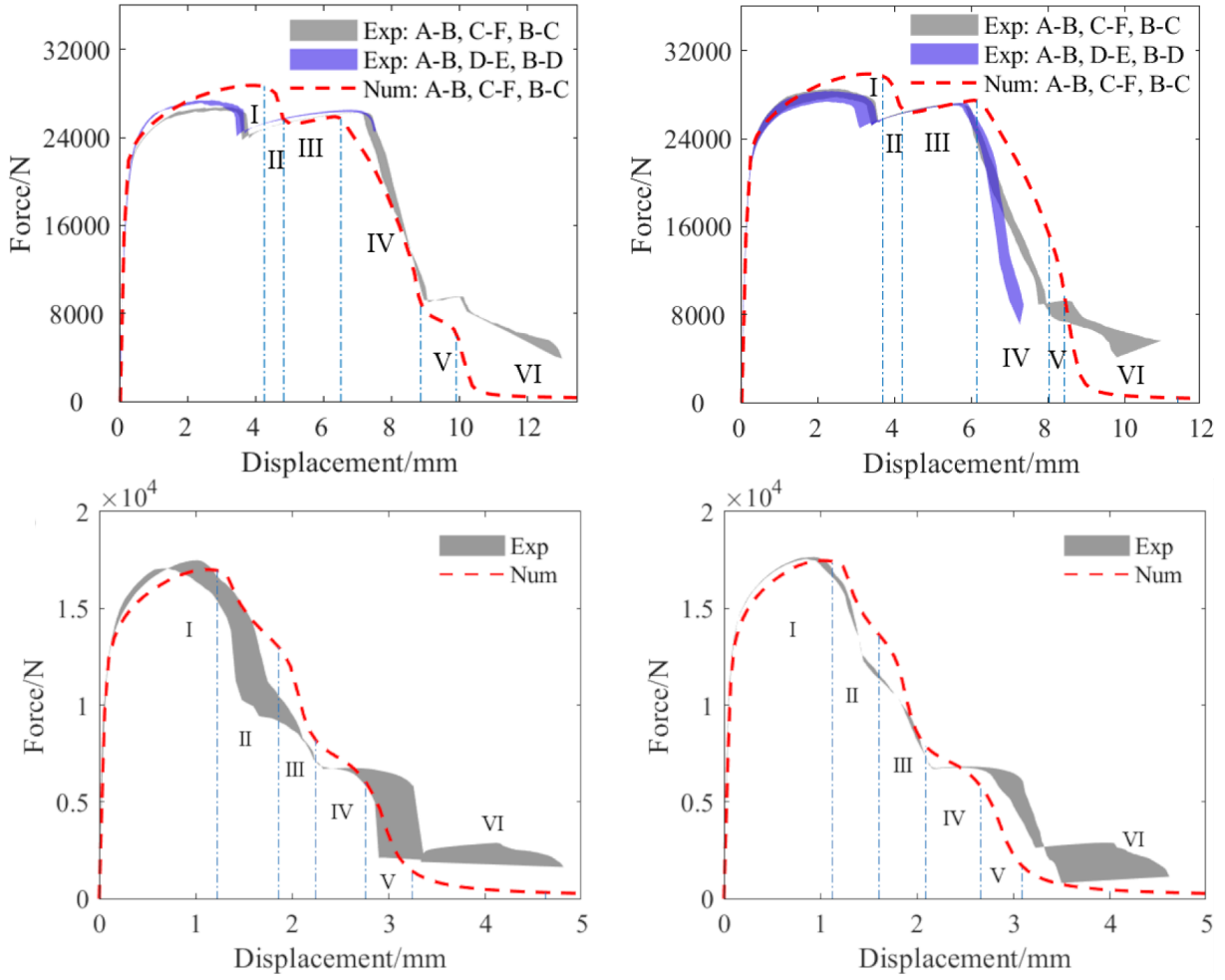


Figure 2.22: Comparison of numerical and experimental results for various specimens built at various orientations relative to the build direction. Taken from [134]

Quantifying and predicting the surface finish of the as-built LPBF part can also be addressed with PFM. Li *et al.* of the University of Connecticut, apply PFM to the problem of wetting and balling of molten metal to unmelted powder of the powder bed in order to predict the affect of processing parameters on the final part surface finish [133]. In this application, the order parameter is used to represent the state of the argon atmosphere, the metal powder, and the substrate, as can be seen in Fig. 2.23. Li *et al.* conclude that this approach to PFM results in a numerical simulation that agrees with thermophysical phenomena, i.e. that at low to medium energy density, balling is dominant and Marangoni effects are secondary; as energy density is increased, wetting and Marangoni effects becomes more dominant and balling is no longer observed. It should, however, be noted that whilst the application of the PFM is valid and the observation agrees with what would be expected from the thermophysical phenomena, due to the simplification of the

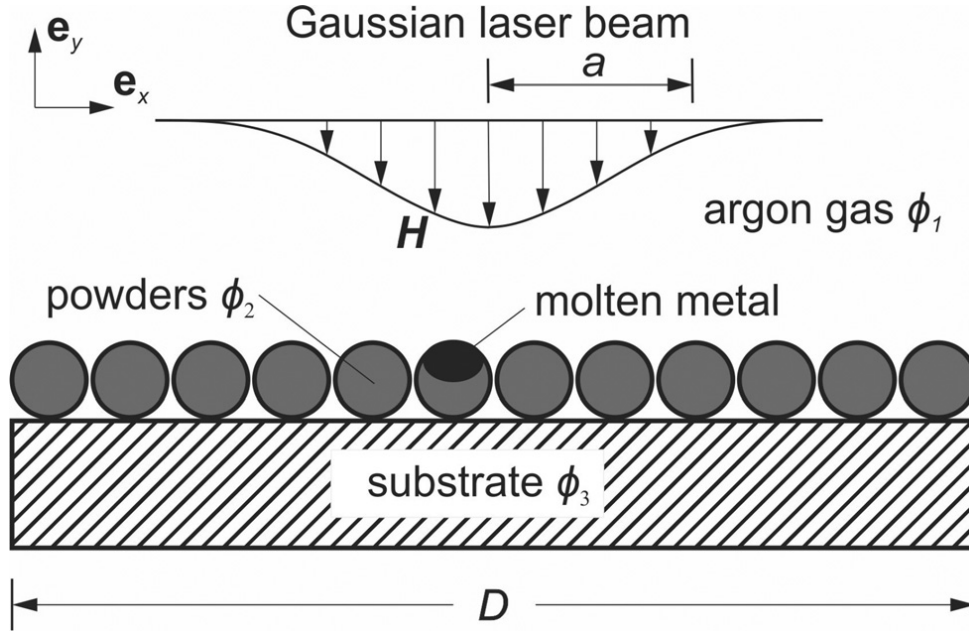


Figure 2.23: Schematic of selective laser melting of a horizontal layer of equal-sized metal powders placed on top of the substrate and surrounded by argon gas. Phase field variables ϕ_1 , ϕ_2 , and ϕ_3 indicate the volume fractions of argon gas, metal powders, and the substrate, respectively. D represents the width of the computational domain, and the Gaussian beam is featured by its irradiation intensity H and a characteristic spot radius a . Taken from [133]

problem the powder bed no longer represents an industrially relevant system. Therefore, the model requires further development before any conclusion from the approach can be applied to a real-world problem. In order to overcome this limitation of this model, a suitable method of powder bed generation needs to be adopted. These algorithms are commonplace in the Mesoscopic Scale Methods, and shall be elucidated next.

2.2.2 Mesoscopic Scale Methods

Mesoscopic methods are employed when phenomena that are of the scale of individual powder particles are being quantified, such as the capillary action of the liquid melt into the powderbed, or the wetting of the meltpool on the surrounding powder. In order to quantify these phenomena, the powder bed cannot be approached stochastically, the powder particles themselves, must be defined and handled explicitly. Therefore, they are reliant on the how a representative volume of the powderbed is generated.

2.2.2.1 Powder Bed Generation

These methods describe the way in which the generation of a representative volume of powder is performed. In general, these methods can be categorised in two ways:

- the "Rainfall" Method,
- and the Discreet Element Method (DEM).

2.2.2.1.1 "Rainfall" Method Meaken and Jullien formalised the use of spherical fractal generators to propose the restructured rainfall method in 1988 [137]. In this algorithm, a basal line is established, then spherical particles of the selected size distribution are sequentially "dropped" onto the basal surface. Under the effect of gravity each powder particle is allowed to come to rest at a local minimum potential energy. If the basal surface is reached the particle moves no further, should a particle come into contact with another particle, it is allowed to freely rotate until a local minimum or the basal surface is found. Once all particles are placed, the algorithm then subtracts particles from the layer in order to achieve the desired packing density. This process is illustrated in [Fig. 2.24](#).

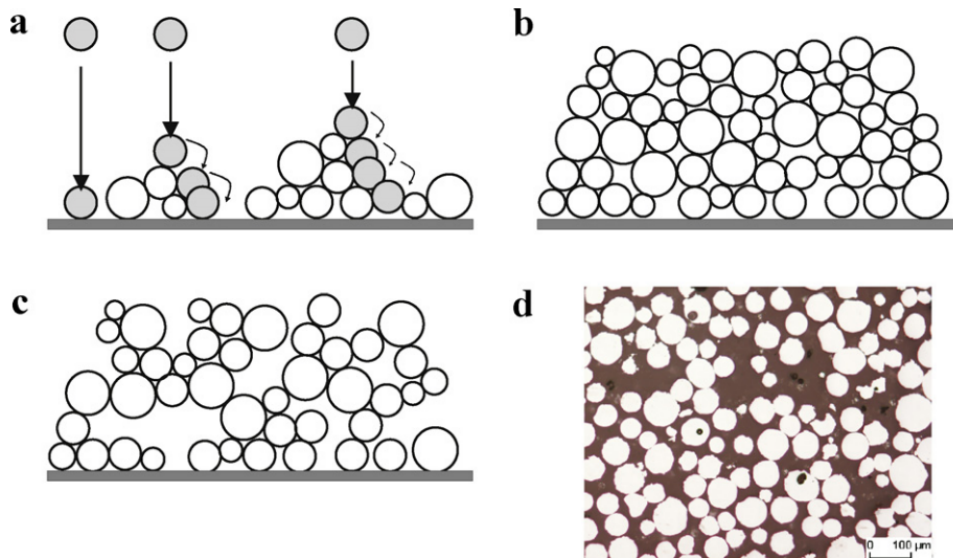


Figure 2.24: Illustration of the Rainfall Method of Powderbed Generation. (a) Schematic of the Rain Model for Random Packing with Rotations. (b) Powderbed Produced by the Rain Model. (c) Adjusting the Relative Density by Removing Some of the Particles. (d) Cross Section of a Real Powderbed (Titanium Alloy.) Taken from [138].

2.2.2.1.2 Discrete Element Method Discrete Element Methods or DEMs are powerful methods of handling volumes of powder particles, whilst handling each particle explicitly. These methods have been utilised across many industries in which the behaviour of powder is of interest, from Powder Metallurgy, to Animation, Pharmaceuticals, and even soil engineering [139–142]. In this method, each powder particle is explicitly resolved with each force acting on it. The forces common to the DEM are:

- contact force,
- rolling resistance,
- friction,
- and gravity.

The former three, act between powder particles, and between powder particles and the processing environment. Each powder particle is subject to Newton’s second law [140]:

$$\mathbf{F}_i = m\ddot{\mathbf{x}}_i \quad (2.70)$$

$$\mathbf{M}_i = I\ddot{\boldsymbol{\omega}}_i \quad (2.71)$$

where $\mathbf{F}_i$ and $\mathbf{M}_i$ are the force and momentum of any particle selected at random, m is the mass, and I is the moment of inertia of said particle. If sufficiently small a timestep is taken (Δt), $\ddot{\mathbf{x}}_i$ and $\ddot{\boldsymbol{\omega}}_i$ can be assumed to be constant before and after the time, t [142].

The linear and angular velocities can be represented:

$$\dot{\mathbf{x}}_i^{t+\Delta t/2} = \dot{\mathbf{x}}_i^{t-\Delta t/2} + \left(\frac{\mathbf{F}_i}{m} \right) \Delta t \quad (2.72)$$

$$\dot{\boldsymbol{\omega}}_i^{t+\Delta t/2} = \dot{\boldsymbol{\omega}}_i^{t-\Delta t/2} + \left(\frac{\mathbf{M}_i}{m} \right) \Delta t. \quad (2.73)$$

Therefore, the position of particles can similarly expressed:

$$\mathbf{x}_i^{t+\Delta t/2} = \mathbf{x}_i^t + \dot{\mathbf{x}}_i^{t+\Delta t/2} \Delta t \quad (2.74)$$

$$\boldsymbol{\omega}_i^{t+\Delta t/2} = \boldsymbol{\omega}_i^t + \dot{\boldsymbol{\omega}}_i^{t+\Delta t/2} \Delta t. \quad (2.75)$$

A criterion must be put in place to discern whether two particles come into contact. This is done by calculating the distance between each particle, and if any of these are less than the sum of their respective radii, then a collision is assumed to have occurred (Eqn. 2.76), a collision is also assumed to have occurred if the position of a particle is within a radius of the volume boundary.

$$\|\mathbf{O}_1 + \mathbf{O}_2\| < r_1 + r_2 \quad (2.76)$$

Once a collision is detected, the contact force must be calculated so that the velocities and momentum can be updated:

$$\mathbf{F}^c = \mathbf{F}^{cn} + \sum d\mathbf{F}^{cs} \quad (2.77)$$

$$\mathbf{F}^{cn} = k_n u_n \mathbf{n} \quad (2.78)$$

$$d\mathbf{F}^{cs} = -k_s \dot{\mathbf{u}}_s dt. \quad (2.79)$$

Here, the contact force $\mathbf{F}^c$ can be resolved into the normal force $\mathbf{F}^{cn}$ and the shear force $\mathbf{F}^{cs}$; k_n and k_s are the elastic normal and shear stiffness respectively; u_n is the overlap distance derived in Eqn. 2.76; $\mathbf{n}$ is the normal unit vector; and $\dot{\mathbf{u}}_s$ is the shear velocity. Due to the variation in particle size, elasticity k is calculated from the macro-scale Young's modulus E_m , and Poisson's ratio ν :

$$k_n = 2E_m \frac{r_1 r_2}{r_1 + r_2} \quad (2.80)$$

$$k_s = \nu k_n. \quad (2.81)$$

In order to quantify the rotation of the particles, thought must be given to the rolling $\mathbf{M}^r$ and twisting $\mathbf{M}^t$ moments of each particle. As these are the resolved components of the rolling resistance $\mathbf{M}^{res}$:

$$\mathbf{M}^{res} = \mathbf{M}^r + \mathbf{M}^t \quad (2.82)$$

$$\mathbf{M}^r = k_r \boldsymbol{\pi}^r \quad (2.83)$$

$$\mathbf{M}^t = k_t \boldsymbol{\pi}^t. \quad (2.84)$$

Here, k_r , k_t , $\boldsymbol{\pi}_r$, and $\boldsymbol{\pi}_t$ are the rotational and torsional stiffness, and the rotational and torsional vectors. All these equations currently describe a perfectly elastic system, with no energy dissipation. Therefore, regardless of the length of simulation, the system will stay in motion. Therefore, terms must be added to allow the energy dissipation through friction and damping. One such source of energy dissipation is the contact shear force, as this is reduced by inter-particle friction. Hence, a coefficient of friction ϕ must be introduced.

$$\mathbf{F}^{cs} > \mathbf{F}_{max}^{cs} = \mathbf{F}^{cn} \tan \phi. \quad (2.85)$$

Each particle is also subject to gravitational force:

$$\mathbf{F}^g = -mg. \quad (2.86)$$

However, these may not be sufficient to produce numerical stability for convergence to quasi-steady state, thus another source of non-viscous damping is also added [143, 144]:

$$\mathbf{F}_i^d = -\Omega \text{sgn}(\dot{x}_i^t) |\mathbf{F}_i|, \quad (2.87)$$

where Ω is the damping coefficient, and sgn is the sign function. The damping coefficient is selected by the operator in order to converge the solution within a reasonable time, however this does create a somewhat artificial result. Thus, the final equations that need to be solved for each particle are:

$$\mathbf{F}^{cm} + \sum d\mathbf{F}^{cs} + \mathbf{F}^g + \mathbf{F}_i^d = m\ddot{x}_i \quad (2.88)$$

$$\mathbf{M}^{res} + \sum (\mathbf{r}_i \times \mathbf{F}^{cs}) = I\ddot{\omega}_i. \quad (2.89)$$

As previously stated, these equations are required to be solved for each particle at each timestep. As the number of particles increases the scale of computational load grows at a rate greater than $O(n)$. This is incredibly limiting on the scale of final volume that can be simulated. A benefit of DEM simulation is that as forces are resolved explicitly, a greater accuracy can be achieved by adding terms to simulate the effect of the recoating method

on the powder bed, making simulations more representative of the conditions within the build chamber.

It is also of note that this simulation is not in itself the ends with respect to the AM process. DEM is required to generate the powderbed, on which further simulation is required. Thus, increased computational load and time at this stage is detrimental to industrial relevant timescales.

2.2.3 Macroscopic Scale Methods

In order to resolve individual powder particles the numerical methods utilised for these simulations require meshes of resolution approximately 10% the mean particle size. Typically the particle size distribution (PSD) of powders utilised in LPBF is 15 to 45 μm for non-reactive materials and 15 to 63 μm for reactive materials [145]. This would mean the resolution of the mesh would need to be between 2 to 4 μm . A full build volume of $250 \times 250 \times 350 \text{ mm}^3$ this would represent 2.734375×10^{15} and $3.41796875 \times 10^{14}$ elements. This would make the computational load for the build gargantuan, and not viable for industrial use. A way to overcome this limitation is to treat the powderbed as a continuum with stochastic representation of key properties. However, this approach, in its pursuit of simplifying representation of the problem, disregards surface representation. This is handled instead by adjustment of the values that govern the laser/powder interaction.

2.2.3.1 Continuum Modelling

With continuum modelling, multiple powder particles are now represented within a single element. Due to this, the model requires the introduction of a new material phase for the properties of the powder. These properties differ from the properties of the bulk [20].

As was discussed in Sec. 2.1.2.2, the effective thermal conductivity of the powderbed can be related to the gas contained between the metallic powder particles due to the lack of inter-particle contact area [146]. However, Gusarov *et al.* also proposed a model with the thermal conductivity of the powderbed being derived from the conduction from

inter-particle contact area [147]. This work showed that when the powderbed approaches the sintering temperature the increased contact area between the powder particles becomes non-negligible as previously assumed. This is also shown to be the case for powderbeds in which the powder recoating method applies a compressive force to the powder.

2.2.3.1.1 Melt Pool Geometry Many of the applications of continuum modelling are focused on approximating the geometry of the meltpool immediately beneath the incident laser. Much of continuum modelling requires the solution of the heat equation 4.1. This also requires taking into account any thermal sinks in the system, such as the radiative losses from the powder bed surface (2.1.2.3); and convective losses to the gaseous atmosphere (2.1.2.4). As was discussed in [Sec. 2.1.3.3](#), when the laser melts the powder and subsequent layers, some of the alloying elements are vaporised. This does incur an enthalpy loss but many continuum models do not quantify this loss but still result in reasonable agreement with Monte Carlo simulations [11]. However, Loh *et al.* show that the ability to ignore the losses due to evaporation is alloy specific. In their work the Aluminium alloy AA6061 was shown to lose almost 50% of the processed material due to evaporation, illustrated in [Fig. 2.25](#). Therefore, the omission of these losses may not always be an appropriate decision. As the meltpool geometry can be inferred from the isotherms of the heat equation solution at each timestep, such simulations can be heavily simplified, and provide the best basis on which fast thermal solutions can be validated. Another possible simplification that can be applied to continuum modelling is the omission of hydrodynamic forces. This omission removes the need for tracking flow of mass as well as the flow of heat. This has some accuracy implications as was discussed in [Sec. 2.1.2.5](#), the presence of minor elements such as sulphur and phosphorous can affect the liquid flow in the molten metal which has direct implications on meltpool geometry [57]. However, as shown by numerous studies, this approach can produce sufficiently accurate results [149, 150].

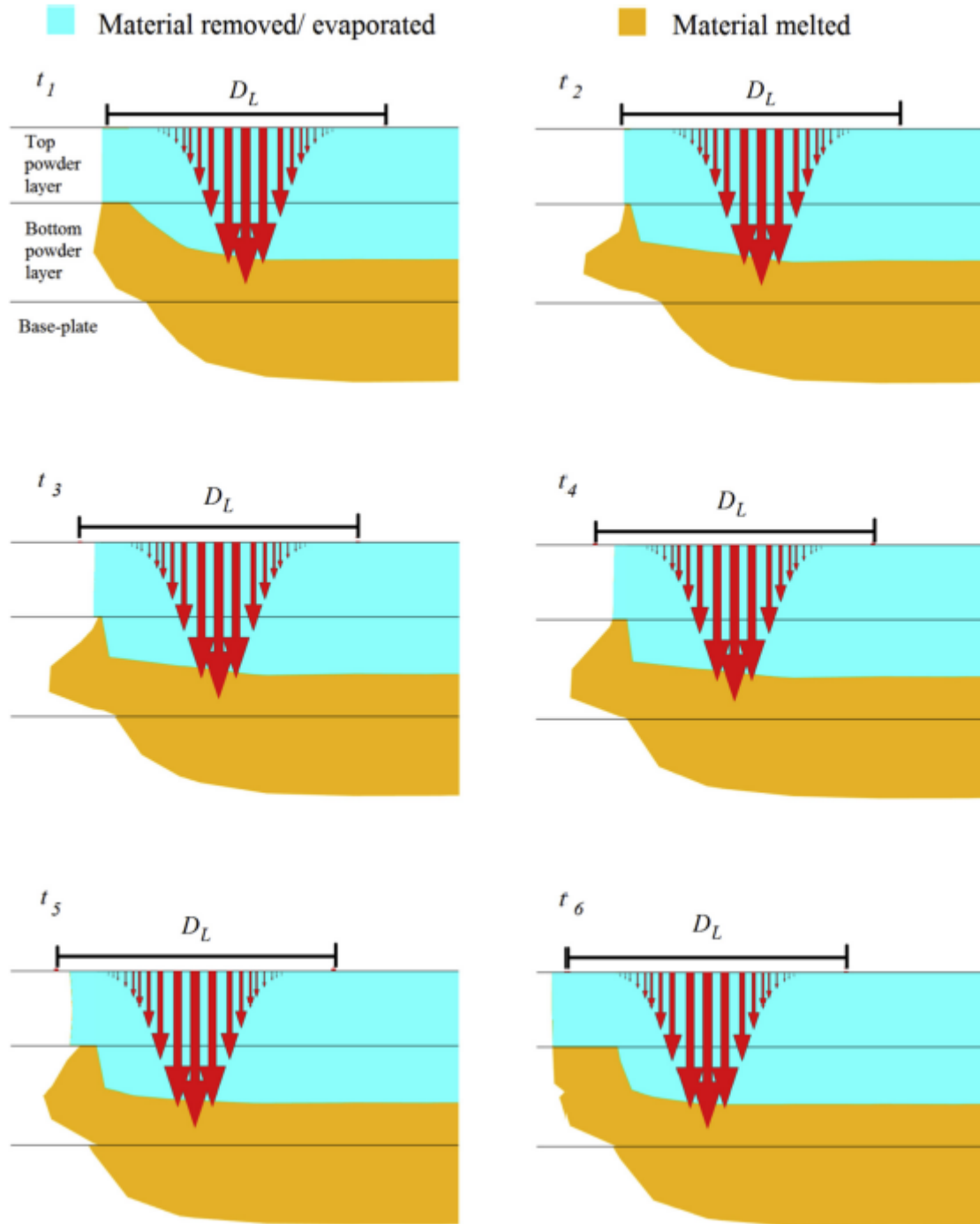


Figure 2.25: Illustration of the Proportion of Melt to Evaporation in AA6061. Taken from [148]

2.2.3.1.2 Residual Stress and Distortion Due to the inhomogenous distribution of thermal field during building of a part, there can be an inhomogenous distribution of residual stresses left in the finished part. This can lead to physical distortion in the final part. Therefore, solution of the thermal field can be used to predict distortions in the final part so that they may be compensated, or laser parameters can be adapted to reduce distortion [151]. Distortion in as-built parts remains a prominent issue in maintaining part compliance in industrial projects and continued work in residual stress calculation [152]. The most market dominant method of distortion calculation is the Inherent Strain (IS) method. The origins of the IS method comes from welding technologies, developed with Ueda *et al.* [153]. IS was repurposed for AM in 2014 by Keller and Ploshikhin [154], with multiple variations on the method being developed [155, 156]. These derivative methods all require coupling to an FEM simulation. Variation between these methods comes from how strongly the IS method is coupled to the FEM simulation. The FEM simulation is fed into the governing equations of the IS method:

$$\rho(T)c_p(T)\frac{\partial T(x, y, z, t)}{\partial t} = \nabla(k(t) \cdot \nabla T(x, y, z, t)) + Q(x, y, z, t) \quad (2.90)$$

$$\nabla \cdot \boldsymbol{\sigma} = 0 \quad (2.91)$$

$$\boldsymbol{\sigma} = \mathbf{D}\boldsymbol{\epsilon}^{el} \quad (2.92)$$

$$\boldsymbol{\epsilon}^{tot} = \boldsymbol{\epsilon}^{el} + \boldsymbol{\epsilon}^{pl} + \boldsymbol{\epsilon}^{th} \quad (2.93)$$

$$\boldsymbol{\epsilon}^{th} = \alpha(T)(T - T_0) \quad (2.94)$$

Full details of the application of the IM method to the AM process is outlined in the work of Gouge *et al.* [157], including the validation using industry benchmark parts (shown in Fig. 2.26). However, it is clear that every derivative and variant implementation of the IM method requires an independent thermal simulation to be coupled with, whether strongly or weakly.

- The original IS method was uncoupled from the thermal analysis, and the heat equation is used purely to calculate the temperature increase from initial temperature T_0 due to the source term.

- A weakly coupled IM method solves the thermal FEM analysis in its entirety to inform the thermal strain matrix. However, the updated displacement matrix is not used to update the node positions of the thermal FEM analysis.
- A strongly coupled IM method also solves the thermal FEM analysis in its entirety, as with the weakly coupled. However, the thermal FEM node positions are updated from the new displacement positions, producing a feedback loop with the thermal FEM.

Thus, the accuracy and speed of the distortion prediction is heavily dependent on the thermal simulation it is coupled to.

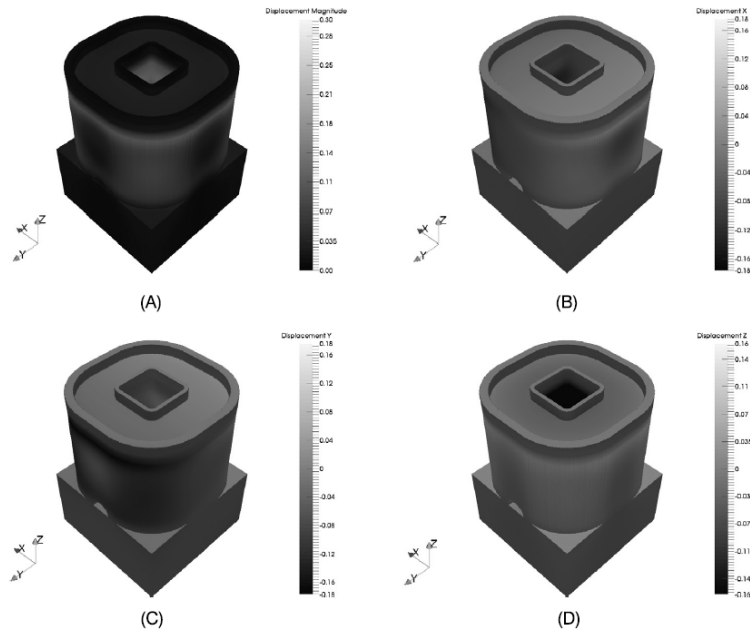


Figure 2.26: Deformation Validation Results. Taken from [157]

2.3 Computational Hardware

Development of simulation algorithms and development of the computational hardware that is used to perform these simulations go hand-in-hand. Therefore to discuss the state of the art of one without discussion of the other would be remiss.

2.3.1 Graphical Process Units

As early as 1951, at the Massachusetts Institute of Technology (MIT) in the US, the Whirlwind I was a vacuum tube based device able to rendering 3-dimensional images for use as a flight simulator for the US Navy during the cold war [158]. Whilst this was one of the very early use of technology to generate 3D representations, it is a far sight from the Graphical Processing standards that are familiar today. The predecessors of today's processors would not arrive until a quarter of a century after Whirlwind I, when RCA released the "Pixie" chip [159]. However, these consumer chipsets were focused on 2D rendering rather than 3D images.

It was the 1990s that saw the shift from a focus on 2D to 3D graphics with the release of 3DFx's Voodoo 1 graphics card in 1995 [160]. This was a dedicated to 3D images, and was a separate component that could be installed into a PC, and the second edition of this product, the Voodoo 2, had three chips to allow concurrent processing of multiple textures in a single pass. This is the first use of concurrent processing, that could be recognisable in comparison to modern graphics cards.

The term Graphics Processing Unit (GPU) was first coined and used by NVIDIA in 1999 with the release of the NVIDIA GeForce 256. The first in the "GeForce" line, that continues as part of the NVIDIA dominance of the GPU landscape. As part of that trajectory, in 2007, NVIDIA released the CUDA Development Environment, the first widely adopted programming paradigm for GPUs. How this differed from conventional CPU programming is shown in [Sec. 2.3.2](#).

The capability of modern day GPUs, when compared to their early predecessors, are order of magnitude more streamlined and functional. Since this point, two major manufacturers have dominated the GPU market, NVIDIA and AMD (formerly ATI Technologies Inc.). The latest generation of GPUs utilise production transistor technologies of the order of approximately 10 nm, as compared to the 220 nm process used for the GeForce 256. This results in modern day GPUs possessing in excess of 76 billion transistors on the NVIDIA RTX 4090, and 58 billion on the AMD Radeo RX 7900 XTX. This makes the 17 million of the GeForce 256 seem paltry in comparison [161–163]. The latest generation of

NVIDIA and AMD GPUs are rated 83 and 61 trillion FLOPS (TeraFLOPS or TFLOPS) respectively [162, 164]. This constant growth and refinement of GPU technology has allowed huge advancements in numerical, data driven technologies, including simulation, machine learning, and data science. Advancements that could not have been handled practically with conventional CPU computation.

2.3.2 Parallel Computation

In order to conceptualise parallel computing, one must first understand its predecessor of serial (or sequential) computing. Consider a simple matrix addition:

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix} \quad (2.95)$$

where x , y , and z are arbitrary vectors of length n . If one were to calculate z manually, one would naturally begin by calculating z_1 , then z_2 and so on. This is reflected in the early computer architectures and arithmetic logic unit (ALU) design, in which each arithmetic action was handled individually, one at a time. Represented in pseudocode this is:

Algorithm 1 Pseudocode Representing Sequential Calculation of a Simple Vector Addition

Require: $n \geq 0$

```

1:  $N \leftarrow 0$ 
2: while  $N < n$  do
3:    $z_N \leftarrow x_N + y_N$ 
4:    $N \leftarrow N + 1$ 
5: end while
```

As can be seen in [Alg. 1](#), as the number of total elements n increases, so does the calculation time of z . At the time of the release of the first dubbed “GPUs” the latest CPU released was the Intel Pentium III single core processor, with a clock speed between 400 MHz and 1.4 GHz and a reported calculation speed of two 32-bit floating point operations per cycle. This would mean at peak performance the Pentium III could perform

approximately 2.8 million 32-bit floating point operations per second (FLOPS). This is sufficient for large arrays of number if simple addition was all that was required. However, in the case of matrix multiplication, which is well established has a base computational complexity of $\mathcal{O}(n^3)$, this would mean that any square matrix with N greater than 141 would require multiple seconds. This is was incredibly limiting for the time, especially with displays. The human eye can register between 24 and 60 frames per second (FPS) of a display [165]. Thus, on a simple 512×512 pixel display, 24 FPS would require the calculation of approximately 6.3 million floating point values per second (6.3 Giga-FLOPS or GFLOPS) which was way beyond the capability of the Intel Pentium III.

Due to the market drive of display hungry applications, a new way of handling such computation was required. Due to the nature of the problem, it was realised that there was no need to handle these calculations serially, the value of a single pixel is independent on the value of any other pixel on the display. Hence, if these values can be calculated concurrently, in parallel, then the time for calculation of the entire display can be reduced by a factor of how many parallel processors are used. This methodology can also be extended to the matrix addition problem of [Eqn. 2.95](#). The value of z_n is independent of any other value of z , therefore this is also a calculation that would benefit from concurrent computing. This revolutionary approach became known as parallelisation.

The modern GPU leverages this parallelisation by implementing multiple simplified processing cores, usually referred to as Graphical Processing Clusters (GPCs). Instead of the full general complexity of a core of a CPU a GPU is streamlined for speed of calculation rather than varied calculation optimisation of the CPU. The CPU is designed to switch between instruction sets more frequently, whereas the GPU is optimised for performing very similar instruction sets across many concurrent cores [166]. An example of GPU architecture can be seen in [Fig. 2.27](#).

Not every problem can benefit from parallelisation, and the viability of a problem to be parallelised must be investigated. [Sec. 4.3](#) will go into full detail on the formation of the enthalpy approach to solving the heat flow equation. However, from its derivation, in [Appendix A](#) and [Appendix B](#) it can be seen that the solution can be represented in

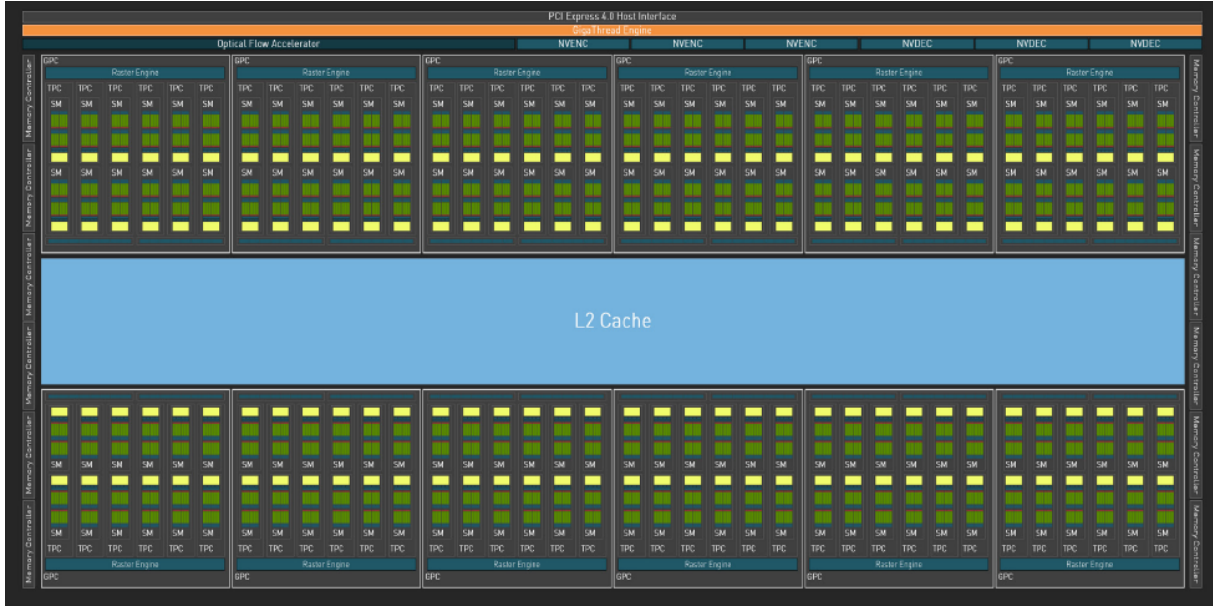


Figure 2.27: Diagram of GPU Chip Layout of Latest NVIDIA Ada Lovelace Architecture. Taken from [161]

matrix form. Inspection of these matrix forms is shown in [Eqn. 4.26](#) and [4.27](#). From these, it can be seen that the calculation of change of enthalpy of a single element in the simulated volume is dependent solely on the surrounding six elements, and is independent of the remaining elements. This indicates that this is a problem that would benefit from the application of parallelisation, where a GPU can be programmed that a single core handles the enthalpy change of a single element, and numerous elements are calculated at the same time to reduce the calculation time of the entire volume [167].

2.4 Concluding Remarks

The literature reviewed in [Chap. 2](#) and identifies the phenomena present during the LPBF process, and the numerical methods utilised in order to quantify and predict them. Based on this literature, it is observed that the LPBF process is an incredibly physically complex process, spanning nanometers to tens of millimeters. Where a multi-physics, multi-scale, unified model would require petabytes of computation. Even with the computational power of the latest NVIDIA and AMD GPUs this would all-encompassing model would be unwieldy for commercially available computing, or incredibly expensive for cloud based solutions [168].

In order to make simulation more manageable, phenomena are aggregated via scale: microscopic, mesoscopic, or macroscopic. However, the varied phenomena across these length scales are thermally coupled. Therefore, a thermal simulation must first be performed, or calculated alongside the additional phenomena simulations. Thus, the advancement that would unilaterally improve performance across all simulations would be to improve the performance of the thermal simulations which all others are coupled with. This will be the aim of this project, and is further expanded on in Chap. 3.

Chapter 3

Research Aims and Objectives

3.1 Research Aims

The overall aim of this project is to develop techniques for increasing the speed performance of heat flow simulation of Laser Powder Bed Fusion, that can be used in conjunction with other established techniques, in order to achieve faster than real-time simulations of industrially acceptable accuracy. If these techniques are to be considered viable, they should be able to predict the meltpool geometry of the LPBF process, whilst outperforming an unmodified simulation in speed.

If successful, these simulation can be used to predict the local thermal history of different geometries present in production parts to identify areas in which the standard parameters may cause overheating and potential build failure ([Sec. 2.1.3](#)). This is a useful preventative tool for Design for Additive Manufacturing (DFAM).

3.2 Research Objectives

In order to accurately evaluate the performance of the coarsening techniques developed in this project a benchmark must be established for comparison, and this benchmark must be validated with physical experiment. Therefore the project objectives are as follows:

1. to produce a base fully fine resolution simulation method to predict the thermal

flow through a macroscale part (Chap. 6);

2. to validate the performance of this benchmark simulation method through utilising it to predict the geometry of meltpools at a range of different processing parameters (Chap. 6);
3. to develop a method of overcoming the limitation of current coarsening strategies that cannot coarsen across materials or material states (Chap. 7);
4. to validate the performance of these coarsening techniques via comparison to the established, validated baseline model (Chap. 7).

Chapter 4

Simulation Methodology

As shown in [Chapter 2](#), due to how the material is processed in LPBF, the physical phenomena that arise are almost exclusively thermally driven. Therefore, when simulating the process, regardless of what methods are undertaken, there is often a need to couple them to a separate thermal simulation to evaluate the thermal state of the volume before all else each time step. Therefore, it stands to reason that in order to improve the performance of these methods, with regard to computational time, when simulating larger and more industrially relevant volumes, one must address the performance of the coupled thermal model on which all the other methods stand. This chapter will describe the computational techniques employed to produce a “baseline” thermal model of the LPBF process and qualify its fidelity via evaluation of the model’s ability to predict melt pool geometry.

4.1 The Heat Equation

The distribution of energy within the build volume is given by the Heat Equation, assuming no heat is lost from the build volume to the wider machine:

$$\dot{T} = \alpha \nabla^2 T + \frac{1}{\rho c} F, \quad (4.1)$$

where T is the short form of $T(x, y, z, t)$ and represents the temperature distribution in the x, y, z directions and time (t); α is the thermal diffusivity of the volume; ρ is the density of the volume; c is the specific heat capacity of the volume; and F is the source term. The full derivation of the heat equation can be found in [Appendix A](#). As can be seen from its derivation the Heat Equation is a second-order linear partial differential equation. A general second-order linear differential equation can be written in the form:

$$au_{xx} + 2bu_{xy} + cu_{yy} + du_x + eu_y + fu = g \quad (4.2)$$

Where the coefficients a, b, c, d, e , and f are known functions of x and y . Here, the subscript u_i represents the first derivative of u with respect to i . In the case of the heat equation, the x and y are replaced with the spatial and temporal domains. The general second-order linear differential equation is presented here in two dimensions for brevity, for how this is shown in three dimensions, please refer to [Appendix B](#). As with any binomial equation, the classification of the equation can be obtained by evaluation of the behaviour of the *discriminant*, $D \equiv b^2 - ac$: if $D < 0$, the equation is parabolic; if $D = 0$, the equation is elliptic; and if $D > 0$, it is hyperbolic. Equations can be of mixed type as the discriminant can vary depending on domain. The Heat Equation ([Eqn. 4.1](#)), sometimes also referred to as the Diffusion Equation, when expressed in three spatial dimensions, can be written in the form:

$$u_t = u_{xx} + u_{yy} + u_{zz}, \quad (4.3)$$

where t represents the temporal dimension. This form of the heat equation represents the prototype of a parabolic equation.

4.2 Discretization

In order to numerically solve the heat equation for the closed volume that is the build volume in LPBF, [Eqn. 4.3](#) must be discretized in all four domains. In the case of the spatial domains, it is trivial to imagine dividing each orthogonal dimension into

equal intervals of arbitrary size h . In other words, dividing the entire build volume into voxels of side length h . Approximation of the second order terms of Eqn. 4.3 (using this discretization) is performed via standard finite difference approximation:

$$u_{xx}(x_i, y_j, z_k) \approx \frac{-2u_{ijk} + u_{i+1,j,k} + u_{i-1,j,k}}{h_x^2} \quad (4.4)$$

$$u_{yy}(x_i, y_j, z_k) \approx \frac{-2u_{ijk} + u_{i,j+1,k} + u_{i,j-1,k}}{h_y^2} \quad (4.5)$$

$$u_{zz}(x_i, y_j, z_k) \approx \frac{-2u_{ijk} + u_{i,j,k+1} + u_{i,j,k-1}}{h_z^2}. \quad (4.6)$$

The temporal domain must also be discretized by approximating Eqn. 4.3 at time steps of Δt and can also be approximated in a similar way through a finite difference approximation. However, in order to generate a system of equations that will give a finite solution (given appropriate initial conditions and boundary conditions), there are two approaches that can be used to perform this finite difference:

- backward difference and,
- forward difference.

4.2.1 Backwards Difference and Implicit Solvers

The backward difference method of finite difference generates a difference equation utilizing the current term and the previous term in the discrete domain. Hence, the solution to the current time step is dependent on the solution of the next time step, this is referred to as an *implicit* method. For demonstration, consider the one-dimensional examples of Eqn. 4.3:

$$u_t = u_{xx} \quad (4.7)$$

Let $u_i^{(k)}$ denote the solution at $x_i = ih$ and $t_k = k\Delta t$. $u_t(z, t)$, which gives rise to the difference equation:

$$\frac{u_i^{(k)} - u_i^{(k-1)}}{\Delta t} = \frac{-2u_i^{(k)} + u_{i+1}^{(k)} + u_{i-1}^{(k)}}{h^2}; \quad i = 1, \dots, n-1; \quad k = 0, 1, \dots \quad (4.8)$$

Which leads to the identity:

$$u_i^{(k)} = u_i^{(k-1)} + \frac{\Delta t}{h^2} \left[-2u_i^{(k)} + u_{i+1}^{(k)} + u_{i-1}^{(k)} \right]. \quad (4.9)$$

In order for the solution to Eqn. 4.3 to be unique, initial conditions and boundary conditions must be defined. If these are defined, and the system of difference equations are expressed in their natural order, the entire solution can be written in the form of a matrix equation $\mathbf{A}x = b$, where:

$$\mathbf{A} = \begin{pmatrix} 1+2\mu & -\mu & & & \\ & -\mu & \ddots & \ddots & \\ & & \ddots & \ddots & -\mu \\ & & & -\mu & 1+2\mu \end{pmatrix}, \quad b = \mu \begin{pmatrix} \alpha \\ 0 \\ \vdots \\ 0 \\ \beta \end{pmatrix} \quad (4.10)$$

Where $\mu = \Delta t/h^2$. In order to achieve a unique solution to the above matrix equation, boundary and initial conditions must be provided. At this point, in order to solve the above equation, one must solve the entire matrix for each time step. This is an implicit method of solution, one such method is the Crank-Nicholson Method. This is computationally demanding for each time step and reduces the viability for industrial application for full build volumes. One advantage of implicit solvers is the stability criteria levied on the values of μ . Due to the requirement of solving the entire matrix backwards through time the use of temperature dependent properties introduces another complexity. This introduces a cyclical problem which the properties to be used at $t = t_{n+1}$ are dependent on the temperature profile at $t = t_n$. However, in order to calculate the temperature at $t = t_n$ the temperature profile at $t = t_{n+1}$ must be known.

4.2.1.1 Stability Criteria of Implicit Methods

Referring back to Eqn. 4.10, one may notice that the matrix $\mathbf{A}$ is a Tridiagonal Symmetric Toeplitz (TST) matrix:

$$\mathbf{A} = \begin{pmatrix} 1+2\mu & -\mu & & \\ -\mu & \ddots & \ddots & \\ & \ddots & \ddots & -\mu \\ & & -\mu & 1+2\mu \end{pmatrix} \equiv \begin{pmatrix} a & c & & \\ b & \ddots & \ddots & \\ & \ddots & \ddots & c \\ & & b & a \end{pmatrix} \quad (4.11)$$

The eigenvalues of such matrices is found using the formula:

$$\lambda_k = a \pm 2\sqrt{bc} \cos\left(\frac{k\pi}{N+1}\right), \quad k = 1, \dots, N \quad (4.12)$$

Where N is the order of matrix $\mathbf{A}$. Thus, the eigenvalues of $\mathbf{A}$ are:

$$1 + 2\mu \pm 2\sqrt{\mu^2} \cos\left(\frac{k\pi}{N+1}\right), \quad k = 1, \dots, N \quad (4.13)$$

and the eigenvalues of $\mathbf{A}^{-1}$:

$$\frac{1}{1 + 2\mu \left(1 - \cos\left(\frac{k\pi}{N+1}\right)\right)}, \quad k = 1, \dots, N. \quad (4.14)$$

Combining the fact that $\mu \equiv \frac{\Delta t}{h^2} > 0$ and $1 - \cos k\pi/N+1 \in (0, 2)$, the eigenvalues of $\mathbf{A}^{-1}$ are always positive and less than one for every value of μ . Thus implicit methods are unconditionally stable for all sizes of discretization in time.

The downfall of such methods in industrial applications comes from the need for each timestep requiring the full solving of matrix $\mathbf{A}$ each iteration, these methods are computationally intensive, and time-consuming. Also, in LPBF, the scanning speeds achievable during processing, if too large a time-step is taken the laser spot may move considerably between times t_n and t_{n+1} . Whilst this does not impose any limitation on the stability of the method, it would undermine the accuracy of the thermal simulation, thus does impose a maximum limit on the size of time step that can be taken.

4.2.2 Forwards Difference and Explicit Solvers

If instead, a forwards difference is used to combine the expressions for discretization of Eqn. 4.3, then the difference equation (Eqn. 4.15) that arises shows that the solution to the next timestep is dependent on the solution to the current timestep, hence is an explicit method.

$$\frac{u_i^{(k+1)} - u_i^k}{\Delta t} = \frac{-2u_i^{(k)} + u_{i+1}^{(k)} + u_{i-1}^{(k)}}{h^2}; \quad i = 1, \dots, n-1; \quad k = 0, 1, \dots \quad (4.15)$$

As with the backwards difference, when expressed in natural order Eqn. 4.15 can be written as a Tridiagonal Symmetric Toeplitz matrix equation:

$$\mathbf{A} = \begin{pmatrix} 1-2\mu & \mu & & & \\ \mu & \ddots & \ddots & & \\ & \ddots & \ddots & \mu & \\ & & \mu & 1-2\mu & \end{pmatrix}, \quad b = \mu \begin{pmatrix} \alpha \\ 0 \\ \vdots \\ 0 \\ \beta \end{pmatrix} \quad (4.16)$$

4.2.2.1 Stability Criteria of Explicit Methods

In order to investigate whether this method of solution is subject to any restrictions with respect to stability, the same approach is used as was undertaken with the backwards difference. The eigenvalues of $\mathbf{A}$ are hence expressed:

$$1 - 2\mu \left(1 - \cos \left(\frac{k\pi}{N+1} \right) \right), \quad k = 1, \dots, N \quad (4.17)$$

This is subject to the same constraint that in order to guarantee stability, the eigenvalues of $\mathbf{A}$ must be greater than -1 and less than 1:

$$\begin{aligned}
-1 &< 1 - 2\mu \left(1 - \cos \left(\frac{k\pi}{N+1} \right) \right) < 1 \\
-2 &< -2\mu \left(1 - \cos \left(\frac{k\pi}{N+1} \right) \right) < 0 \\
0 &< \mu \left(1 - \cos \left(\frac{k\pi}{N+1} \right) \right) < 1
\end{aligned} \tag{4.18}$$

As $1 - \cos(k\pi/(N+1))$ has a maximum value of 2, when $k\pi/(N+1) = \pi$. This leads to:

$$\begin{aligned}
2\mu &< 1 \\
\mu &< \frac{1}{2} \\
\frac{\Delta t}{h^2} &< \frac{1}{2}.
\end{aligned} \tag{4.19}$$

Therefore, unlike the implicit methods, explicit methods have a strict restriction in the relationship between values of both Δt and h that maintain convergence to the correct solution. Due to this restriction the viable values of Δt used in explicit methods are often orders of magnitude smaller than the equivalent implicit methods. However, due to the explicit nature of the solution, there is no need to solve a full system of equations each time step, unlike the implicit method. This condition was first formalised by Courant, Lewy, and Friedrichs in 1928 in their paper “Über die partiellen Differenzengleichungen der mathematischen Physik”, and is often referred to as the Courant-Lewy-Friedrichs Condition [169]. The reduced complexity of the explicit method can be used to overcome the stability restrictions and can allow explicit methods to exceed the computational speed of implicit methods.

4.3 An Enthalpy Approach to the Forward Euler Method of Numerical Solution for Heat Diffusion

The first law of thermodynamics, first formalised by Robert Clausius in 1850 in their paper “Ueber die bewegende Kraft der Wärme und die Gesetze, welche sich daraus für die Wärme-lehre selbst ableiten lassen”, states that the internal energy of a closed system is the sum of the heat supplied to or withdrawn from the system and the work done on the system [170]. Mathematically:

$$\Delta H = Q + W, \quad (4.20)$$

Where H is the internal energy, or enthalpy; Q is heat; and W is work. Therefore, if the build volume is considered a closed system, and is discretized as with [Section 4.2](#), then the change in internal energy of any single cubic element is equal to the heat flow from any surrounding element and/or the heat supplied by the laser. In order to quantify the heat flow between adjacent elements in the volume Fourier’s Law of thermal conduction [171]:

$$\frac{\Delta Q}{\Delta t} = -kA \frac{\Delta T}{\Delta x}. \quad (4.21)$$

Consider two cubic elements of dimension h , in contact through a single face, as illustrated in [Fig. 4.1](#). Heat flow from element 1 to element 2 can be shown to be:

$$\Delta Q_{12} = -k_{12}A_{12}\Delta t \frac{T_2 - T_1}{\Delta x}. \quad (4.22)$$

The thermal conductivity, k_{12} , can be expressed as a combination of the thermal resistivity of cubes one and two, and the respective distances from the cell centres. Also, the area

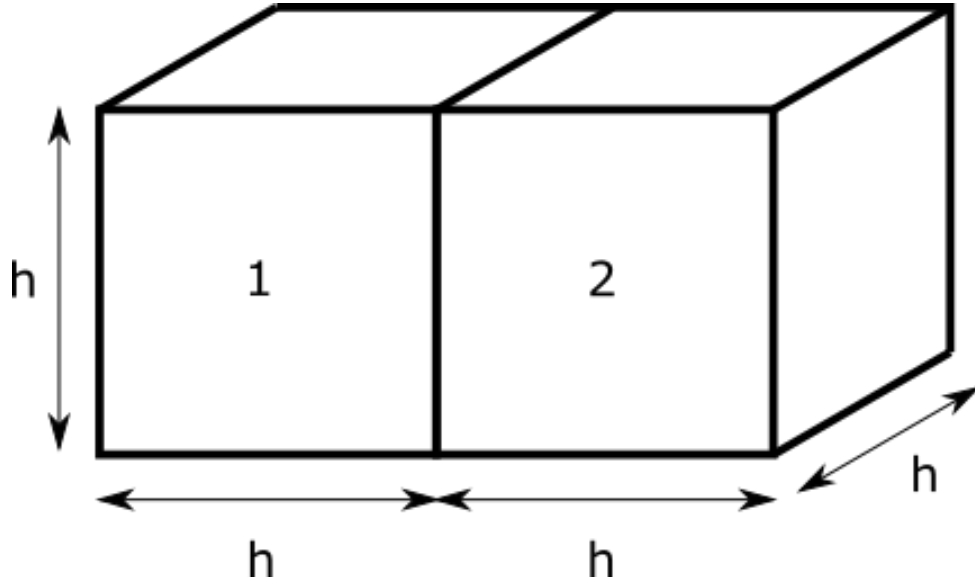


Figure 4.1: Schematic showing two adjacent cubic elements of dimension h .

of contact, A_{12} can be seen to be equal to h^2 . Hence, Eqn. 4.22 becomes:

$$\begin{aligned}\Delta Q_{12} &= -h^2 \Delta t \frac{T_2 - T_1}{\frac{h}{2} R_1 + \frac{h}{2} R_2} \\ \Delta Q_{12} &= -2h \Delta t \frac{T_2 - T_1}{R_1 + R_2}.\end{aligned}\tag{4.23}$$

As there is no internal work being done to or by each cube, the heat flow can be related to the specific enthalpy through the expression:

$$\Delta H = \frac{\Delta Q}{V \rho}.\tag{4.24}$$

Where V is the volume, and ρ is the density. Thus, the change of specific enthalpy of element 1 due to heat transfer between itself and element two can be summarised as:

$$\begin{aligned}\Delta H_1 &= -2 \frac{h \Delta t}{V_1 \rho_1} \left(\frac{T_2 - T_1}{R_1 + R_2} \right) \\ \Delta H_1 &= -2 \frac{h \Delta t}{h^3 \rho_1} \left(\frac{T_2 - T_1}{R_1 + R_2} \right) \\ \Delta H_1 &= -2 \frac{\Delta t}{h^2 \rho_1} \left(\frac{T_2 - T_1}{R_1 + R_2} \right).\end{aligned}\tag{4.25}$$

Extending into a full volume in three dimensions, the expression for the enthalpy change for any given element through heat flow between adjacent cubic elements can be expressed:

$$\begin{aligned} \Delta H_{x,y,z,t+\Delta t} = & \frac{2\Delta t}{h^2 \rho_{x,y,z}(T)} \left(\frac{T_{x+1,y,z,t} - T_{x,y,z,t}}{R_{x+1,y,z,t} + R_{x,y,z,t}} + \frac{T_{x-1,y,z,t} - T_{x,y,z,t}}{R_{x-1,y,z,t} + R_{x,y,z,t}} + \right. \\ & + \frac{T_{x,y+1,z,t} - T_{x,y,z,t}}{R_{x,y+1,z,t} + R_{x,y,z,t}} + \frac{T_{x,y-1,z,t} - T_{x,y,z,t}}{R_{x,y-1,z,t} + R_{x,y,z,t}} \\ & \left. + \frac{T_{x,y,z+1,t} - T_{x,y,z,t}}{R_{x,y,z+1,t} + R_{x,y,z,t}} + \frac{T_{x,y,z-1,t} - T_{x,y,z,t}}{R_{x,y,z-1,t} + R_{x,y,z,t}} \right), \end{aligned} \quad (4.26)$$

or more concisely in matrix notation:

$$\Delta h = \frac{2\Delta t}{h^2 \rho_{x,y,z}(T)} \mathbf{A} \mathbf{r}^T \mathbf{I} \mathbf{u}. \quad (4.27)$$

Here, $\mathbf{r}$ and $\mathbf{u}$ are vectors containing the conductivity and the temperatures as time t of each element in the volume in their natural order respectively; $\mathbf{I}$ is the identity matrix; and $\mathbf{A}$ is a Tridiagonal Banded Toeplitz (TBT) Matrix:

$$\mathbf{A} = \begin{pmatrix} \mathbf{T} & \mathbf{I} & & & & & \\ & \mathbf{I} & \mathbf{T} & & & & \\ & & \mathbf{I} & \mathbf{T} & & & \\ & & & \ddots & \ddots & \ddots & \ddots \\ & & & & \mathbf{I} & \mathbf{T} & \mathbf{I} \\ & & & & & \mathbf{I} & \mathbf{T} \\ & & & & & & \mathbf{I} & \mathbf{T} \end{pmatrix}, \quad \text{where} \quad \mathbf{T} = \begin{pmatrix} -6 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -6 \end{pmatrix}. \quad (4.28)$$

Therefore, it is plain to see that the calculation of the net heat flow from a single element at any given time is only dependent on the state of seven elements in the volume. This reduction in computational load and suitability of GPU technology to parallelise matrix arithmetic can be leveraged against the increased restriction on the size of time step that maintains stability in order to exceed the performance of implicit models.

Another advantage of an enthalpy approach to solution of the heat equation is that the lack of dependence of the solution on the temperature variant specific enthalpy that

temperature based solutions must incorporate.

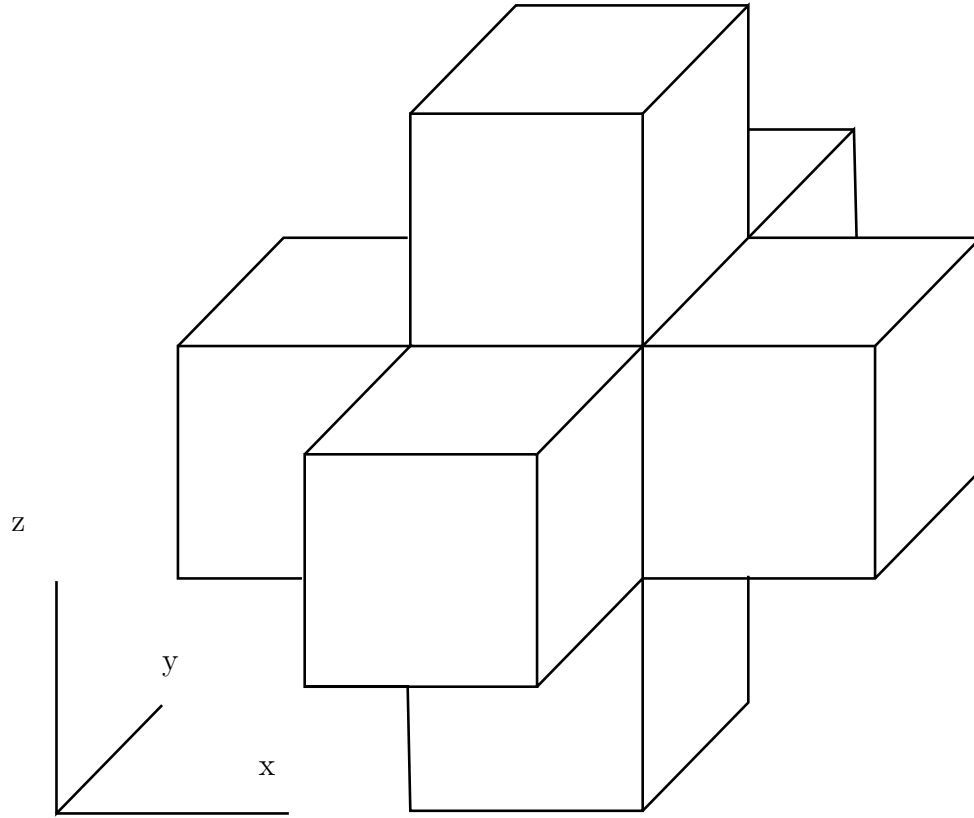
4.3.1 Derivation of Maximum Stable Time step for an Explicit Enthalpy Approach to Solving the Heat Diffusion Equation

As was shown in [Sec. 4.2.1.1](#) and [4.2.2.1](#), in order to quantify the maximum stable time step that must be observed by the solver, the eigenvalues of the matrix $\mathbf{A}r^T\mathbf{I}$ must be evaluated and the magnitude of these need to be less than one. However, in three dimensions this matrix, as shown in [Eqn. 4.28](#), is a TBT Matrix. The eigenvalues of this matrix is decidedly less trivial to evaluate than the TST Matrix in two dimensions [172, 173]. Therefore, a different approach to the purely mathematical is required.

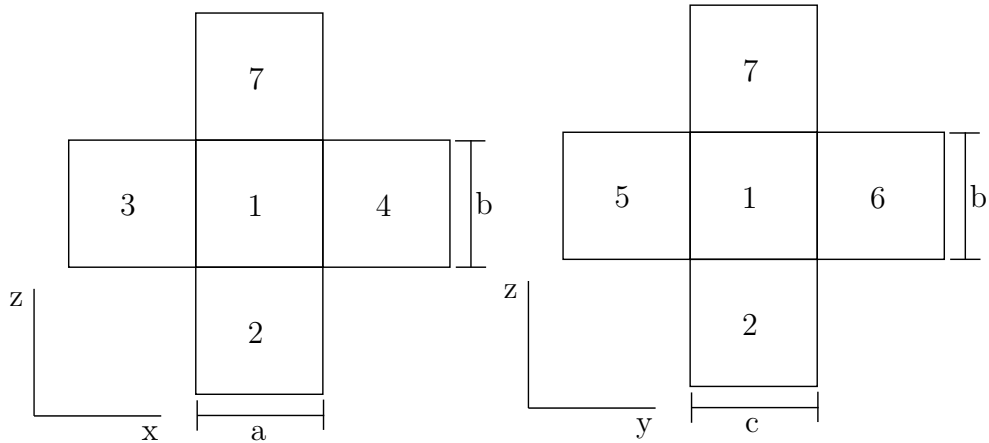
First, consider a neighbourhood of cubic elements, shown in [Fig. 4.2](#). The expression of heat flow into the central element (element one) is given by [Eqn. 4.26](#). This can be used to calculate the time taken for the central element to reach a target temperature. If the target temperature is the mean temperature of all elements in the immediate neighbourhood, then this calculated time would represent the minimum time step that would be required to reach a steady state. Thus, would be sufficient time that would not cause oscillation in the neighbourhood of cells, and would give reasonable estimation of the maximum stable time step. The change in temperature corresponding to the homogenisation of the central element is expressed in [Eqn. 4.29](#).

$$\Delta T_1 = T_t - T_1 = \frac{1}{6} \sum_{i=2}^7 (T_i - T_1). \quad (4.29)$$

Relating the change in temperature of the the central element to the heat flow from the neighbouring elements is done through the combination of [Eqn. 4.26](#) and the identity $c_p = dH/dT$. This gives rise to the expression for the case of cubic elements (where $a =$



(a) Schematic of element and six neighbouring elements



(b) XZ section of elements

(c) YZ section of elements

Figure 4.2: Schematics and sections of an arbitrary element and its six neighbouring elements

$b = c = h$):

$$\Delta T_1 = \frac{2\Delta t}{c_p h^2 \rho_1(T)} \left(\frac{T_7 - T_1}{R_7 + R_1} + \frac{T_6 - T_1}{R_6 + R_1} + \frac{T_5 - T_1}{R_5 + R_1} + \frac{T_4 - T_1}{R_4 + R_1} + \frac{T_3 - T_1}{R_3 + R_1} + \frac{T_2 - T_1}{R_2 + R_1} \right). \quad (4.30)$$

Setting Eqn. 4.29 equal to Eqn. 4.30 and solving for Δt for the worst case ($R_1 = R_2 = R_3 = R_4 = R_5 = R_6 = R_7 = \min(R(T))$, $c_p = \min(c_p(T))$, $\rho = \min(\rho(T))$) yields an expression for the maximum timestep:

$$\Delta t = \frac{\min(c_p(T)) h^2 \min(\rho(T)) \min(R(T))}{6}. \quad (4.31)$$

This expression fulfills the Courant-Lewy-Friedrichs condition for the three-dimensional explicit numerical solution to the heat diffusion equation.

4.3.2 Representing Laser Power Input

Whether LPBF or EBPF is utilised for the production of metallic parts, the heat source/beam intensity profile that is assumed is Gaussian. This is due to the method of production of each of these beams. Thus the two-dimensional intensity profile of the laser, as received at the surface of the coupon, is given by:

$$I(x, y) = \frac{\eta P}{2\pi\sigma_x\sigma_y} \exp\left(-\frac{x^2 + y^2}{2\sigma_x\sigma_y}\right). \quad (4.32)$$

Where η is the optical absorptivity of the material at the frequency of the laser or electron beam; P is the nominal power of the laser; σ_x and σ_y are the beam spot diameters of the beam at the focal point on the material in the x and y directions respectively (these are often given as the diameter at which laser intensity is $1/e^2$ its maximum). Thus, when integrated over the full range ($\pm\infty$) the result is ηP as expected. The absorptivity η of the material can be related to the emissivity of the material ε through Kirchhoff's Law [174]. This is believed to hold during the LPBF process, as observed break down of this relationship only happens in extreme conditions [175].

However, as with the welding technology that preceded PBF, surface profiles of heat input were found to be insufficient for simulation and modelling, as due to the penetration of the beam into the material, the heat source acts as a volumetric source within the material/meltpool [176–178]. Thus, a third dimension term must be added to the intensity profile to represent this. There has been much investigation into the appropriate z-profile for these heat sources, Zhang *et al.* provide an excellent summary of the commonly used volumetric heat sources, and are shown in Fig. 4.3 [179].

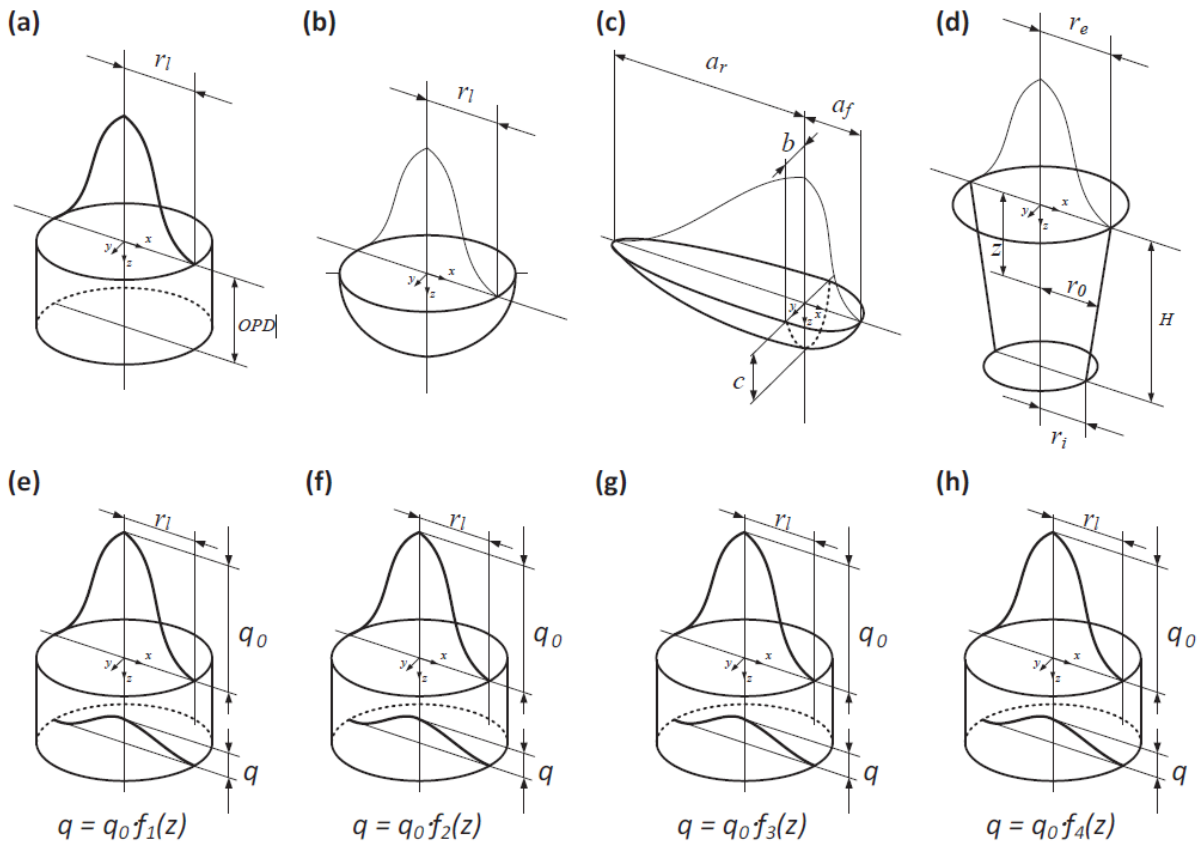


Figure 4.3: Schematics of Commonly Utilised Volumetric Heat Sources for Modelling and Simulation of LPBF, (a) Cylindrical; (b) Semi-spherical; (c) Semi-ellipsoid; (d) Conical; (e) Radiation Transfer Method; (f) Ray-Tracing Method; (g) Linearly Decaying Method; (h) Exponentially Decaying Method. Taken from [179].

Zhang *et al.* conclude that all of these volumetric heat source profiles result in approximately 40% under-prediction of meltpool depth compared to physical experiments. However, the topic of the absorptivity utilized in the numerical prediction was weakly formed and may account for this inaccuracy. The results show that the predicted lengths of each of these heat sources for equivalent volumes results in a maximum variation in prediction

of 15 μm . Therefore, the choice of heat source shape becomes arbitrary. As the aim of the project is speed of simulation it was then decided that a cylindrical profile should be used as this can easily be defined, requiring the fewest calculations per element:

$$I(x, y) = \frac{\eta P}{2\pi\sigma^2 h} \exp\left(-\frac{x^2 + y^2}{2\sigma^2}\right). \quad (4.33)$$

Where h is the assumed penetration depth of the laser, and assumes that the beam radius is constant in x , and y ; i.e. $\sigma_x = \sigma_y = \sigma$. A natural assumption for the value of h is that it is equal to the layer thickness. Eqn. 4.33 is subject to the same results constraints as the two dimensional expression in Eqn. 4.32 that:

$$\int_0^h \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} I(x, y, z) dx dy dz \equiv \eta P. \quad (4.34)$$

Due to the requirement to discretize heat input to an individual cell of the mesh, consider an individual element i , with x , y , and z coordinates x_i , y_i , and z_i respectively. The expression for the enthalpy increase of element i due to the laser input is then:

$$\begin{aligned} & \frac{1}{\rho_i n^3} \int_{z_i - n/2}^{z_i + n/2} \int_{y_i - n/2}^{y_i + n/2} \int_{x_i - n/2}^{x_i + n/2} I(x, y, z) dx dy dz = \\ & \frac{1}{\rho_i n^3} \int_{z_i - n/2}^{z_i + n/2} \int_{y_i - n/2}^{y_i + n/2} \int_{x_i - n/2}^{x_i + n/2} \frac{\eta P}{2\pi\sigma^2 h} \exp\left(-\frac{x^2 + y^2}{2\sigma^2}\right) dx dy dz = \\ & \frac{\eta P}{4h\rho_i n^2} \left(\operatorname{erf}\left(\frac{x_i + n/2}{\sqrt{2}\sigma}\right) - \operatorname{erf}\left(\frac{x_i - n/2}{\sqrt{2}\sigma}\right) \right) \left(\operatorname{erf}\left(\frac{y_i + n/2}{\sqrt{2}\sigma}\right) - \operatorname{erf}\left(\frac{y_i - n/2}{\sqrt{2}\sigma}\right) \right) \end{aligned} \quad (4.35)$$

Where ρ_i is the element density, n is the dimension of the cubic elements, erf is the error function, and $0 \leq z \leq h$. One benefit of this, is that if the element size for the irradiated elements is constant for the entire simulation, these values of power input can be calculated in advance to reduce simulation time. As the pre-computed values can be used rather than increasing the number of calculations per element.

4.3.3 Losses

4.3.3.1 Radiative Losses

It is assumed that radiative losses are only relevant in the top surface of the part. As discussed earlier in [Sec. 2.1.2.3](#) the absorptivity/emissivity of the surface is dependent on the oxidation present. In the case of the most heavily oxidised samples can approach 1.0 at low wavelengths. Therefore, in order to cater to these “worst-cases”, radiative losses are calculated using an emissivity of 1.0. Hence the enthalpy loss of an element due to radiative losses is:

$$\Delta H_i = 5.670373 \times 10^{-8} n^2 (T_i - T_0)^4 \quad (4.36)$$

where T_0 is the ambient temperature of the build chamber/inert gas flow, which is assumed to be constant.

4.3.3.2 Convective Losses

Similarly to radiative losses, convective losses are assumed to be limited to the top surface of the part which has contact with the chamber gas flow. Li *et al.* performed numerous experiments in order to derive a relationship between observed convection coefficient for various SLM alloys of varied part geometry [50]. From this work an approximate value of convective coefficient can be obtained, and was selected to be 11.6. Due to the comparative orders of magnitude of the conductive losses with respect to the radiative and conductive losses it is assumed that the approximate value is sufficient as most work discussed in [Chap. 2](#) assume them to be negligible.

4.4 Combining Multiple Materials into Hybrid Elements for Mesh Coarsening

As with all numerical solvers for matrix problems, the scaling of finite methods is proportional to the number of elements or nodes [180]. Therefore, a method of reducing the computational time required for simulation is to reduce the number of elements that

define the volume. This, intuitively, means that element size must be increased. However, to increase the dimensions of all elements uniformly in the volume would reduce the information that can be inferred from the results, i.e. [Chap. 2](#) discusses the resolution of simulation methods that each thermophysical and metallurgical phenomena requires and if the element size is increased beyond this then this information is unable to be inferred. Finite element methods are able to produce greater detail of conditions within the element than the resolution allows by utilizing higher order nodes within the element [181]. However, by increasing the number of nodes within an element, the number of calculations per element is increased. Thus, the exponential convergence is undermined by the increase in computational load. A natural progression of this element-based approach then requires the element size to be gradated, from fine elements in the regions of interest to coarse elements in the very bulk of the part. This then requires a strategy that either naturally, or explicitly handles the transition from fine to coarse elements. Current methods of mesh coarsening for finite volume solvers are limited to coarsening elements that are of the same material status, i.e. powder elements must be coarsened with other powder elements; and solid elements must be coarsened with other solid elements. This limits the maximum coarsening that can be performed. Extreme examples of this limitation are lattice structures [182] due to their thin sections and complex geometry that effectively prevent mesh coarsening due to the constant transition of the build volume from solid to powder. Therefore, a novel method of element coarsening is proposed that allows for hybrid powder/solid elements to overcome this limitation.

The method described provides an algorithm to generate a resistivity vs temperature curve for any cubic element consisting of a combination of both powder and solid. This value cannot be calculated from first principles at this time. Consider [Fig. 4.4](#), where the grey elements are solid and the dotted elements are powder. The traditional method of calculation of the equivalent thermal resistivity of the entire volume, R_{TOT} is given in [Eqn. 4.37](#):

$$R_{TOT} = \left(\frac{1}{R_1 + R_4 + R_7} + \frac{1}{R_2 + R_5 + R_8} + \frac{1}{R_3 + R_6 + R_9} \right)^{-1}. \quad (4.37)$$

However, this method poses an issue for the fringe case of the example shown. If the top surface of elements 1, 2, and 3 are held at an elevated temperature, T_h , and the bottom surface of elements 7, 8, and 9 are held at a reduced temperature, T_l , intuition would show that heat would flow from the top surface to the bottom. The predominant route of heat flow would be via the solid elements: 1, 4, 5, 6, then 9. However, Eqn. 4.37 would indicate that should the resistivity of the powder increase and tend to the near infinite, regardless of the resistivity of the solid, R_{TOT} would tend to zero. This would mean no heat flow would occur between the top and bottom surfaces, which can be seen by inspection would be incorrect. Thus, this approach is insufficient for calculating the equivalent thermal resistivity of a hybrid element.

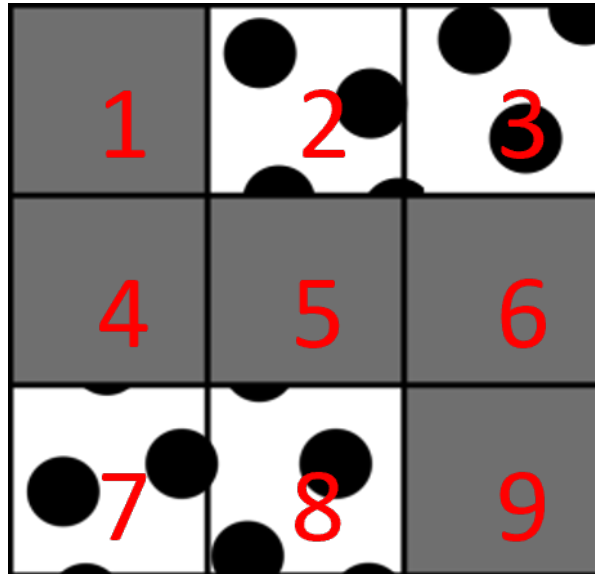


Figure 4.4: Schematic of a 2-Dimensional Volume Consisting of Both Powder and Solid

The proposed alternative takes inspiration from the historic method of measuring the thermal conductivity of materials [104]. In this method a sample of material is held between two surfaces of fixed, but differing temperature, creating a thermal gradient like the one proposed above. The time taken for the sample to reach a thermal equilibrium is measured, and is used to calculate the thermal conductivity of the sample:

$$k = \frac{Qd}{At(\theta_1 - \theta_2)}. \quad (4.38)$$

Here, Q is the power in watts consumed by the maintenance of the thermal gradient at steady state, d is the thickness of the sample, A is the area of the sample, t is the time taken to reach thermal equilibrium, and $\theta_1 - \theta_2$ is the difference in temperature between the top and bottom surfaces.

Over the next century the method described by Griffiths *et al.* was superseded by the transient hot wire method [183], this was mostly due to the fact that the static method takes considerably greater time than the dynamic, transient method. Materials with considerably low thermal conductivity reach thermal equilibrium slowly, and therefore in order to create a curve of conductivity versus temperature requires the measurement needs to be taken multiple times of a number of temperature ranges, which is a considerable time investment.

The new proposed method utilises the heat flow methods outlined in [Sec. 4.3](#), and the static method of measurement outlined above. By simulating a volume of both powder and solid, with a fixed thermal gradient across the volume, to steady state an equivalent thermal conductivity for the volume can be calculated. This is done using Fourier's Law:

$$Q = -k \frac{A \Delta t}{L} \Delta T. \quad (4.39)$$

Q is the heat flow, k is the thermal conductivity, A is the area through which the heat flows, Δt is the time over which heat has flowed, L is the length over which the heat flows, and ΔT is the temperature gradient. Applying Fourier's Law to the previous example volume, at steady state, the total heat flow between the top and bottom surfaces would be equal to the heat flow between the top row of elements and the second row of elements and so on. Therefore, this can be leveraged to calculate an equivalent resistivity value for the entire volume.

By inputting the relevant values for the total simulated volume into [Eqn. 4.39](#) and setting it equal to the value of heat flow from element layer to element layer. The choice of adjacent layers is arbitrary as at steady state the heat flow is constant through any cross

section normal to the thermal gradient. Thus:

$$\begin{aligned}
 -k_{TOT} \frac{(3n)^2 \Delta t}{3n} (T_h - T_l) &= \Delta H \Delta t \\
 -3k_{TOT} n (T_h - T_l) &= \Delta H \\
 k_{TOT} &= -\frac{\Delta H}{3n(T_h - T_l)}.
 \end{aligned} \tag{4.40}$$

Where n is the side length of a single cubic element. The equivalent resistivity of any hybrid element at any temperature must lie between the the values of the value for the resistivity of the solid and powder at the same temperature. This can be expressed as a linear interpolation:

$$\begin{aligned}
 R_{equiv} &= R_{solid} + \alpha(R_{powder} - R_{solid}) \\
 &= R_{solid} + \alpha R_{powder} - \alpha R_{solid} \\
 &= (1 + \alpha)R_{solid} + \alpha R_{powder}.
 \end{aligned} \tag{4.41}$$

If instead Eqn. 4.41 is solved for α , this value can be used to produce a full $R(T)$ curve for the hybrid. Thus, a single value can be saved for use in the simulation rather than require another look-up array per each geometry of hybrid element (Eqn. 4.42).

$$\alpha = \frac{R_{equiv} - R_{solid}}{R_{powder} - R_{solid}} \tag{4.42}$$

This value of α is then specific to the orientation of powder and solid in the direction of the thermal gradient. This means that the value of alpha needs to be calculated in the x , y , and z directions, and handled separately during simulation of the build volume. Due to the reliance on R_{solid} and R_{powder} on temperature, this would mean that Eqn. 4.42 would also be temperature dependent. This is explored in Sec. 7.2.1.

4.4.1 The Fully Fine to Coarse Element Boundary

Due to the difference in element size between fully fine and coarsened elements Eqn. 4.27 no longer holds. Heat transfer between fully fine and coarsened elements must

be handled explicitly. Fig. 4.5 shows a boundary between cubic, fully fine elements of side length h , and a coarsened, cubic element of side length $5h$.

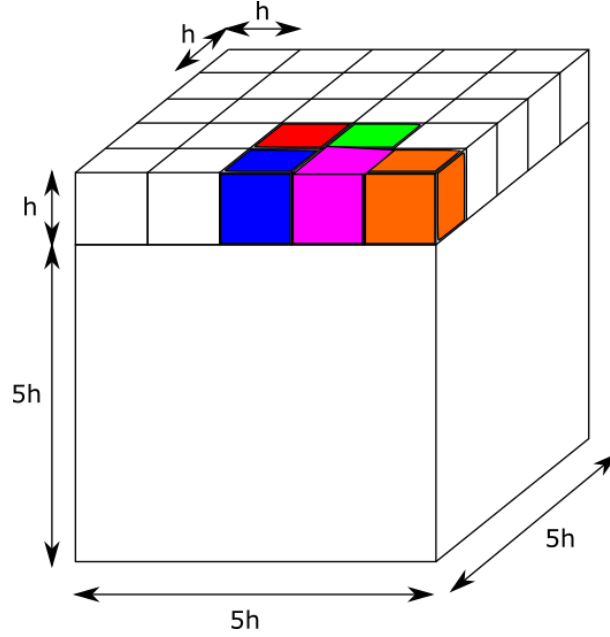


Figure 4.5: Diagram of Boundary between Fully Fine and Coarsened Elements

From the diagram, Eqn. 4.22 now must incorporate the adjustment in geometry between cell centres. If the distance between the cell centres of the fully fine and coarsened elements in the x , y , and z directions are given as Δx , Δy , and Δz respectively then Eqn. 4.22 becomes:

$$\Delta Q = -2h \sin(\theta) \frac{\Delta T}{R_1 + 5R_2}, \text{ where} \quad (4.43)$$

$$\theta = \arctan \left(\frac{\Delta z}{\sqrt{\Delta x^2 + \Delta y^2}} \right) \quad (4.44)$$

The color coding of Fig. 4.5 shows the five non-trivial cases. However, as the relationship between the cell centres is fixed, the values of theta can be precomputed to save on computational time during simulation. The conversion from enthalpy to temperature is unchanged by the alteration to geometry.

Chapter 5

Materials and Methods

5.1 Physical Experiments

Physical experiments were performed using the open architecture machine developed at Heriot Watt university, Edinburgh by Andrew Moore *et al.* [184]. The machine is equipped with a SPI 400W single mode, continuous wave, 1070 nm wavelength fibre laser. The laser position is controlled using a Raylase MS-II-14 scanner with a 163 mm focal length, f-theta lens. The coupon and its actuators are enclosed in a detachable, 5 mm thick, transparent, perspex chamber, which is then drawn down to a vacuum before being filled with argon inert gas. The machine set-up is shown in [Fig. 5.1](#).

The substrate used in the open architecture machine were wrought 316L stainless steel coupons of dimensions $80 \times 50 \times 5 \text{ mm}^3$. A schematic of the substrate coupons can be found in [Fig. 5.2](#). These coupons were exposed to a continuous wave (CW) laser of varying power and scanning speeds. In order to ascertain the meltpool geometries for comparison to the simulation experiments, each coupon was sectioned using electro-discharge machining (EDM) on a GF Cut 30 EDM. Then mounted ground and polished to an OPS 0.04 μm finish using standard metallographic procedure. The samples were electrochemically etched using a 10% solution of oxalic acid in deionised water at a voltage of 5 V for 30 seconds each. Optical microscopy was performed on a Zeiss Axioskop 2 equipped with a monochrome charge-coupled device (CCD) camera and motorised stage. Meltpool geometries were measured using ImageJ open source analysis software.

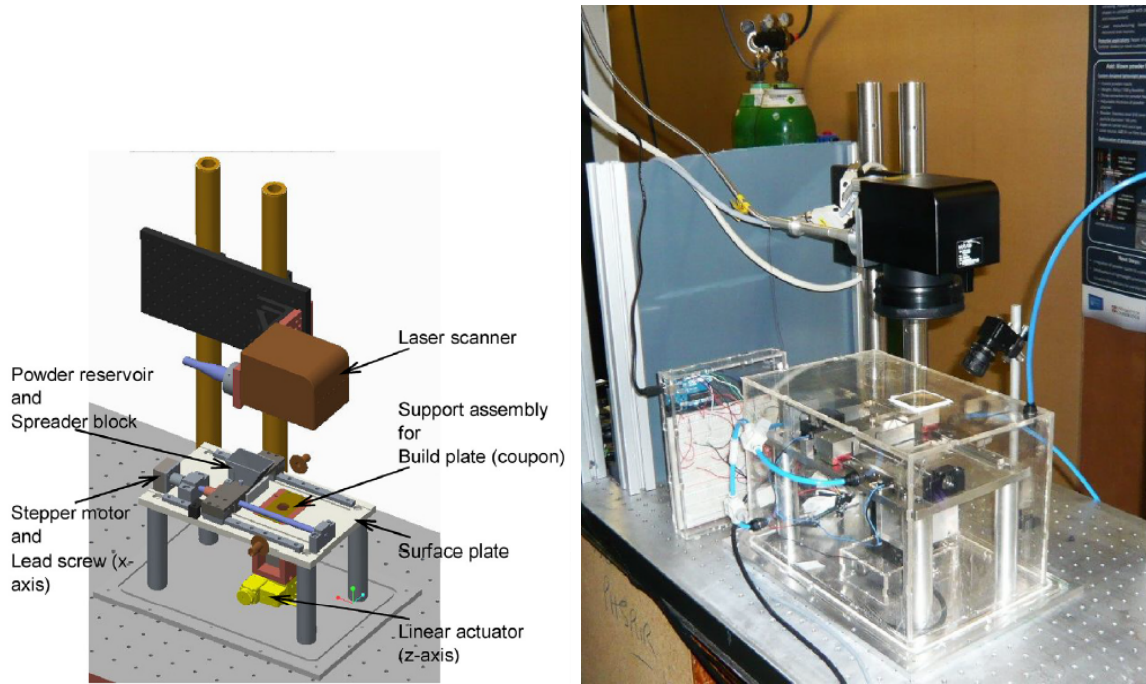


Figure 5.1: Images of the Open Architecture Rig. Taken from [184].

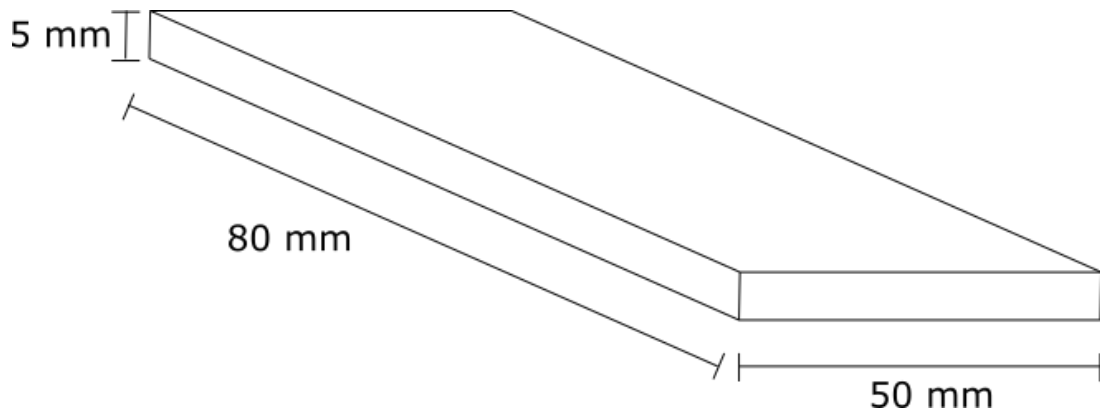


Figure 5.2: Schematic of Stainless Steel Substrate Coupons

5.1.1 Validation Experiment 1: Single Track Experiment

The first validation experiment, referred to as the “Single Track Experiment”, used fixed values of laser power and scanning speed. The purpose of this experiment was to verify the accuracy of the numerical experiment at predicting the amount of energy transferred into the substrate by laser exposure. A total of forty 10 mm line scans were exposed on the surface of the substrate. The layout of these exposures can be seen in [Fig. 5.3](#). The spacing between each exposure was set to 3 mm, this was to ensure that the point of exposure of each line scan was not subject to any “preheating” effect from the previous exposure.

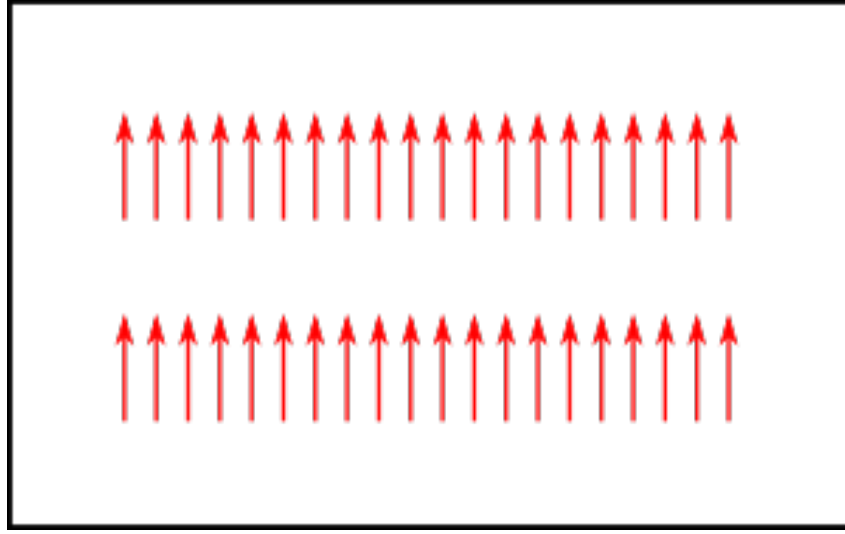


Figure 5.3: Schematic of Vector Layout of Single track Experiments

The laser parameters used in this experiment can be seen in [Tab. 5.1](#).

Table 5.1: Table showing the Laser Parameters used for Validation Experiments

Laser (W)	Power	Scanning Speed (mm/s)	Scanning Strategy	Track Length (mm)	Spot (μm)	Size
200		600	Single Track	10	50	

The cross section of the meltpools were then measured (as per the method described in [Sec. 5.1](#)) and compared to the results of the numerical experiment described in [Sec. 5.2.1](#).

5.1.2 Validation Experiment 2: Island Scan Experiment

The second validation experiment, referred to as the “Island Scan Experiment” or the “Meander Experiment” was performed in order to verify the numerical model’s ability to quantify the “preheating” that the substrate experiences due to the laser exposure of the previous scan vector. In this experiment four $10 \times 10 \text{ mm}^2$ areas (or islands) were exposed onto the surface of the substrate. They were distributed equidistant from the centre of the the coupon, as displayed in [Fig. 5.4](#). The meander strategy was used when scanning the islands. This is a scanning strategy in which the laser is not turned off in between each adjacent scan vector of each island. Instead a small scan vector is added to join the end of one 10 mm scan vector to the start of the next, as shown in [Fig. 5.5](#).

The laser parameters used in this experiment are described in [Tab. 5.2](#). As can be observed

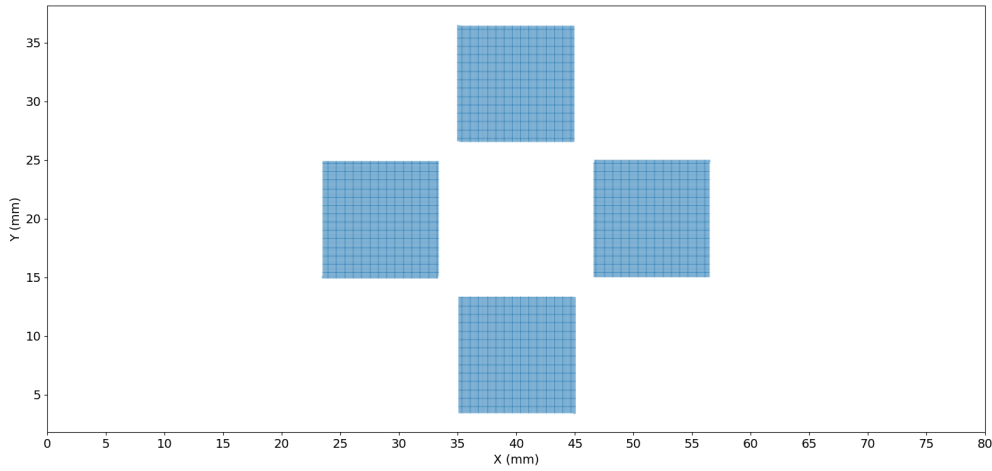


Figure 5.4: Schematic of Vector Layout of Meander Experiments

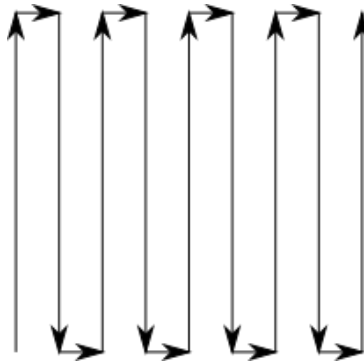


Figure 5.5: Schematic of Meander Scanning Strategy

in addition to the parameters used in the single track experiment, the “Hatch Distance” is also required. This parameter defines the distance between each of the long parallel tracks of the island.

Table 5.2: Table showing the Laser Parameters used for Validation Experiments

Laser Power (W)	Scanning Speed (mm/s)	Scanning Strategy	Hatch Distance (um)	Track Length (mm)	Spot Size (um)
200	850	Meander	100	10	70

The meltpool geometries were measured (as per the method described in [Sec. 5.1](#)) and compared to the numerical results of [Sec. 5.2.2](#).

5.1.3 Validation Experiment 3: Parameter Matrix Experiment

The third, and final, physical validation experiment performed was the “Parameter Matrix Experiment”. This experiment was performed in order to evaluate the accuracy of the numerical model when the processing mode transitions from conduction to keyhole mode. To this end, a series of laser parameters were selected varying both laser power and scanning speed to create a matrix of energy densities and processing modes. This way any limitation of the numerical model could be identified.

Each parameter was scanned as a single track, each was positioned the same was as described in [Sec. 5.1.1](#) [Fig. 5.3](#). The parameters selected for this experiment are shown in [Tab. 5.3](#).

The meltpool geometries were measured (as per the method described in [Sec. 5.1](#)) and compared to the numerical results of [Sec. 5.2.3](#).

5.2 Simulation Experiments

The method of discretization and solution, described in [Chapter 4](#), was implemented in C++/CUDA using the Nvidia CUDA Toolkit v10.7, on Windows 10 PC with a 9th Generation Core i7 CPU, 16GB RAM, and Nvidia RTX 2060 GPU. The properties of each cell were stored in three-dimensional 32-bit floating point arrays of length N , where N is the total number of elements. The arrays were arranged in ‘natural order’, where elements are listed in ascending order of i , then j , then lastly k . Element size was selected to be $50 \mu m^3$, this allowed for sufficient resolution for isotherm inference without exceeding the theoretical maximum value of 32-bit float of specific enthalpy values for each element. Each property stored in an independent array, one each for temperature, thermal resistivity, enthalpy, density. As heat flow is calculated using enthalpy, a system of conversion from enthalpy to temperature and *vice versa* is required. This is handled using look-up arrays, also 32 bit floating point. Due to the scales of magnitude of temperatures, the look-up array for temperature to enthalpy conversion contains per degree specific enthalpy values, thus the index value can be used to reference the correct en-

Table 5.3: Table showing the Parameters Matrix

Laser Power (W)	Scanning (mm/s)	Speed	Track Length (mm)	Spot Size (um)
40	100		10	50
40	500		10	50
40	900		10	50
40	1300		10	50
40	1700		10	50
90	100		10	50
90	500		10	50
90	900		10	50
90	1300		10	50
90	1700		10	50
140	100		10	50
140	500		10	50
140	900		10	50
140	1300		10	50
140	1700		10	50
190	100		10	50
190	500		10	50
190	900		10	50
190	1300		10	50
190	1700		10	50
240	100		10	50
240	500		10	50
240	900		10	50
240	1300		10	50
240	1700		10	50

thalpy value, decimals of degrees kelvin are handled through simple linear interpolation. However, due to the scales of magnitude of the enthalpy values it is not practical nor possible to store per Jkg^{-1} increments. Therefore, indexing is performed using $kJkg^{-1}$ increments, with linear interpolation being used for decimal values. A separate look-up array was used for each state of matter: solid, powder, gas; thus an integer array was required to track the state of each cell and must be updated at each time step. Melt pool location and dimension is inferred through bilinear interpolation of isothermal contours, i.e. any area of the volume where temperature exceeds the liquidus temperature of the alloy. Analysis of the output temperature array was performed using Python scripts developed with standard NumPy and Matplotlib packages.

The simulation experiments described in this section provide the full details of each simulation experiment performed. Values for the thermophysical properties of 316L Stainless Steel were taken from the extensive work performed by Kenneth Mills [185] and are summarised in [Tab. 5.4](#). The values marked with an asterisk are not quoted in the work of Kenneth Mills, these values are a linear extrapolation from the quoted data, but is a simulatory necessity. Due to the element size, the maximum theoretical enthalpy and temperature reached by the element at the centre of the beam far exceeds the maximum value of the standard arrays. Therefore, in order to prevent an indexing error this value must be included. [Tab. 5.5](#) shows the static thermophysical properties used.

It should be noted that whilst it is known that density will also vary with temperature, due to the method of measurement of the specific enthalpy (described in [Sec. 2.1.4.2](#)) the variation of density is embedded in the variation of this value. Also, if variation of density is taken into consideration, the variation in the coefficient of ΔH is minuscule. This is shown in [Fig. 5.6](#), which shows the value of the coefficient of ΔH versus temperature. The variation of density was calculated using the empirical relationship derived by Kenneth Mills [185], shown in [Eqn. 5.1](#). This shows that when density is varied with temperature, that if the mass of the cell is maintained, the increase in surface contact area between elements results in a variation of the value of ΔH per degree is less than 0.0004 below the

Table 5.4: Table of Temperature Variant Thermophysical Properties used in Simulation. Taken from [185].

T (K)	H (J/kg)	R (mK/W)
0	0	0.0513
297	136591	0.0513
374	173882	0.0469
473	221826	0.0435
574	277784	0.0413
673	331072	0.0402
775	387027	0.0375
871	445663	0.0360
974	504289	0.0347
1073	568264	0.0342
1174	629565	0.0328
1273	693540	0.0323
1371	762861	0.0330
1470	826835	0.0346
1570	898823	0.0332
1656	954803	0.0332
1721	1267302	0.0332
1772	1307302	0.0332
1872	1384636	0.0332
50273*	3887800*	0.0332*

Table 5.5: Table of Static Thermophysical Properties. Taken from [185].

T_l (K)	T_s (K)	$\rho(kg/m^3)$	η	c_{pp} (J/Kg)
1703	1645	7950	0.3	450

solidus temperature. Hence, for simplification, a constant value of density is sufficient.

$$\rho(T) = \begin{cases} 7950 - 0.501(T - 273) & T < T_{sol} \\ 6881 - 0.77(T - 1713) & T > T_{liq} \end{cases} \quad (5.1)$$

5.2.1 Single Track Simulation of Validation Experiment 1

For the single track simulation, it was decided for efficiency, that instead of simulating the entire coupon (Fig. 5.2) with 40 identical laser exposures, a single laser exposure would be sufficient to provide the meltpool geometry for comparison. Dimensions of the simulation domain were selected so that contribution to the meltpool geometry were negli-

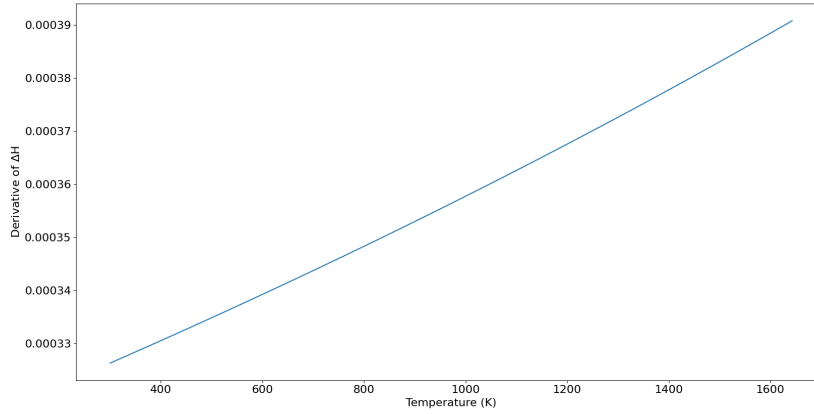


Figure 5.6: Plot of Derivative of Coefficient of ΔH With Respect to Temperature When Calculated Using Variable Density.

gible, whilst allowing the meltpool to reach steady state along the scan vector. Therefore, the dimensions of the simulated volume and the element dimensions used are given in [Tab. 5.6](#).

Table 5.6: Table of Simulation Domain and Element Dimensions for the Single Track Simulation

Dimension	Length (mm)
Domain X	4.00
Domain Y	25.00
Domain Z	6.25
Element X	0.05
Element Y	0.05
Element Z	0.05

Boundary conditions were set such that:

- Heat flux across the domain boundary at all domain boundaries except the top surface was zero.
- Heat flux across the domain boundary of the top surface was via radiation and convection only.

The simulation time-step was calculated using [Eqn. 4.31](#) and the properties given in [Tab. 5.4](#) and [5.5](#). Here h is the side length of the simulation elements, given in [Tab. 5.6](#). Thus, the calculated maximum simulation time-step is $4.95224 \times 10^{-5} s$. The laser param-

eters used in this simulation were selected to match that of the Single Track Experiment (Sec. 5.1.1), and are given in Tab. 5.1.

5.2.2 Island Scan Simulation of Validation Experiment 2

The island scan simulation, due to the total energy that would be transferred into the coupon by the laser, the entire coupon geometry was simulated. Therefore, the simulation volume matched that of the stainless steel coupons (Fig. 5.2), and the dimensions are given in Tab. 5.7.

Table 5.7: Table of Simulation Domain and Element Dimensions for the Island Scan Simulations

Dimension	Length (mm)
Domain X	80.00
Domain Y	40.00
Domain Z	5.00
Element X	0.05
Element Y	0.05
Element Z	0.05

Boundary conditions were the same as with Sec. 5.2.1: that:

- Heat flux across the domain boundary at all domain boundaries except the top surface was zero.
- Heat flux across the domain boundary of the top surface was via radiation and convection only.

The simulation time step was also calculated to be $4.95224 \times 10^{-5} s$, the same as Sec. 5.2.1. In order to match the laser parameters of Sec. 5.1.1 the laser parameters used were those listed in Tab. 5.2. The layout of the laser scan vectors was that given in Fig. 5.4, creating four $10 \times 10 \text{ mm}^2$ islands. The scanning order of each island is shown in Fig. 5.7.

The time of travel between the end of one island and the beginning of the next island was taken to be negligible.

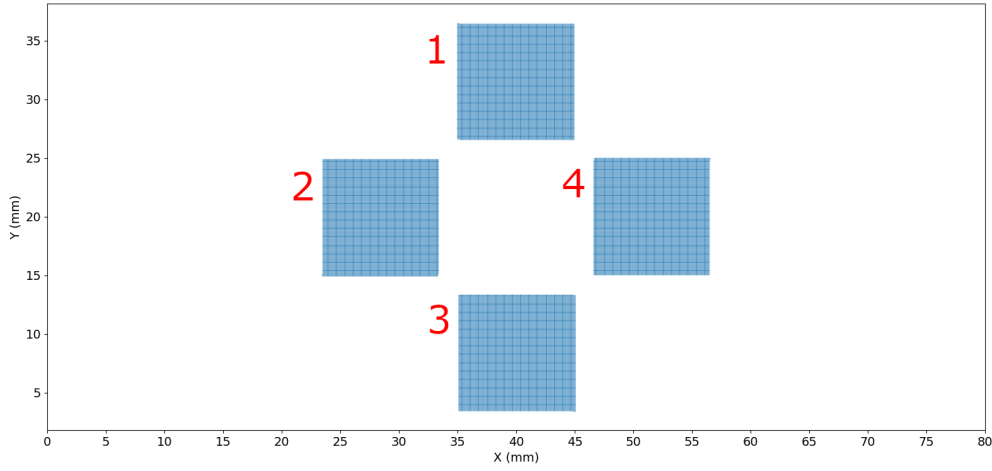


Figure 5.7: Schematic of Order of Island Scans

5.2.3 Parameter Matrix Simulation of Validation Experiment 3

The parameter matrix simulation performed was a repeat of the single track simulation (Sec. 5.2.1). However, in this simulation instead of the fixed single laser parameter set, the processing parameters simulated were varied to match the matrix parameters selected for Sec. 5.1.3 (shown in Tab. 5.3). The simulated volume for each track was the same as Tab. 5.6, similarly to avoid edge effects. The boundary conditions for the simulated domain also remained the same:

- Heat flux across the domain boundary at all domain boundaries except the top surface was zero.
- Heat flux across the domain boundary of the top surface was via radiation and convection only.

The simulation time step was also calculated to be $4.95224 \times 10^{-5} s$, the same as Sec. 5.2.1. The meltpool geometry of each simulation was compared to the corresponding track from the Parameter Matrix Experiment to analyze any limitation of the model with respect to predicting the processing mode of the laser parameter.

5.2.4 Coarsening Validation Simulation

In order to validate the method of coarsening from small elements to larger elements outlined in [Sec. 4.4.1](#), a repeat of the Single Track simulation ([Sec. 5.2.1](#)) was conducted. This repeat was the same in domain size, boundary conditions, and laser parameters. However, the top five layers of elements were “fully-fine” size of $50\mu m$, and the remaining layers were of “coarsened” size of $250\mu m$. The dimensional details are given in [Tab. 5.8](#).

Table 5.8: Table of Simulation Domain and Element Dimensions for the Fully Fine with Coarsening Simulation with Laser Heat Input

Dimension	Length (mm)
Domain X	4.00
Domain Y	25.00
Domain Z	6.25
Fine Element X	0.05
Fine Element Y	0.05
Fine Element Z	0.05
Hybrid Element X	0.25
Hybrid Element Y	0.25
Hybrid Element Z	0.25

Boundary conditions were set such that:

- Heat flux across the domain boundary at all domain boundaries except the top surface was zero.
- Heat flux across the domain boundary of the top surface was via radiation and convection only.

The simulation time step was also calculated to be $4.95224 \times 10^{-5} s$, the same as [Sec. 5.2.1](#).

5.2.5 Multiple Layer Simulation

5.2.6 Hybrid Element Thermophysical Property Simulation

In order to explore the methodology set out in [Sec. 4.4](#), a series of simulations were conducted to compare the equivalency of the hybrid elements to the same simulation conditions without any hybrid coarsening. To this end, it was decided to select a “unit

cell” to be used as a repeated hybrid element. The geometry selected for the unit cell must be representative of the realistic build geometry, whilst demonstrating the ability to overcome the pitfall of the traditional method for calculating the thermal conductivity of complex volumes also described in [Sec. 4.4](#). Thus, the selected geometry can be seen in [Fig. 5.8a, b, and c](#). Here, the solid areas are displayed as solid grey, and powder is represented as the dotted areas.

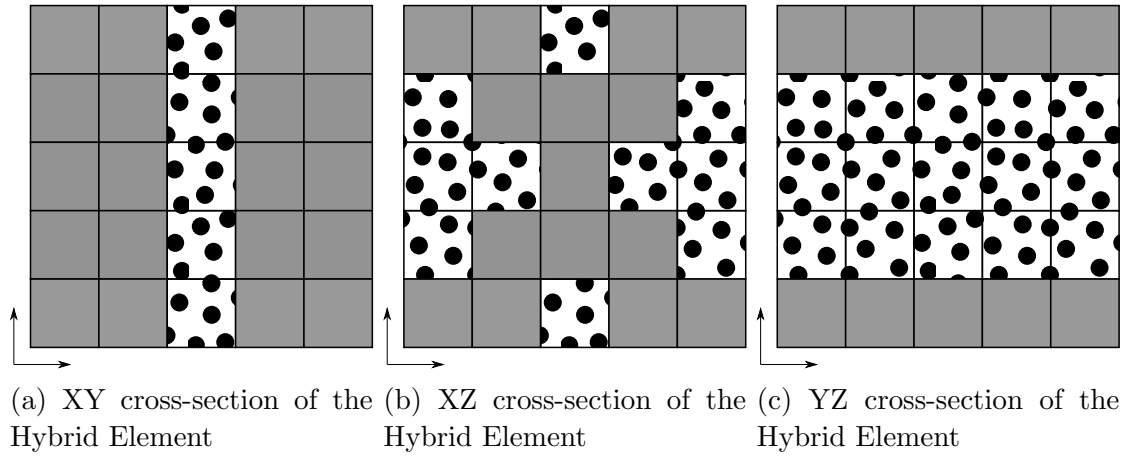


Figure 5.8: Cross Sections of the Hybrid Elements

As can be seen from the schematic cross-sections of the unit cell, there is a clear path for heat flow from the top YZ surface to the bottom YZ surface. However, if the thermal resistance of the powder-filled areas (as shown by the dotted areas) were to tend to infinite (perfect insulators) the conventional method for calculation of the equivalent thermal resistivity of the hybrid volume would tend to zero.

In order to ascertain the equivalent thermal conductivity of the unit cell hybrid element, a simulation was conducted to generate the Resistivity versus Temperature curve for the Z direction. The simulation domain used in this case was that of a single unit cell, consisting of $5 \times 5 \times 5$ elements. The dimensions are summarized in [Tab. 5.9](#).

The simulation time step was also calculated to be $4.95224 \times 10^{-5} s$, the same as [Sec. 5.2.1](#).

Boundary conditions for the volume were as follows:

- Heat flux across the domain boundary at all domain boundaries was zero.
- The temperature of the top surface was maintained at T_h .

Table 5.9: Table of Simulation Domain and Element Dimensions for the Calculation of the Thermal Resistivity of the Hybrid Elements

Dimension	Length (mm)
Domain X	0.25
Domain Y	0.25
Domain Z	0.25
Element X	0.05
Element Y	0.05
Element Z	0.05

- The temperature of the bottom surface was maintained at T_l .

In this simulation, a fixed temperature gradient was applied along the Z axis of the unit cell ($T_h - T_l = 400$). The gradient was maintained for 200,000 simulation time steps to ensure that steady state is achieved. once steady state was achieved, the mean heat flux in the XY plane was taken at all internal element boundaries, and the mean temperature of each internal element (T_m) was taken, both of these values were used to calculate the equivalent thermal conductivity of the volume (as per Eqn. 4.40) and the corresponding α value was also obtained (as per Eqn. 4.42). The direction of heat flow is shown in Fig. 5.9.

This process was repeated for a range of T_m from 300 K to the solidus temperature of

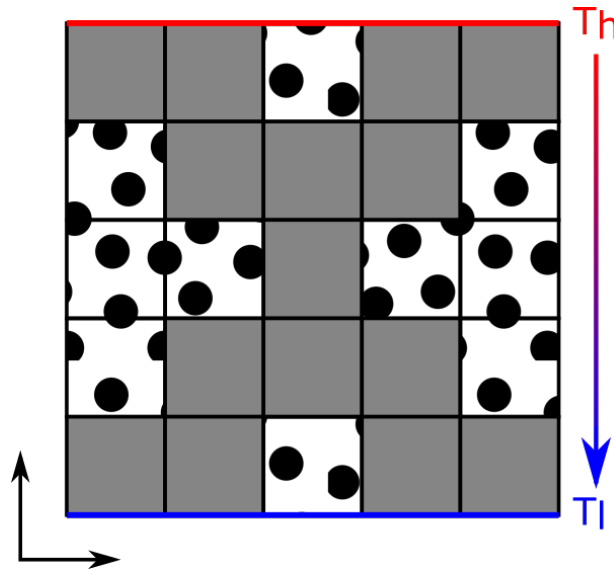


Figure 5.9: Schematic of the Simulation Setup for Calculating the Thermal Conductivity of the Hybrid Element Unit Cell

the material. This curve of thermal conductivity versus temperature was then used to inform the behavior of the hybrid elements in subsequent simulations.

5.2.7 Hybrid Element Volume Simulation

The intent of this simulation experiment was to quantify and evaluate the performance of the Hybrid Elements from [Sec. 5.2.6](#) when used to represent a larger volume. To this end, a simulation of much larger domain size was simulated in which each element of the domain was a single hybrid element unit cell. The conductivity versus temperature curve used for each element was the curve calculated in [Sec. 5.2.6](#). The domain and element sizes for this simulation are given in [Tab. 5.10](#).

Table 5.10: Table of Simulation Domain and Element Dimensions for the Hybrid Element Volume Simulation

Dimension	Length (mm)
Domain X	6.25
Domain Y	6.25
Domain Z	6.25
Element X	0.25
Element Y	0.25
Element Z	0.25

As the intent of this simulation was to evaluate only the performance of the Hybrid Elements alone, a laser heat source was not incorporated into the simulation. Instead, the top layer of elements of the domain was set to an elevated temperature ($T_h = 1000$ K) and the diffusion of the heat through the domain was evaluated. Boundary conditions were as follows:

- Heat flux across the domain boundary at all domain boundaries was zero.

The simulation was run for a total of 1 s of simulated time (20,193 simulated time steps). A representative diagram of the simulated domain is shown in [Fig. 5.10](#), due to the true domain being $25 \times 25 \times 25$ elements in size, for simplicity and clarity a 5×5 representation is provided.

Here, the solid black line show the element boundaries, solid grey represents solid metal, and the dotted regions represent those filled with powder. In order to evaluate the performance of the hybrid elements, a “high fidelity”, “fully-fine” simulation was performed. The details of this simulation are presented in [Sec. 5.2.8](#), below.

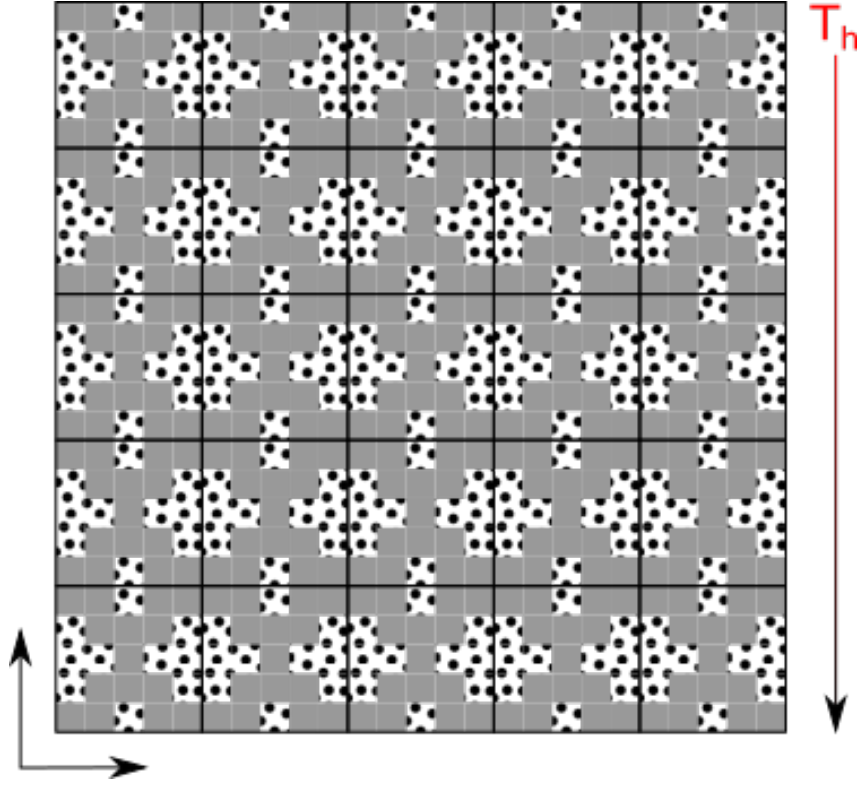


Figure 5.10: Representative Diagram of the Simulation Setup for Evaluating the Conductive Performance of the Hybrid Elements in a Large Volume.

5.2.8 Fully Fine Unit Cell Volume Simulation

The purpose of this simulation was to provide a high fidelity baseline for the coarsened volume of [Sec. 5.2.7](#). To this end, the domain, boundary conditions, and initial conditions were exactly the same as [Sec. 5.2.7](#). The difference, being that instead of using a coarsened $25 \times 25 \times 25$ element volume, this simulation used a 100×100 element volume. Each element consisting of a single material; solid metal or powder. [Tab. 5.11](#) gives details of the domain and element dimensions.

Table 5.11: Table of Simulation Domain and Element Dimensions for the Fully Fine, Unit Cell Volume Simulation

Dimension	Length (mm)
Domain X	6.25
Domain Y	6.25
Domain Z	6.25
Element X	0.05
Element Y	0.05
Element Z	0.05

A representative diagram of the simulated domain is shown in [Fig. 5.10](#), due to the true

domain being $100 \times 100 \times 100$ elements in size, for simplicity and clarity a 25×25 representation is provided.

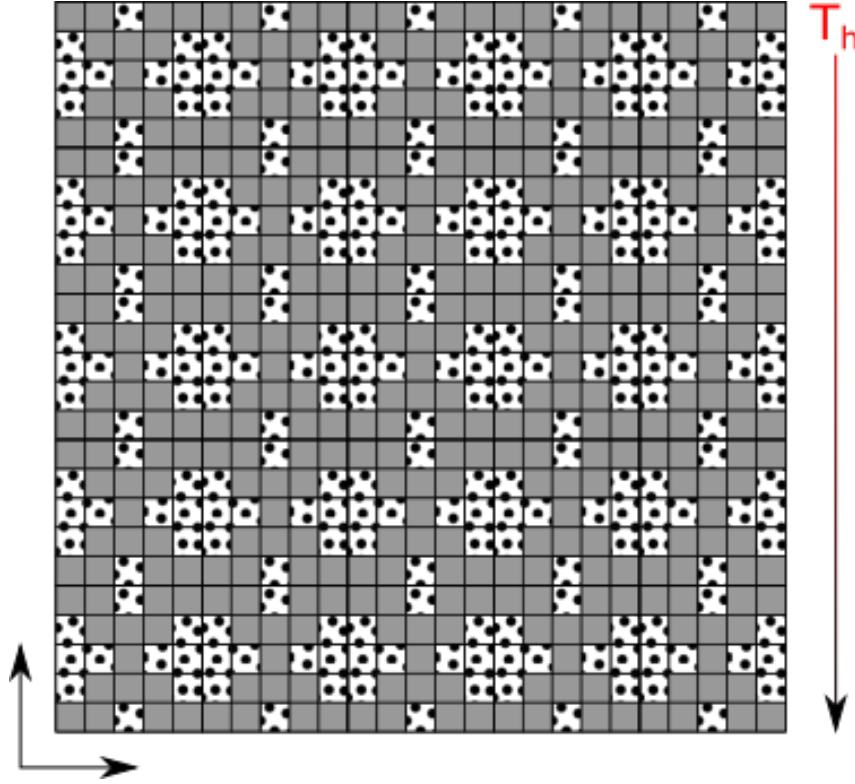


Figure 5.11: Representative Diagram of the Simulation Setup for Evaluating the Conductive Performance of the Hybrid Elements in a Large Volume.

Here, the solid black line show the element boundaries, solid grey represents solid metal, and the dotted regions represent those filled with powder. Comparison to [Fig. 5.10](#), shows the smaller element size of single material.

5.2.9 Single Track with Hybrid Element Coarsening Simulation

In order to test the performance of the hybrid elements in a simulation with realistic laser heat input, it was decided to perform a single track simulation, like that performed in [Sec. 5.2.1](#). However, in a real application, the laser exposure would not be directly onto the hybrid elements. Therefore, a number of the “fully-fine” elements would be placed on top of the layers of hybrid elements, which would receive the laser exposure. A representative diagram of the arrangement of fully fine and hybrid elements is shown in [Fig. 5.12](#). In the simulation performed, five layers of fully-fine elements were placed on

top of 24 layers of hybrid elements.

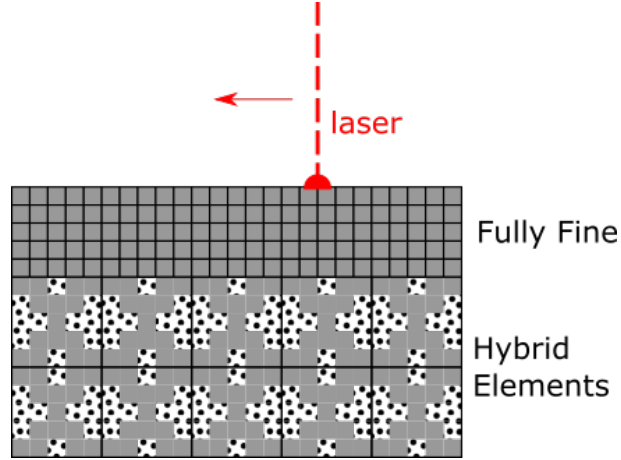


Figure 5.12: Representative Diagram of the Simulation Setup for Evaluating the Conductive Performance of the Hybrid Elements with Fully Fine Elements, and Laser Exposure.

The full domain volume and element sizes are shown in [Tab. 5.12](#). As the properties of the fully fine elements would be the most inhibiting to the largest stable simulation time step, this is what was used for calculation of the simulation time-step. The time-step was calculated to be $4.95224 \times 10^{-5} s$. As would be expected when using the same element and material properties as [Sec. 5.2.1](#) and [5.2.2](#).

Table 5.12: Table of Simulation Domain and Element Dimensions for the Fully Fine and Hybrid Element Coarsened Simulation with Laser Heat Input

Dimension	Length (mm)
Domain X	4.00
Domain Y	25.00
Domain Z	6.25
Fine Element X	0.05
Fine Element Y	0.05
Fine Element Z	0.05
Hybrid Element X	0.25
Hybrid Element Y	0.25
Hybrid Element Z	0.25

For consistency, the laser parameters used were the same as [Sec. 5.1.1](#), and are given in [Tab. 5.1](#). Boundary conditions were also kept the same. As described in [Sec. 4.4.1](#), the heat flow across the fully fine to coarsened boundary is handled explicitly. In order to quantify the impact that coarsening with hybrid elements had on the moltpool geometry an equivalent “fully-fine” simulation was performed ([Sec. 5.2.10](#)) for comparison.

5.2.10 Single Track without Hybrid Element Coarsening Simulation

The intent of this simulation was to provide an uncoarsened baseline for comparison of [Sec. 4.4.1](#). Therefore, arrangement of solid metal and powder within the domain, boundary conditions, laser parameters, and simulation time step were all maintained from [Sec. 4.4.1](#). [Tab. 5.13](#) shows the domain and element dimensions used in this simulation.

Table 5.13: Table of Simulation Domain and Element Dimensions for the Uncoarsened Simulation with Laser Heat Input

Dimension	Length (mm)
Domain X	4.00
Domain Y	25.00
Domain Z	6.25
Fine Element X	0.05
Fine Element Y	0.05
Fine Element Z	0.05

Chapter 6

Heat Flow Simulation of Laser Powder Bed Fusion and Validation

The results and analysis found within this chapter covers the measured meltpool geometries from numerous Physical Experiments and Numerical Simulations. The list below shows the Physical Experiments and Numerical Simulations that are covered herein, along with references to the corresponding method descriptions in Chap. 5.

1. Single Track Experiment, Sec. 5.1.1;
2. Island Scan Experiment, Sec. 5.1.2;
3. Parameter Matrix Experiment, Sec. 5.1.3;
4. Single Track Simulation, Sec. 5.2.1;
5. Island Scan Simulation, Sec. 5.2.2;
6. Parameter Matrix Simulation, Sec. 5.2.3;
7. Multilayer Simulation, Sec. 5.2.5.

6.1 Results

6.1.1 Single Track Experiment Results

An optical micrograph of one of the forty meltpools generated during the single track experiment can be seen in [Fig. 6.1](#). The laser parameters used for this experiment can be found in [Tab. 5.1](#).

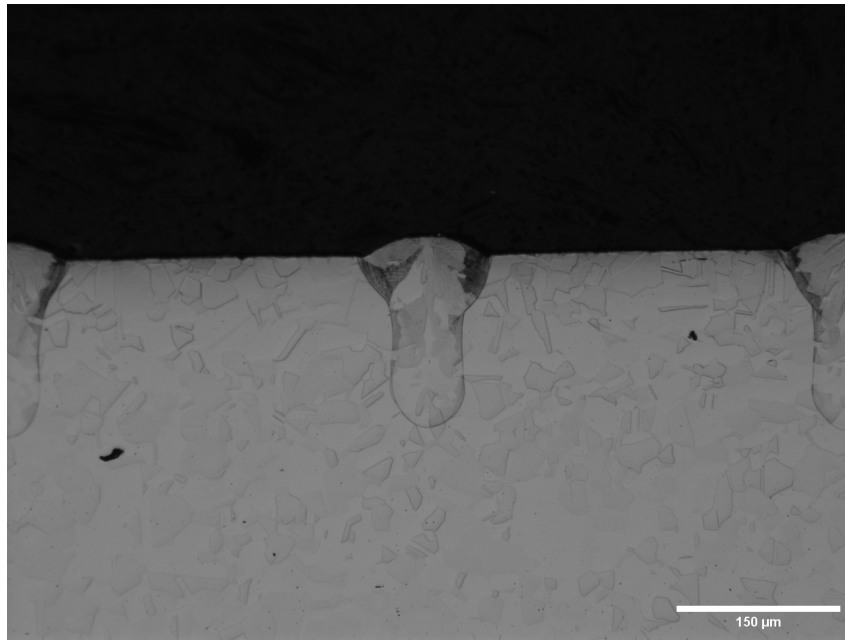


Figure 6.1: Optical Micrograph Showing Cross-section of the Single Track Meltpool.

Boxplots of the measured widths and depths are shown in [Fig. 6.2](#). The error associated with these measurements is believed to be $\pm 1\mu m$. The aspect ratio of the measured widths and depths shows that the selected parameter meets the criteria for being in the transition to keyhole processing mode. It is also possible to see from [Fig. 6.1](#) the change from the equiaxed grain structure of the substrate to the directional grain structure within the meltpool, as is expected in LPBF material.

6.1.2 Single Track Simulation Results

Temperature heat-map results from the single track simulations ([Sec. 5.2.1](#)) can be seen in [Fig. 6.3](#). Meltpool geometry was inferred through bilinear interpolation of the solidus and liquidus isotherms, and are marked in black.

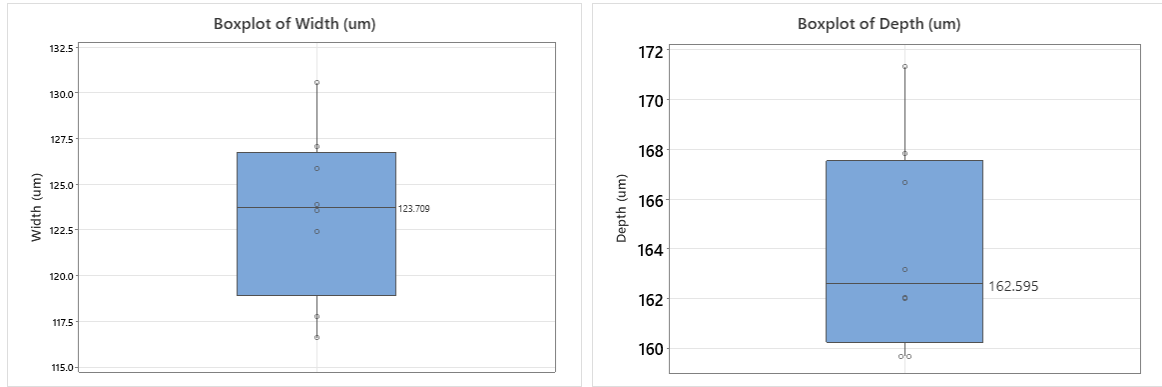


Figure 6.2: Boxplots of Meltpool Dimensions of Single Track Samples (a) Width (b) Depth

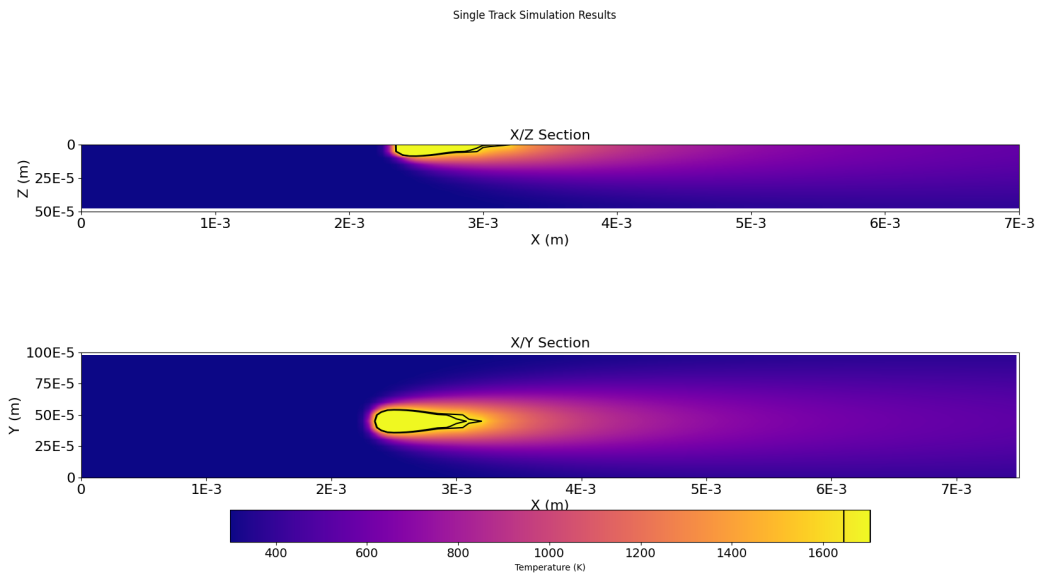


Figure 6.3: Single Track Simulation Heat-Map Results with Solidus and Liquidus Isotherms Marked.

The measurements of the inferred meltpool are shown in [Tab. 6.1](#). These measurements are believed to have an accuracy of $\pm 1\mu m$.

Table 6.1: Table of Meltpool Measurements from the Single Track Simulation

Width (μm)	Depth (μm)
159	85

The computational resources required for the single track simulation can be seen in [Tab. 6.2](#). The total simulated time was 0.025 ms, and the time taken was 60 s. Hence, the ratio of simulated time per element per time step to computational time per element per time step is 1:2400.

Table 6.2: Table of Computational Resources Used by the Single Track Simulation

CPU (%)	Usage	CPU RAM Us- age	GPU (%)	Usage	GPU Ram Us- age	Time Taken (s)
33%		504 MB	100		1.0 GB	60

6.1.3 Island Scan Experiment Results

An optical micrograph of a section through the island scan can be seen in Fig. 6.4. The laser parameters can be found in Tab. 5.2. Boxplots of the measured widths and

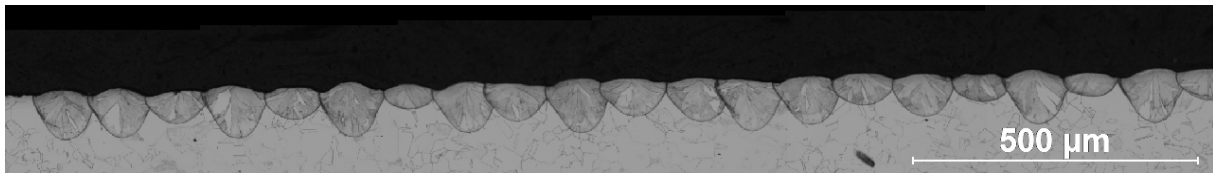


Figure 6.4: Optical Micrograph Showing the Cross-section of the Meander Track Meltpool.

depths are shown in Fig. 6.5. The error associated with these measurements is believed to be $\pm 1\mu m$. The aspect ratio of the measured widths and depths shows that the selected parameter results in conduction mode processing. This was consistent between all island scans.

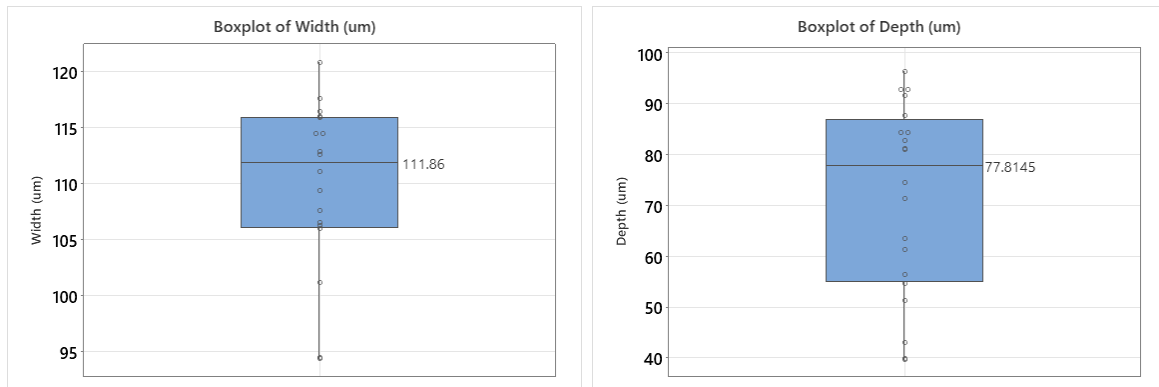


Figure 6.5: Boxplots of Meltpool Dimensions of Meander Track Samples (a) Width (b) Depth

6.1.4 Island Scan Simulation Results

Temperature heat-map results from the island scan simulations (Sec. 5.2.2) can be seen in Fig. 6.6. Melt pool geometry was inferred through bilinear interpolation of the solidus and liquidus isotherms, and are marked in black. The measurements of the in-

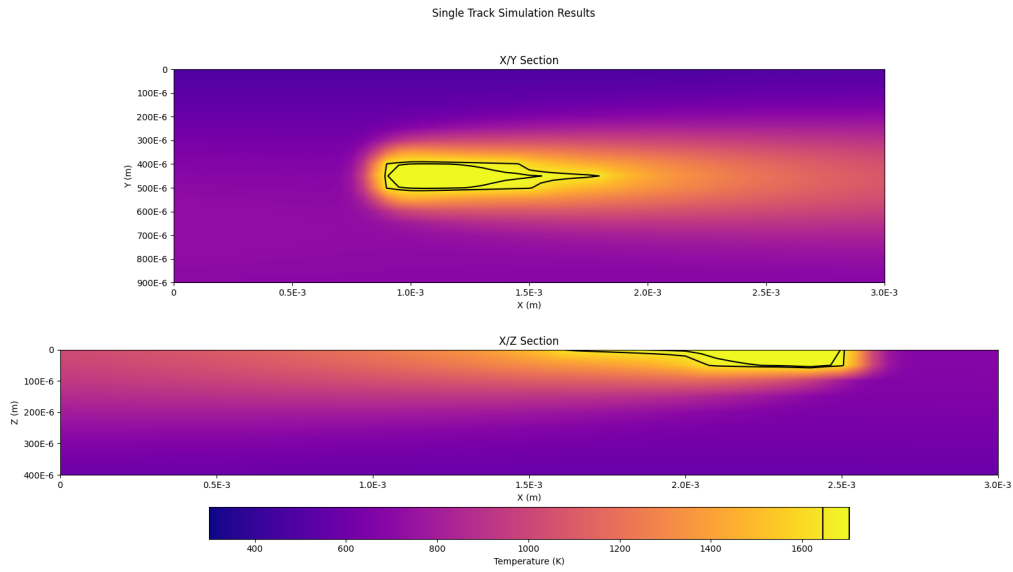


Figure 6.6: Island Scan Simulation Results

ferred melt pools are shown in [Tab. 6.3](#). These measurements are believed to have an accuracy of $\pm 1\mu m$.

Table 6.3: Table of Melt pool Measurements from the Island Scan Simulation

Width (um)	Depth (um)
103	54

The computational resources required for the single track simulation can be seen in [Tab. 6.4](#). The total simulated time was 3.92217408 s, and the time taken was 29607 s. Hence, the ratio of simulated time per element per time step to computational time per element per time step is 1:7549. The ratio of discrete elements of the Island Scan simulation to the Single Track simulation is approximately 26:1; and the ratio of simulation time-taken per element is approximately 6:1.

Table 6.4: Table of Computational Resources Used by the Simulation Methods

CPU Usage (%)	CPU RAM Usage	GPU Usage (%)	GPU Ram Usage	Time Taken (s)
34%	3 GB	100	1.5 GB	29607

6.1.5 Parameter Matrix Experiment Results

The measured meltpool geometries for each parameter listed in [Sec. 5.1.3](#) are shown in [Tab. 6.5](#). Surface plots of the measured widths and depths of the meltpools vs the scanning speed and laser power used are shown in [Fig. 6.7](#). Examples of each of the processing modes are shown in [Fig. 6.8](#), which are all taken from the micrographs collected from the matrix parameters.

Table 6.5: Table of Measurements of Matrix Parameters

Power (W)	Scanning (mm/s)	Speed	Width (um)	Depth (um)
40	100		103	31
40	500		59	20
40	900		52	15
40	1300		47	14
40	1700		39	7
90	100		212	176
90	500		84	43
90	900		63	22
90	1300		55	18
90	1700		52	14
140	100		276	325
140	500		129	108
140	900		89	55
140	1300		71	34
140	1700		62	21
190	100		317	450
190	500		146	161
190	900		108	79
190	1300		82	53
190	1700		79	40
240	100		314	649
240	500		160	240
240	900		113	109
240	1300		88	70
240	1700		90	54

6.1.6 Parameter Matrix Simulation Results

The measured meltpool geometries for each of the parameters listed in [Tab. 5.3](#) are shown in [Tab. 6.6](#). The error in these measurements is believed to be $\pm 3\mu m$. Surface

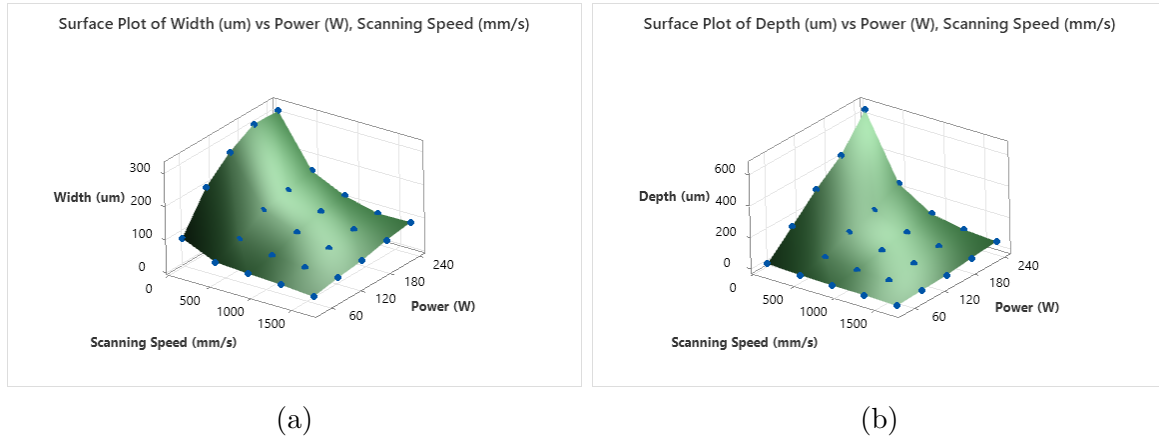


Figure 6.7: Surface Plots of Width and Depth of the Matrix Parameters (a) Width (b) Depth

plots of the measured widths and depths of the melt pools vs the scanning speed and laser power used are shown in [Fig. 6.7](#).

6.1.7 Coarsened Fully Fine Simulation Results

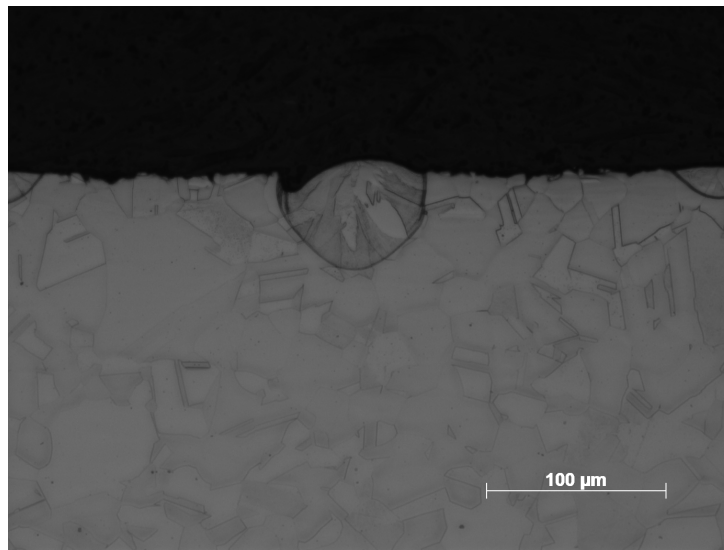
The melt pool prediction for the coarsened simulation is shown in [Fig. 6.10](#). The measured melt pool dimensions are shown in [Table 6.7](#). As previously stated in [Sec. 6.1.1](#), the error associated with these measurements is $\pm 3 \mu m$. The computational resources utilised by this simulation are shown in [Table 6.8](#).

6.1.8 Multilayer Simulation Results

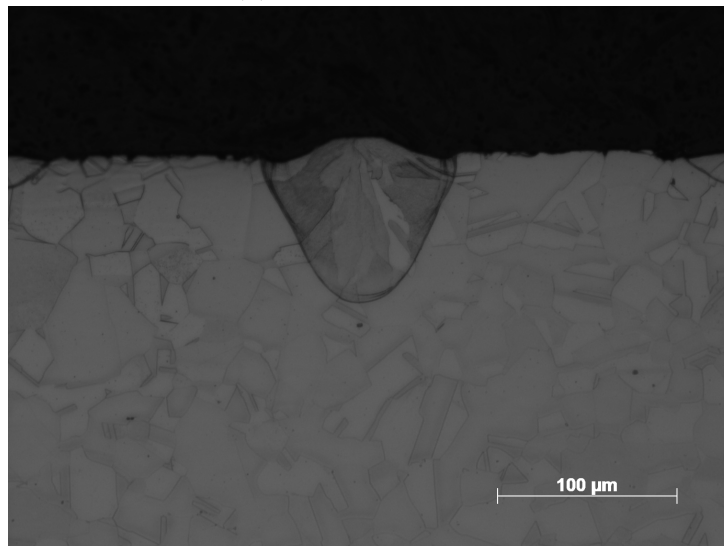
6.2 Discussion

6.2.1 Computational Resources

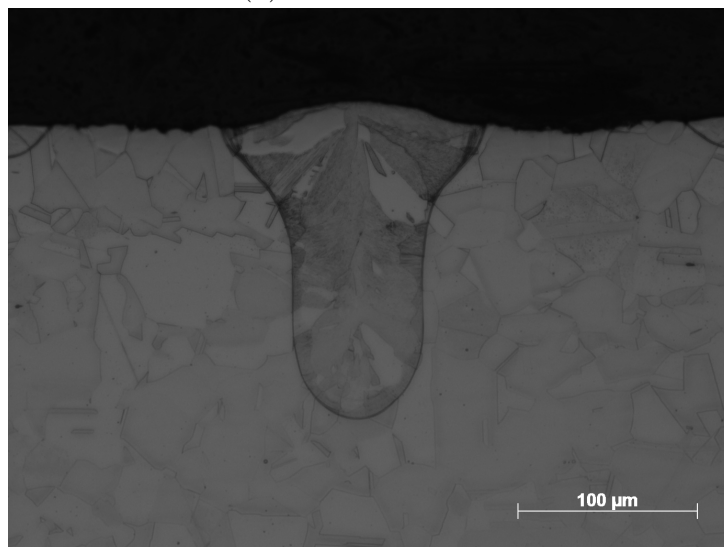
In the case of the meander simulation, Liu *et al.* displayed the use of adaptive mesh coarsening on macroscale simulation [186]. The first test case used in the reported simulation experiment utilised a twin Intel® Xeon® Gold 6150 CPU with clock speed 2.7GHz. The use of a CPU simulation implies that the computation was handled serially, with minor parallelisation via multithreading. The volume simulated was a single layer of 142 scan vectors on a $20 \times 40 \times 3 \text{ mm}^3$ volume. The adaptive meshing strategy resulted



(a) Conduction Mode



(b) Transition Mode



(c) Keyhole Mode

Figure 6.8: Micrographs Showing Examples of the Observed Processing Modes

Table 6.6: Table of Numerical Results for Matrix Parameters

Sorted Power (W)	Scanning (mm/s)	Speed	Simulated (μm)	Width	Simulated (μm)	Depth
40	100		66		33	
40	500		34		22	
40	900		25		19	
40	1300		26		17	
40	1700		25		10	
90	100		253		117	
90	500		87		49	
90	900		60		24	
90	1300		49		20	
90	1700		50		18	
140	100		316		158	
140	500		176		88	
140	900		95		58	
140	1300		68		36	
140	1700		57		22	
190	100		376		170	
190	500		155		94	
190	900		116		55	
190	1300		79		52	
190	1700		77		41	
240	100		479		216	
240	500		218		93	
240	900		130		60	
240	1300		89		67	
240	1700		91		53	

Table 6.7: Table of Simulation Measurements of Coarsened Volume

Strategy	Width (μm)	Depth (μm)
Single Track with Coarsening	168	78

in a total simulation time of 8 hours. In comparison the meander simulation presented in [Sec. 5.2.2](#), the volume Liu *et al.* utilised was over eight times smaller by volume, and consisted of fewer than a sixth of the vectors by number (1.6 times fewer by length). However, as shown in [Sec. 6.2](#), the time of this simulation without any coarsening was 8.25 hours. This clearly shows the power of parallelisation through use of the use of the GPU can be. If GPU parallelisation and meshing techniques can be used in tandem then the viability of close-to-real-time simulation can be recognised.

It should be noted that this simulation was performed in an Nvidia RTX 2060 GPU.

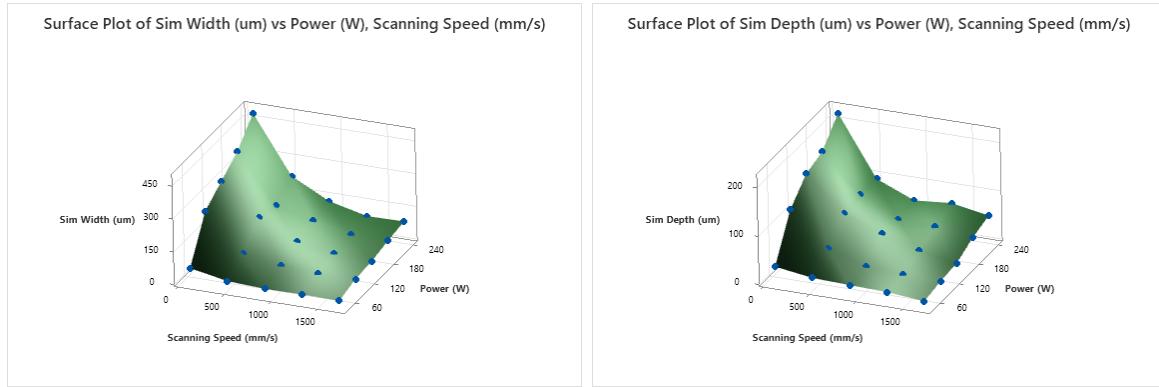


Figure 6.9: Surface Plots of Width and Depth of the Simulated Matrix Parameters (a) Width (b) Depth. For Comparison to the Simulation Results See [Fig. 6.13](#) and [6.14](#).

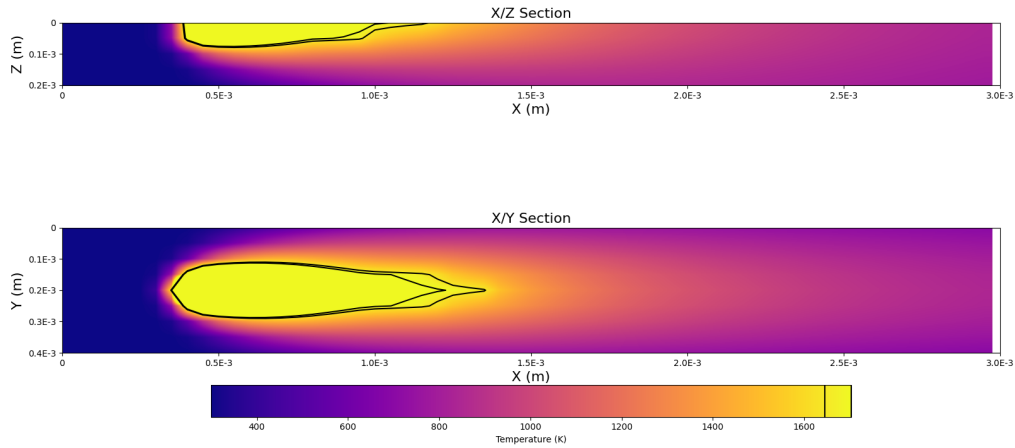


Figure 6.10: Coarsened Simulation Results

Since this point, the RTX line of GPUs have undergone two generational advancements. The current flagship RTX GPUs (the 40 series) are stated to benchmark at 83 TFLOPS versus the RTX 2060's 7 TFLOPS [164]. It is natural to observe that the continued drive of GPUs will passively increase the speed of parallelised simulation methods.

Table 6.8: Table of Computational Resources Used by the Coarsened Simulation

Simulation Type	CPU Usage (%)	CPU RAM Usage	GPU Usage (%)	GPU Ram Usage	Time Taken (s)
Coarsened	8%	392 MB	100	1.0 GB	4

6.2.2 Comparison of Simulation and Physical Results

The comparison of the simulation results and the optical micrograph results are shown in Fig. 6.11, and it can be seen that the simulated results fall within the measured ranges of the optical micrographs. Whilst the simulation results are within range, they

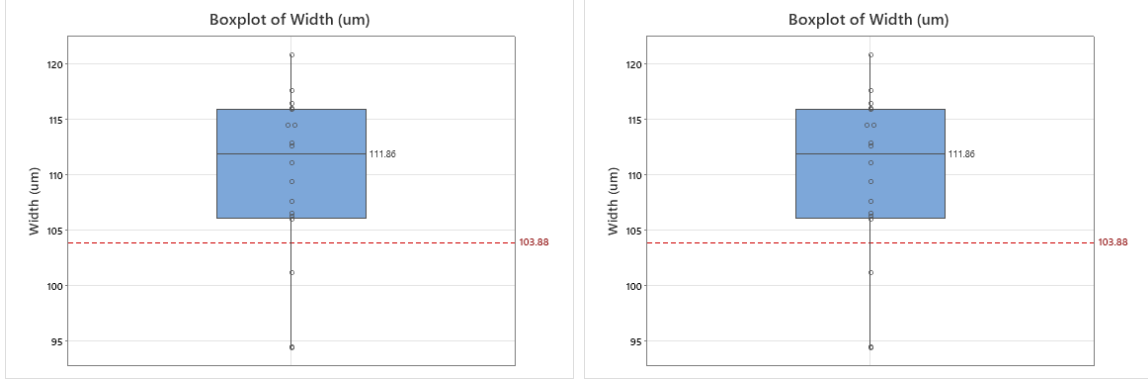


Figure 6.11: Boxplots of Meander Melt pool Geometries with Reference Lines of the Simulation Results for Comparison (a) Width (b) Depth

are consistently lower for both the width and depth. The reasons for this discrepancy are believed to be due to uncertainty of the representation of the heat source rather than a failing of the calculation of heat flow.

There have been few experiments to measure the in situ absorptivity of metals and their powders when irradiated by a laser [24, 41, 187], and it has been shown that absorptivity varies due to numerous effects. The temperature of the irradiated surface, the roughness and oxidation state of the irradiated surface, the degree of melting and fluid flow, and the gas flow within the chamber all have an effect. Trapp and Matthews *et al.* show that the laser parameters affect the measured absorptivity of an irradiated surface, and hypothesise that this is in part due to the degree of melting [24, 187]. As the irradiated material melts, low melting point temperature elements are vaporised causing recoil pressure at the liquid surface. This can cause the liquid surface to bow inwards creating a concave liquid surface that can cause rays of the laser to be reflected into the substrate, increasing the ratio of absorbed photons. As energy density increases, the greater the amount of vaporisation, the greater the concavity of the liquid surface, which continues to increase the observed absorptivity. This phenomenon is most commonly associated with keyhole mode processing, however Bitharas *et al.* show through schlieren imaging, that this gas

cavity begins to form long before keyhole mode is reached [188]. Thus, the absorptivity used for these simulations may not remain constant as assumed by the simulation, and may be a contributing factor to the discrepancy of the simulation results to the measured meltpool geometries. It is possible to incorporate a temperature dependent absorptivity value into the simulation, however no robust source can be found, similar to the published tables of thermophysical properties from Kenneth Mills [185], to generate this curve for use. Also, due to the dependence displayed by the absorptivity on the processing parameters, one would need to know the thermal effects of the parameters to predict the absorptivity, which in then be used to predict the thermal effects of the parameters. This would form a cyclical problem. Therefore, a fixed, representative, empirical, estimate would be preferred; as was done here.

The role of the gas flow is not incorporated into the simulation, but cannot be ignored when interpreting the results of the physical experiments. A further effect of the vapourisation from the molten meltpool was observed by Bidare *et al.* [27]. It was shown that when exposed to the laser, the meltpool produces a “plume” of vapour. This plasma can interact with the laser by “shielding” the substrate from the laser exposure reducing the effective absorptivity of the substrate. The plasma plume generated is highly dependent on the laser parameters used for exposure, and is shown to vary in stability [27, 29, 188]. This may account for some of the variation observed in the physical measurements, and may provide a general shift in the measurements of the physical samples.

Another source of potential error comes from the assumed spot size used in the simulation. The open architecture rig used for the physical experiments [184] utilises only a single z-axis actuator for the control of the substrate height/working distance for the laser. The distance is also checked through an analogue height gauge, which typically have an error of approximately $20\ \mu m$. Thus, the spot size may vary from coupon to coupon as they are manually removed and installed, due to a change in working distance.

The comparison of the single track simulation results to the measured meltpool geometries is shown in [Fig. 6.12](#), and can be seen that the simulated geometries vary greatly from the measured meltpools. In order to elucidate, one must refer back to the micrograph of

the sectioned coupon given in Fig. 6.1. The example of given, shows that the aspect ratio of the melt pool is greater than those shown in Fig. 6.4, and show the distinctive shape of transition/keyhole mode processing [84].

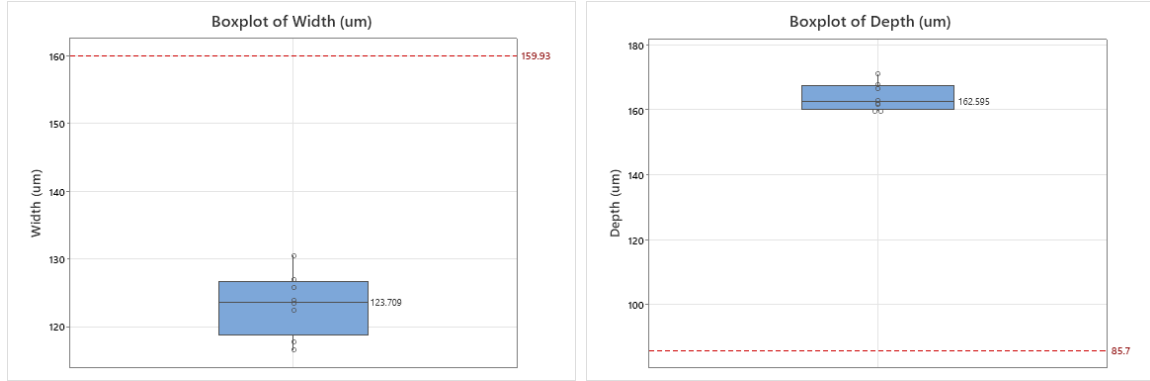


Figure 6.12: Boxplots of Single Track Melt pool Geometries with Reference Lines of the Simulation Results for Comparison (a) Width (b) Depth

These results imply that the volumetric heat source used for simulation of non-conduction mode processing are not sufficient. In order to corroborate this the results of the matrix of parameters should be consulted, as the distribution of laser powers and scanning speeds should show a variety of all three processing modes. As can be observed in Fig. 6.8, conduction mode is identified by the semicircular shape, and aspect ratio less than 0.8; transition mode is identified by its almost triangular shape, with aspect ration between 0.8 and 1.25; and keyhole mode is identified by the characteristic, elongated melt pool shape and large aspect ratio.

Table 6.9 shows the difference of between each simulation result and the corresponding optical micrograph measurement result. A comparison of the simulated melt pool measurements to the optical micrographs are shown in Appendix C. The error associated with the melt pool measurements is estimated to be approximately $\pm 1\mu m$. Comparison of these values and the estimated error associated with both the physical measurement and measurement of the simulate melt pools show that the simulated melt pool values are in excellent agreement with the physical experiments when the observed processing mode is conduction mode. These values are also summarised in Fig. 6.13 and 6.14, from these figures it can be inferred that the simplified heat source representation used in the simulation is appropriate for conduction mode melt pool prediction, but breaks down when

the process parameters result in keyhole mode processing. As touched on earlier, this is due to the fluid flow and plasma production of the irradiated meltpool. As plasma is produced, a recoil pressure acts on the surface of the molten metal, and causes the surface to dip inwards. If sufficient plasma is produced, the meltpool takes on the characteristic keyhole shape shown in Fig. 2.10. This results in a central cavity that allows repeated reflection of incident photons, effectively trapping them and considerably increasing the ration of absorbed energy of the laser beam. Hence, the increased effective absorptivity measured by Trapp *et al.* [24]. It is evident that in the case of keyhole mode processing, the simulation must use an alternative volumetric heat source scheme in order to increase the accuracy of meltpool prediction. An alternative method for heat source modelling was proposed by Ross *et al.* as an extension of the Goldrak triple ellipsoid [189]. However, the values used for the absorptivity, ellipse radius, and ratio of front to rear radius was calibrated first via experimental result, rather than be calculated or derived from first principles. Therefore, would reduce its use in a predictive setting for new materials etc. in an industrial context without first performing DOEs which would then negate the need for a predictive model.

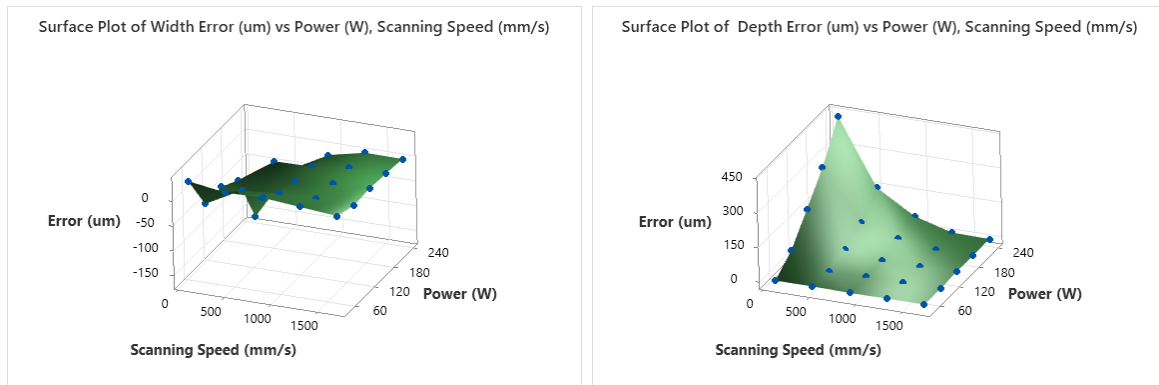


Figure 6.13: Surface Plots Showing the Difference Between Simulated and Measured Geometries (a) Width (b) Depth

Philo *et al.* proposed an alternate approach to volumetric heat source modelling for keyhole mode, extending the work of Gusarov *et al.*, in which the laser intensity profile transferred into the powderbed and substrate was based on the sum of directed, reflected, and scattered radiation [190, 191]. This approach showed excellent performance in prediction of meltpool morphology in both conduction and keyhole mode processing. Thus,

Table 6.9: Table Showing the Error in Simulation Results Compared to the Observed Processing Mode

Power (W)	Scanning Speed (mm/s)	Width (um)	Error	Depth (um)	Error	Processing Mode
40	100	37		-1		Conduction
40	500	26		-1		Conduction
40	900	27		-4		Conduction
40	1300	21		-3		Conduction
40	1700	14		-2		Conduction
90	100	-42		59		Keyhole
90	500	-2		-6		Transition
90	900	3		-2		Conduction
90	1300	6		-3		Conduction
90	1700	2		-4		Conduction
140	100	-40		168		Keyhole
140	500	-47		20		Keyhole
140	900	-6		-3		Transition
140	1300	3		-2		Conduction
140	1700	5		0		Conduction
190	100	-59		279		Keyhole
190	500	-9		68		Keyhole
190	900	-8		24		Transition
190	1300	3		2		Conduction
190	1700	3		-2		Conduction
240	100	-165		433		Keyhole
240	500	-57		147		Keyhole
240	900	-17		49		Transition
240	1300	-1		3		Transition
240	1700	-1		1		Conduction

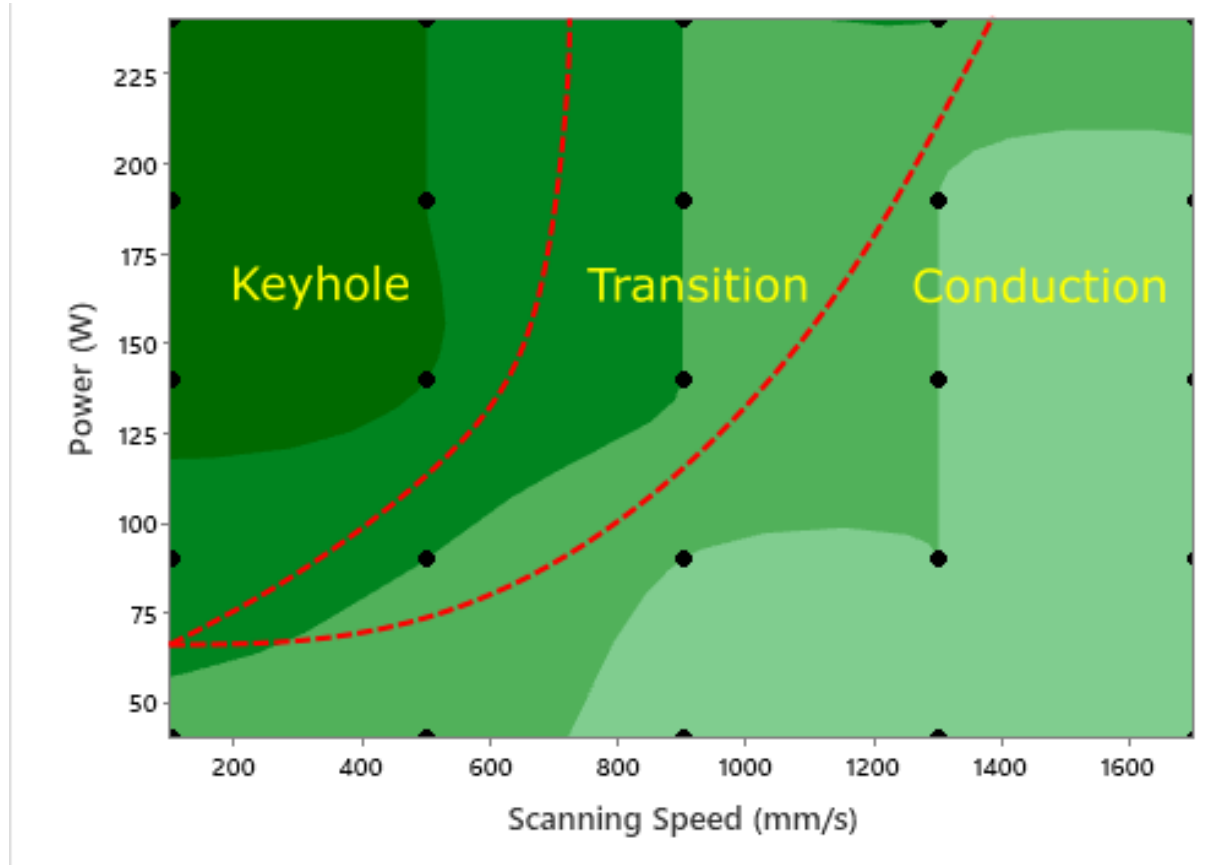


Figure 6.14: Contour Plot Showing the observed Processing Mode vs the Laser Power and Scanning Speed.

conduction only thermal solvers are limited only by the pedigree of the thermophysical data, and the accuracy of the heat input representation. As discussed in [Sec. 2.1.2.5](#), the concentrations of trace elements such as phosphorous and sulphur can have a massive effects on the fluid flow in the meltpool [61]. Therefore, a conduction-only volumetric heat source would require a way to represent the hydrodynamics through variation of the other properties. Philo *et al.* emphasize the importance on powder layer thickness, and beam width on the threshold at which conduction to keyhole mode occurs [191], something that was not accounted for in the previous work of King *et al.* and Hann *et al.* [78, 192]. It is believed that this more adaptive volumetric heat source should be more suitable for the high resolution regions of any coarsened simulations, but it can be shown that the method of solution is suitable for investigation of the thermal flow within the part.

6.3 Conclusions

The validation experiments described here, and the resulting analysis have shown that the use of GPU parallelisation to accelerate thermal flow simulation results in a reduction in computational time comparable to that reported by Liu *et al.* without any specialist coarsening techniques [186]. If these techniques were to be used in tandem then the goal of real-time simulation becomes realisable in the near future. Liu *et al.* claim that the adaptive meshing scheme that they propose resulted in a speed up of factor seven, if the same speed up can be achieved with a GPU simulation, then this would result in a simulation whose ratio of simulated time to real time is 9.275×10^{-4} . However, it is easy to surmise that if this adaptive meshing scheme was implemented in a CPU, like the coupled heat flow simulation, that it could not also somewhat benefit from GPU acceleration in some way. Thus, further pushing the ratio of simulated time to real time, closer to unity. This is also complimented in the continuous development and advancements made in GPU technology [164]. As throughput of the GPU cards climbs ever higher, such large computational tasks that were previously limited to cluster sized data centers, are then able to be performed by desktop workstations, and eventually on the production machines themselves.

It is also shown, that the method implemented to predict the heat flow through the volume using a “conduction only” scheme was sufficient in predicting the meltpool geometries of parameters that result in conduction mode processing. The simulation design implemented here, was limited only by the representation of the volumetric heat source as processing transitioned into keyhole mode. This is due to various changes in laser/metal interaction resulting in the assumed value of absorptivity, and the effective geometry of the heat source no longer being valid. A more sophisticated method, such as that proposed by Philo *et al.* should be adopted in order to maintain simulation integrity in these higher energy density processing regimes [191]. This approach uses the absorptivity of the material to predict the laser penetration into the powderbed and the flat surface. This circumvents the need to continually adapt values of the absorptivity of the powder and solid based on the processing mode.

Finally, through comparison of the computational resources and predicted meltpool geometries of the fully fine simulation and coarsened simulation, shows that the computational time can be reduced by over 90% whilst producing results error of less than 10%. This does not circumvent the inaccuracy caused by the oversimplification of the heat source representation in non-conduction processing modes.

Chapter 7

A Hybrid Meshing Strategy for Finite Volume Methods

As with all numerical solvers for matrix problems, the scaling of finite methods is proportional to the number of elements or nodes [180]. Therefore, a method of reducing the computational time required for simulation is to reduce the number of elements that define the volume. This, intuitively, means that element size must be increased. However, to increase the dimensions of all elements uniformly in the volume would reduce the information that can be inferred from the results, i.e. [Chapter 2](#) discusses the resolution of simulation methods that each thermophysical and metallurgical phenomena requires and if the element size is increased beyond this then this information is unable to be inferred. Finite element methods are able to produce greater detail of conditions within the element than the resolution allows by utilizing higher order nodes within the element [181]. However, by increasing the number of nodes within an element, the number of calculations per element is increased. Thus, the exponential convergence is undermined by the increase in computational load. A natural progression of this element-based approach then requires the element size to be gradated, from fine elements in the regions of interest to coarse elements in the very bulk of the part. This then requires a strategy that either naturally, or explicitly handles the transition from fine to coarse elements. Current methods of mesh coarsening for finite volume solvers are limited to coarsening elements that are

of the same material status, i.e. powder elements must be coarsened with other powder elements; and solid elements must be coarsened with other solid elements. This limits the maximum coarsening that can be performed. Extreme examples of this limitation are lattice structures [182] due to their thin sections and complex geometry that effectively prevent mesh coarsening due to the constant transition of the build volume from solid to powder. Therefore, a novel method of element coarsening is proposed that allows for hybrid powder/solid elements to overcome this limitation.

The numerical method proposed is outlined and discussed in [Sec. 4.4](#). The chapter herein will present the results of:

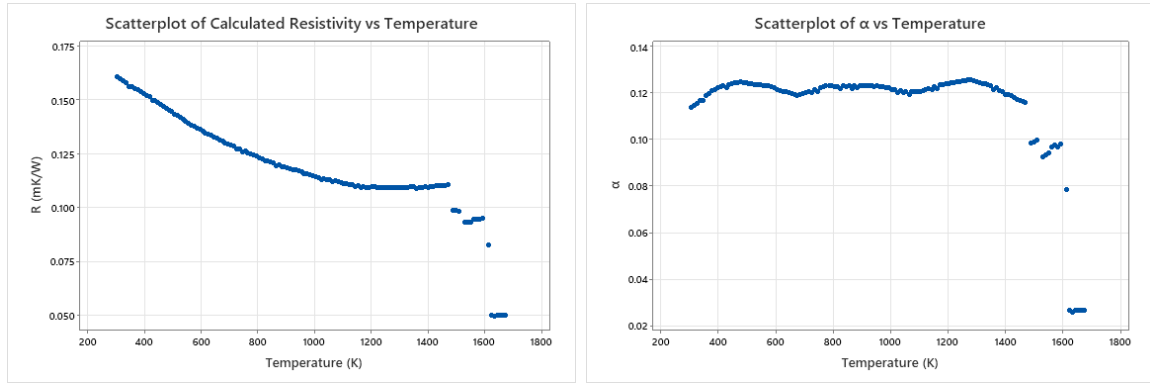
1. Hybrid Element Thermophysical Property Simulation, [Sec. 5.2.6](#);
2. Hybrid Element Volume Simulation, [Sec. 5.2.7](#);
3. Fully Fine Unit Cell Volume Simulation, [Sec. 5.2.8](#);
4. Single Track with Hybrid Element Coarsening Simulation, [Sec. 5.2.9](#);
5. Single Track without Hybrid Element Coarsening Simulation, [Sec. 5.2.10](#)

7.1 Results

7.1.1 Properties of Hybrid Elements Results

The curve of resistivity versus temperature that was calculated for the hybrid volume, and the corresponding values of α , are shown in [Fig. 7.1](#). It can be seen that the calculated values of R and α follow the expected trends, but break down at high temperatures. The calculated resistivity curve was the one was used for the hybrid elements used in the coarsened volume. The temperatures used in the volume simulation are lower than the temperatures at which the curve appears to break down. The computational load required by the generation of the resistivity curve are given in [Tab. 7.1](#).

The time taken referred to in [Tab. 7.1](#) corresponds to 125 individual simulations. This



(a) Generated Resistivity versus Temperature Curve (b) Generated Alpha value versus Temperature

Figure 7.1: Calculated Properties of the Hybrid Solid/Powder Elements

Table 7.1: Table of Computational Resources Used by Resistivity Curve Generation

CPU (%)	Usage	CPU RAM Us- age (MB)	GPU (%)	Usage	GPU RAM Us- age (MB)	Time Taken (s)
7		405	100		100	4238

means, that the mean time per simulation is 33.90 seconds. The factors that govern this time are investigated and discussed in [Sec. 7.2.2](#).

7.1.2 Hybrid Element Simulation Results

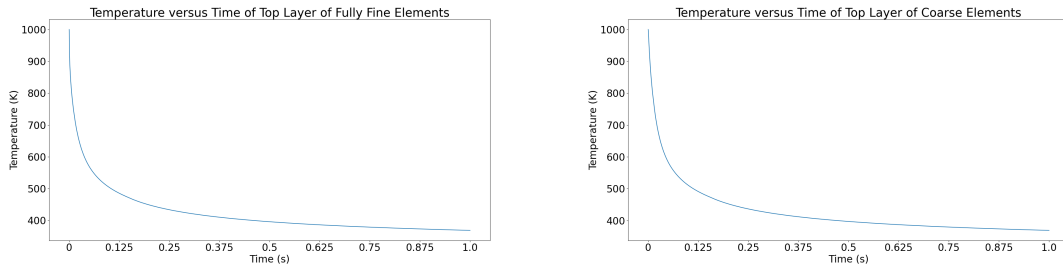
The temperature profiles for the top and bottom layers of both the fully fine and coarsened volumes is shown in [Fig. 7.2](#). The behaviour of the hybrid volume is in keeping with the expected behaviour, and comparable to the fully fine fine simulation established as a benchmark in [Chap. 6](#).

The computational load consumed by the simulation of the fully fine and hybrid volumes are shown in [Tab. 7.2](#).

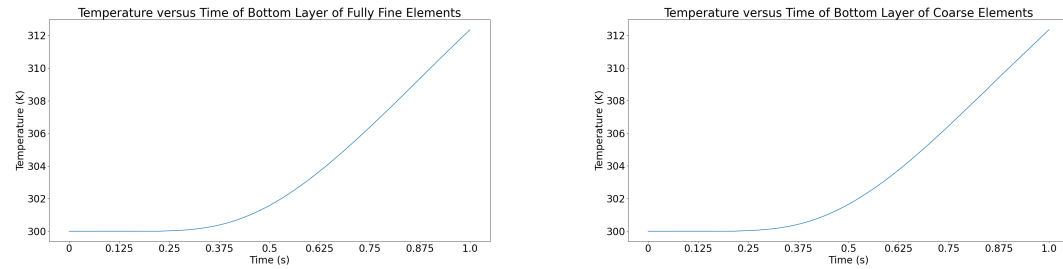
Table 7.2: Table of Computation Resources Required by Each Type of Simulation

Simulation Type	CPU Usage (%)	CPU RAM Usage (MB)	GPU Usage (%)	GPU RAM Usage (MB)	Time Taken (s)
Fully Fine	7	423	32	800	177.86
Hybrid	7	402	32	101	4.08

The times given for the fully fine and hybrid element simulations correspond 1 second of simulation time representing 5.622×10^{-3} and 0.245 seconds of real time respectively.



(a) Temperature Profile versus Time of Top Layer of Fully Fine Volume (b) Temperature Profile versus Time of Top Layer of Coarse Volume



(c) Temperature Profile versus Time of Bottom Layer of Fully Fine Volume (d) Temperature Profile versus Time of Bottom Layer of Coarse Volume

Figure 7.2: Temperature Profiles of Select Parts of Both Fully Fine and Coarse Simulation Volumes

This is a speed up of approximately 44 times.

7.1.3 Coarsening with Hybrid Elements

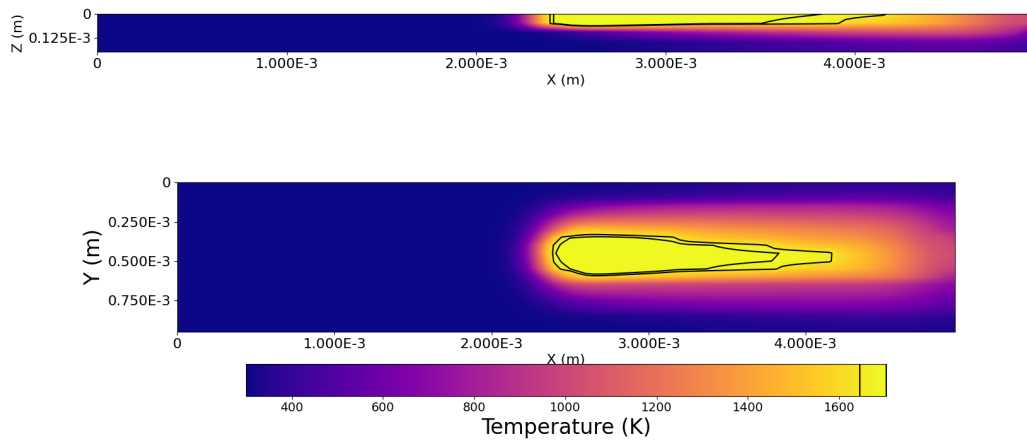
The resultant meltpool predictions for both simulations can be seen in [Fig. 7.3](#). Here, it can be seen that due to the asymmetry of solid and powder distribution either side of the point of laser irradiation of the top surface, the resultant meltpool is also asymmetric. The asymmetry of the powder and solid means that heat flow away from the point of laser irradiation is non-uniform, thus the asymmetry of the predicted meltpool is expected.

The measurements for each meltpool can be seen in [Table 7.3](#) below.

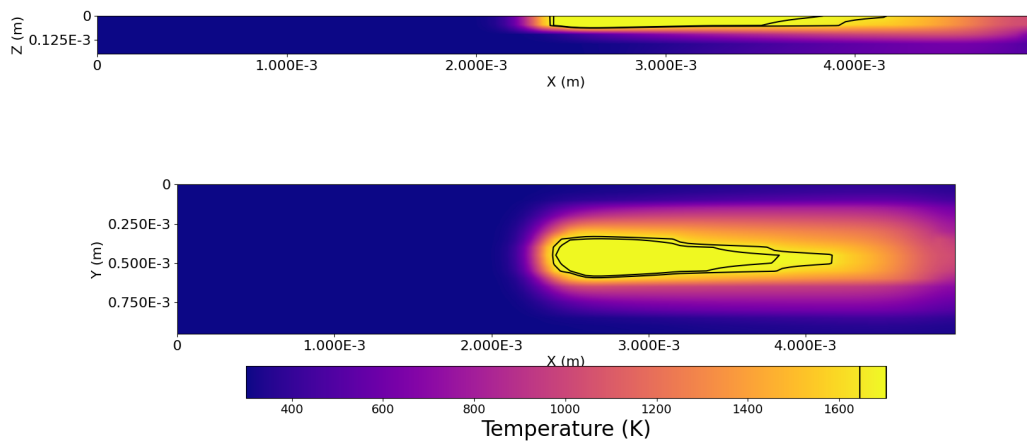
Table 7.3: Table of Meltpool Measurements and Simulation Time of Fully Fine and Coarsened Simulations

Simulation	Width (μm)	Depth (μm)	Simulation Time (s)
Fully Fine	231	58	3.01
Coarsened	230	57	0.58

Fully Fine Single Track Simulation Results



(a) Predicted Meltpool for Fully Fine Simulation
Coarsened Single Track Simulation Results



(b) Predicted Meltpool for Simulation Coarsened with Hybrid Elements

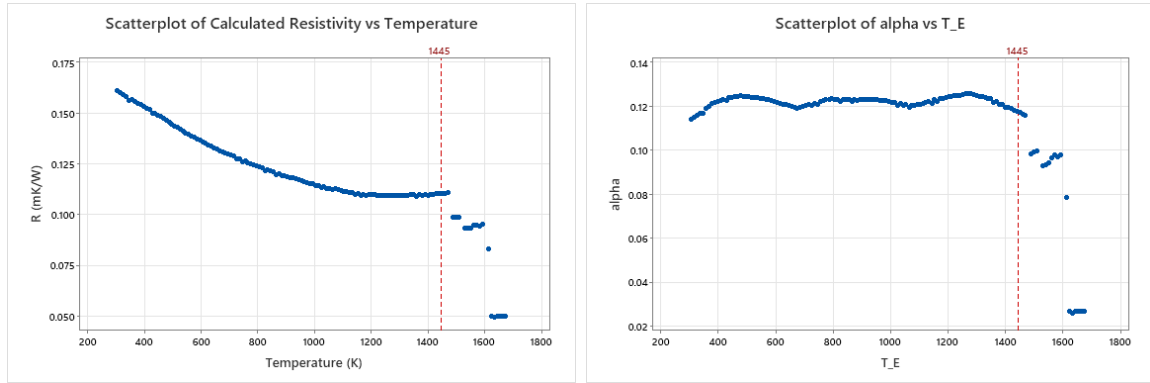
Figure 7.3: Predicted Meltpools for Fully Fine and Hybrid Element Coarsened Simulations

7.2 Discussion

7.2.1 Generation of Resistivity Curve

It was noted in [Sec. 7.2.1](#) that [Fig. 7.1 \(a\)](#) shows that at the higher temperatures of the simulation the generation of the resistivity curve appears to break down. In order to explain this breakdown, the construction of the resistivity simulation must be examined. In order to generate the resistivity for a certain temperature, a thermal gradient of 400 K is applied across the $5 \times 5 \times 5$ element volume. This gradient is created by taking the desired temperature and increasing one side by 200 degrees, and reducing the other side by 200 degrees. As the higher temperatures of the scale are reached this creates the possibility that at steady state the elements of the raised temperature side have met the melting temperature of the material. This then produces the break down in the method as shown by the results. This would suggest that the valid range of these results is below the solidus temperature of the material, minus half the fixed thermal gradient between the two sides (which in this case is 200 K). [Fig. 7.4](#) shows the temperature limit of the simulation for the 316L stainless steel properties used. However, this temperature limitation on the calculation can easily be overcome when the use case is considered in its context. Hybrid elements are used when the mesh requires to be coarsened. It is well established that mesh coarsening is only suitable for regions of the simulation volume that are at a reasonable distance from the region of interest [186]. This region of interest is commonly the position of laser incidence, as the maximum resolution is required there. The temperatures of these regions of the build volume should not approach the temperature of the resistivity curve breakdown.

Comparing [Tab. 7.1](#) and [7.2](#) one can note that the time taken to generate the resistivity versus temperature curve takes more time to calculate than even the fully fine simulation. It should also be recalled that the resistivity curve is dependent on the distribution of powder and solid in the volume. Thus, depending on coarsening strategy, a curve would need to be calculated for each different hybrid volume. This would far exceed the time for a fully fine simulation.



(a) Generated Resistivity versus Temperature Curve (b) Generated Alpha value versus Temperature

Figure 7.4: Calculated Properties of the Hybrid Solid/Powder Elements with Reference Temperature Marked

Alternatively, as the distribution of powder and solid is geometry dependent, these could be computed prior to simulation. Then the values would be used as look-up tables to save time. An alternate approach to reduce time would be based on the inspection of [Fig. 7.1 \(b\)](#). If the values of α that were calculated at temperatures greater than the breakdown at 1445 K are assumed to be outliers, the value of α has a very small distribution about a median value of 0.121921. This can be seen in the boxplot of α of [Fig. 7.5](#).

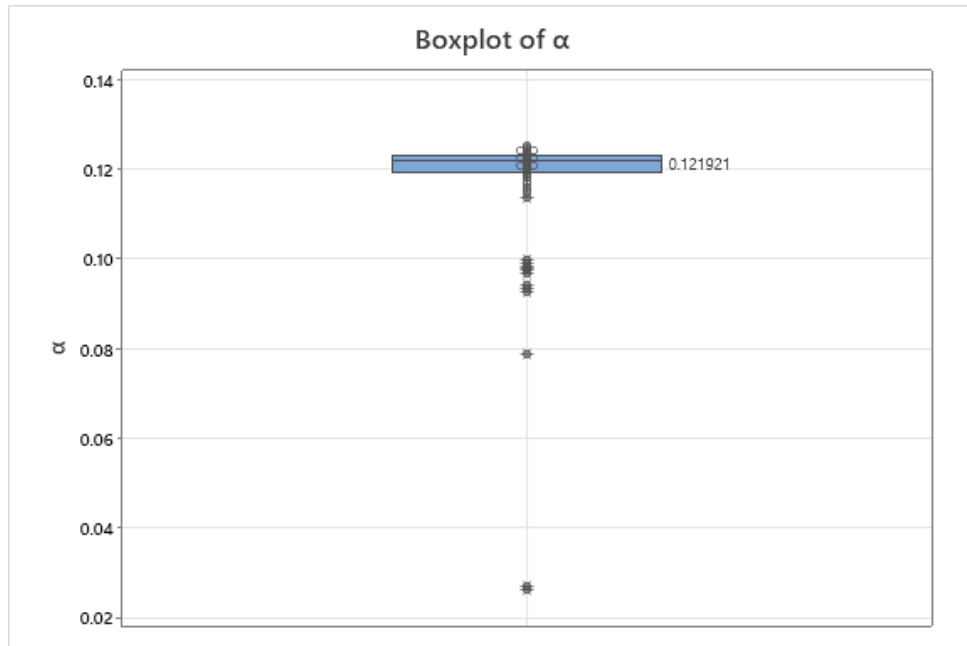


Figure 7.5: Boxplot Showing the Distribution of α Values

If α appears to be near constant in the valid region, this could then present a suitable

method to circumvent the lengthy simulation time. A single value of α or a reduced sample set can be calculated, and α could then be used to generate the entire resistivity versus temperature curve. Fig. 7.6 shows the comparison of three resistivity curves:

1. R_E - the resistivity curve calculated from the simulations;
2. R_A - the resistivity curve calculated from the median α value;
3. R_A_single - the resistivity curve calculated from a single α value calculated from an arbitrary temperature (500 K).

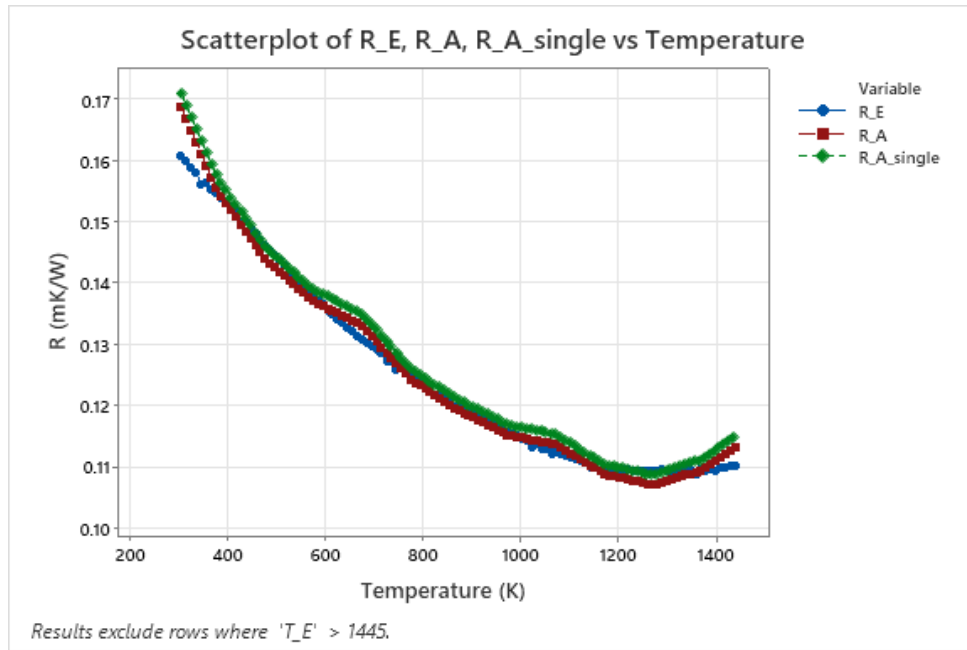


Figure 7.6: Scatterplot Comparing the Calculated Resistivity Curves

Here it can be seen that a reduced set, or even a single value of α , can produce a resistivity versus temperature curve that is comparable to the calculated resistivity curve generated by the full range of simulations. This can further reduce the time taken to coarsen elements as only one steady state simulation need be performed in order to obtain the full resistivity curve. This method of reducing generation of the resistivity curve through calculation of a single α value is limited by assuming a constant relationship between

R_{solid} and R_{powder} . Consider Eqn. 4.41, if differentiated with respect to temperature:

$$\begin{aligned}\frac{\partial}{\partial T} R_{equiv} &= \frac{\partial}{\partial T} ((1 + \alpha) R_{solid} + R_{powder}) \\ &= -\alpha \frac{\partial R_{solid}}{\partial T} - R_{solid} \frac{\partial \alpha}{\partial T} + \alpha \frac{\partial R_{powder}}{\partial T} + R_{powder} \frac{\partial \alpha}{\partial T} \\ &= (R_{powder} - R_{solid}) \frac{\partial \alpha}{\partial T} + \alpha \left(\frac{\partial R_{powder}}{\partial T} - \frac{\partial R_{solid}}{\partial T} \right).\end{aligned}\tag{7.1}$$

Here, if the resistivity of the powder is taken to be a multiple of the resistivity of the powder, then the value of α is temperature independent. As α depends purely on the powder distribution within the hybrid element, relative to the thermal gradient, and the powder packing density. Neither of which vary with temperature. Thus, if $\partial\alpha/\partial T = 0$ and $R_{powder} = kR_{solid}$:

$$\begin{aligned}\frac{\partial R_{equiv}}{\partial T} &= \alpha \left(k \frac{\partial R_{solid}}{\partial T} - \frac{\partial R_{solid}}{\partial T} \right) \\ &= \alpha(k - 1) \frac{\partial R_{solid}}{\partial T}\end{aligned}\tag{7.2}$$

some literature suggests that the resistivity of the powder is closer related to the gaseous environment of the build chamber than the properties of the solid [25]. If this is to be believed then the value of α cannot be assumed to be constant as the relationship between the resistivity of the solid and powder phases will vary depending on temperature. However, the work of Chin *et al.* only explored the relationship between the conductivity and temperature to a maximum temperature of 473 K, much below the operating temperature range that would be experienced by the powder bed during LPBF [25]. Also, the gaseous environment used in their experiments was not representative of the gaseous environment used in commercial LPBF machines [30]. At temperatures greater than 473 K the surface contact area between powder particles can increase due to partial sintering, thus the gaseous transport between particles may no longer be the dominant mechanism. Also, as discussed in Sec. 2.1.2.2, the gaseous flow in LPBF machines varies wildly from machine to machine. Therefore, simulation methods must be tailored to the gaseous flow of each machine for true accuracy. This then means that simulation method cannot ever

be machine agnostic. Thus, using a fixed relationship between R_{solid} and R_{powder} is machine agnostic, reduces the amount of calculation that is required per hybrid element, and produces sufficient results in the final simulation. These, three principles are the key to realising an industrially relevant simulation tool for the LPBF industry.

A further reduction of calculation time can be implemented though dynamic testing of simulation steady state. Currently, the steady state simulation runs each temperature gradient through 200,000 time steps so as to ensure steady state is achieved. This can be shortened by breaking the simulation loop as soon as steady state is achieved, thus requiring fewer time steps. As an exercise to test the extent at which the time for the steady state simulation could be reduced, a “worse case” time for steady state was calculated for the diffusion time t_d :

$$t_d = \frac{d^2}{2D(T)}. \quad (7.3)$$

Here, d is the diffusion distance, and $D(T)$ is the thermal diffusivity of the volume at temperature T . The thermal diffusivity of the volume was calculated using the assumption that the volume is composed purely of powder as this would result in the slowest diffusion time, and is equal to:

$$D(t) = \frac{1}{R_{powder}(T)\rho c_{pp}}. \quad (7.4)$$

Eqn. 7.3 generates a curve of shown in [Fig. 7.7](#), if normalised versus number of time steps, as can be seen this gives a maximum number of time steps for steady state as 20. Assuming a safety factor of 10, this gives a value of the number of time steps required for steady state to be 200, a thousand fold improvement on the initial value of 200,000. The simulation was repeated with this new value, and the comparison of results are shown in [Fig. 7.8](#). The time taken for the generation of the resistivity versus temperature curve with a 200 time step steady state simulation was 6046434 μs , this indicates that the effective time for a single steady state simulation was reduced from 3.15 seconds to 4.50 milliseconds.

As can be seen in [Fig. 7.8](#) the 200 time step steady state simulation produces incredibly

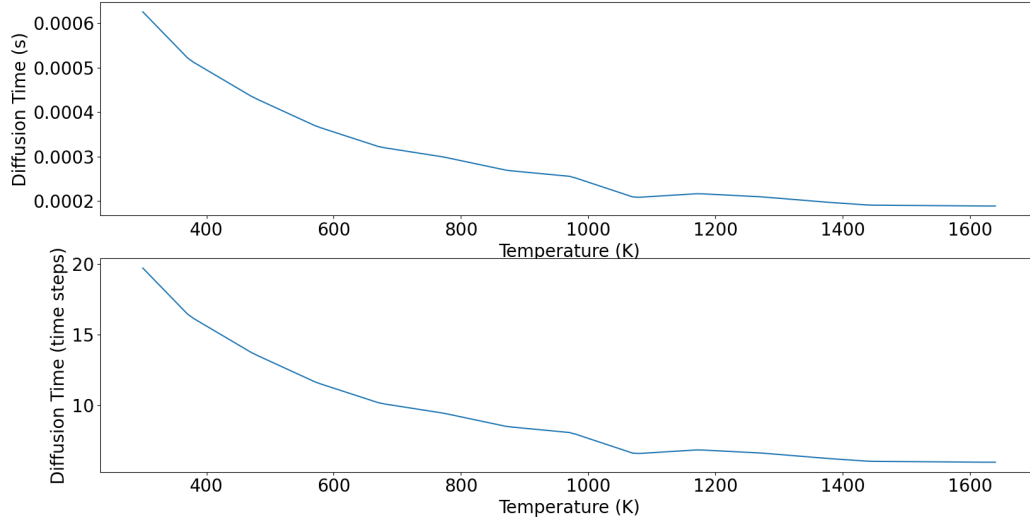


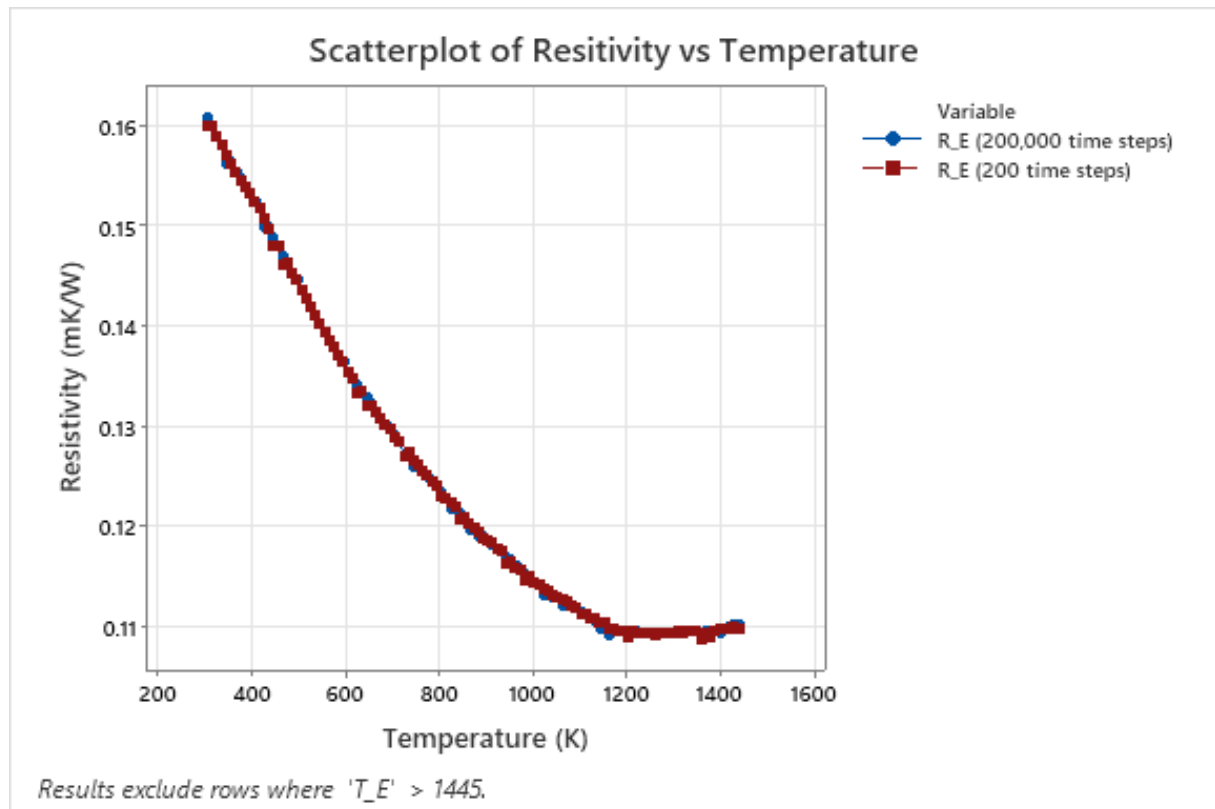
Figure 7.7: Plot of Calculated Diffusion Time versus Temperature (a) Time in Seconds (b) Time in Simulation Steps

similar results to the 200,000 time step steady state simulation. The entire resistivity versus temperature curve for the hybrid element can be calculated from a single α value, in less than a two-hundredths of a second. This, makes the calculation of the resistivity properties of hybrid volumes much more viable to be performed alongside adaptive meshing techniques, like that proposed by Liu *et al.* [186].

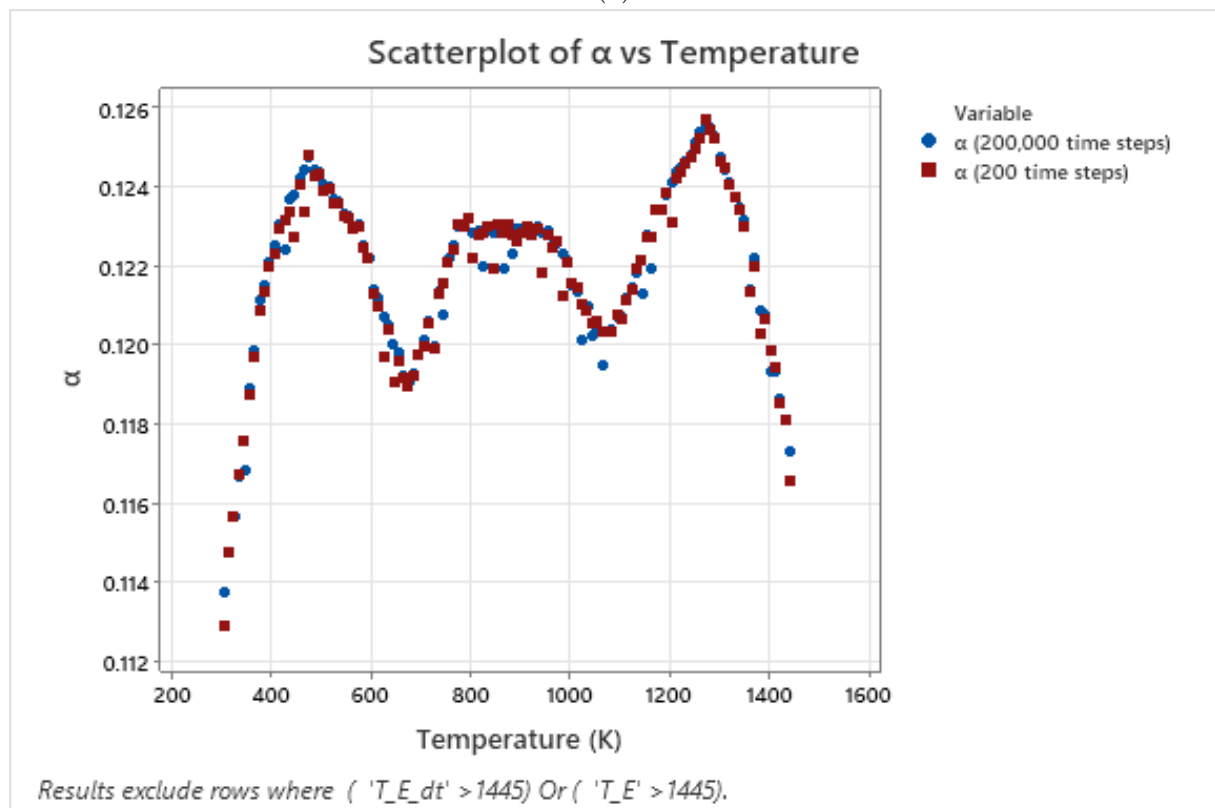
It is suggested that further work on this topic could be performed to investigate the role of machine learning to circumvent the need for steady state simulations. If a data set of α values can be generated given various solid/powder combinations and material properties, then a machine learning model can be used to infer the value of α without the need of the steady state simulations. Thus, reducing time required to coarsen the mesh.

7.2.2 Comparison of Fully Fine Simulated Volume to the Hybrid Element Volume

The performance of the fully hybrid element volume was evaluated against the heat flow of the equivalent fully fine volume. The temperature profiles against time of the top and bottom layers of each volume are plotted in [Fig. 7.2](#). It should be noted that the behaviour of both systems appear to have very similar profile. [Fig. 7.9](#) shows the



(a)



(b)

Figure 7.8: Comparative Plots of Results from 200 and 200,000 Time Step Steady State Simulations

percentage difference in temperature profiles of the top and bottom layers of the volumes.

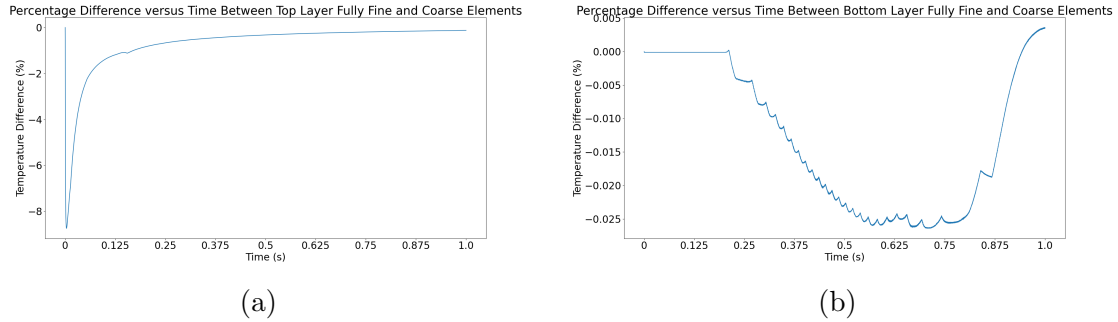


Figure 7.9: Percentage Temperature Difference versus Time Between Fully Fine and Hybrid Volumes (a) Top Layer (b) Bottom Layer

Fig. 7.9 shows that the greatest error between the fully fine and hybrid volumes occurs at the initial period of simulation. The reasoning for this is due to how the hybrid elements geometrically differ from those of the fully fine elements, not believed to be a failing of the simulated properties. This is illustrated in Fig. 7.10. As can be seen in the illustration,

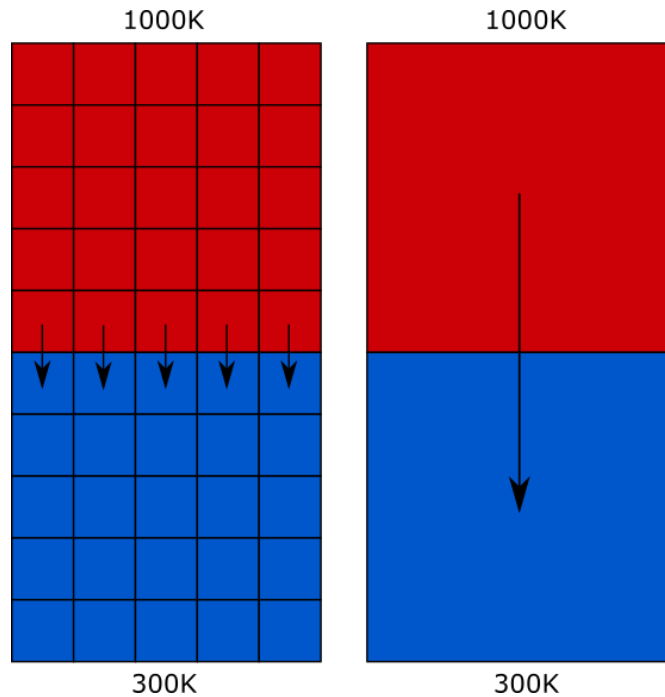


Figure 7.10: Illustration of Initial Heat Flow in Fully Fine and Hybrid Element Simulations

in order for the simulation volumes to be equivalent, the top five layers of the fully fine element volume and the top one layer of the hybrid element volume must be set to 1000 K.

However, in this FVM properties are assumed to reside at the cell centre. Thus, at the point that the simulation begins in the fully fine simulation, heat flows from the centre of layer five to the centre of layer six. A distance of $50\ \mu\text{m}$. However, in the hybrid simulation, the distance between cell centres is $250\ \mu\text{m}$. The equivalent areas of contact between these layers are the same in both simulations. Thus, the increased length scale of the hybrid elements means that the initial heat flow out is reduced, and the rate of heat flow is initially reduced. However, as the initial abrupt rate of thermal change is reduced, so is the error between the two volumes. This is shown in [Fig. 7.11](#). However, this discrepancy in rate of heat flow is shown in [Fig. 7.9](#) to result in a maximum percent difference in temperature of 8.7%. In the bottom layer of the volume the maximum percentage error is less than 0.027%. This abrupt thermal gradient is only expected in the areas closest to the meltpool, and would not be the area of the built part that the hybrid elements are required for use. Hence, whilst showing an 8.7% temperature error in these results, this would not be the case when deployed in full part-scale simulations.

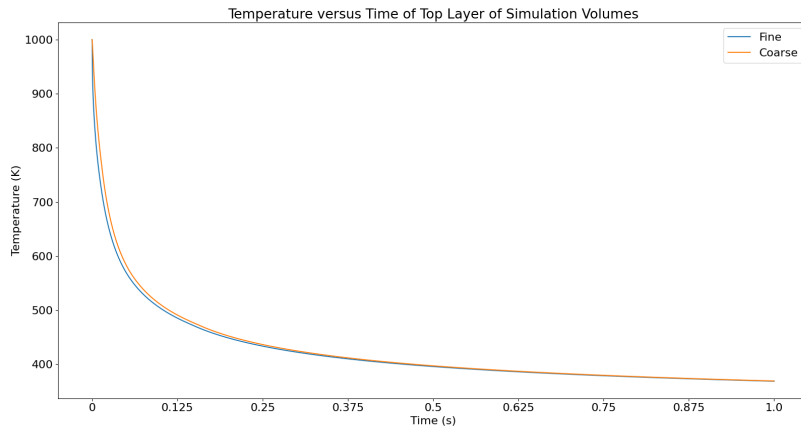
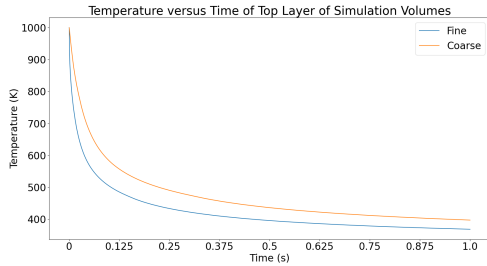
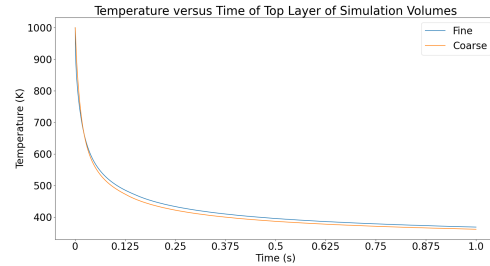


Figure 7.11: Comparison of Temperature Profiles versus Time for both Fully Fine and Hybrid Element Simulations

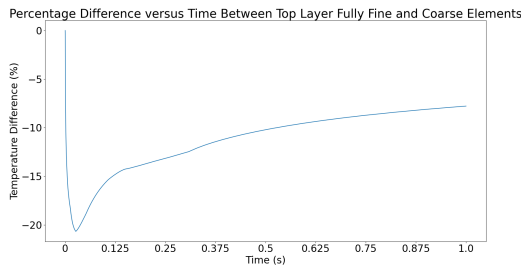
This leads to a further investigation on the error that is incurred in the volume simulation through the choice of thermal gradient used in the steady state generation of the resistivity curve. The initial steady state simulation a gradient of 400 K was chosen as an arbitrary gradient. For comparison, the experiment was repeated with a 200 K and 500 K gradient. The results of these simulations are shown in [Fig. 7.12](#).



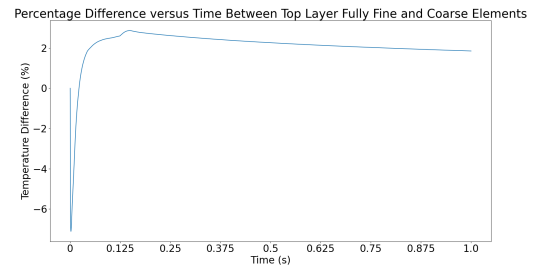
(a) Comparison of Temperature Profiles of Top Layer in Fully Fine and Hybrid Element Simulations with Resistivity Curve Generated with 200 K Gradient



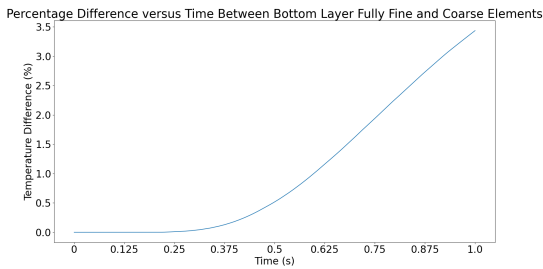
(b) Comparison of Temperature Profiles of Top Layer in Fully Fine and Hybrid Element Simulations with Resistivity Curve Generated with 500 K Gradient



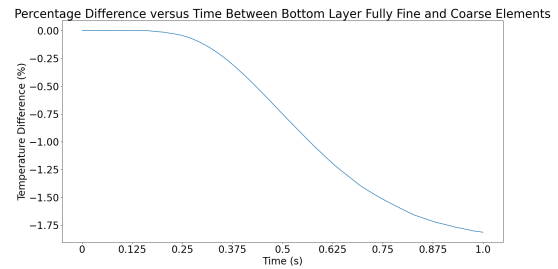
(c) Percentage Difference Between Top Layers of Fully Fine and Hybrid Element Simulations with Resistivity Curve Generated with 200 K Gradient



(d) Percentage Difference Between Top Layers of Fully Fine and Hybrid Element Simulations with Resistivity Curve Generated with 500 K Gradient



(e) Percentage Difference Between Bottom Layers of Fully Fine and Hybrid Element Simulations with Resistivity Curve Generated with 200 K Gradient



(f) Percentage Difference Between Bottom Layers of Fully Fine and Hybrid Element Simulations with Resistivity Curve Generated with 500 K Gradient

Figure 7.12: Performance of Simulations Using Varied Temperature Gradients to Generate Resistivity Curves

These additional experiments show that the gradient at which the steady state simulations are performed to generate the resistivity versus temperature curve affect the accuracy at which heat flows in the hybrid element simulation. The reduction of the fixed thermal gradient to 200 K resulted in an increase in error in both top and bottom layers. The maximum error observed in the top layer of the volume increased from 8.7% to 20.7%, and the maximum error in the bottom layer increased from 0.027% to 3.4%. When the fixed thermal gradient was increased to 500 K resulted in a reduced error in the top layer (from 8.7% to 7.1%). However, error in the bottom layer increased from 0.027% to 1.8%. This shows that there is a dependency of the accuracy of the equivalent resistivity value to the size of gradient applied during the steady state simulations. For example, the temperature gradient across the fine/coarse element boundary in the coarsened simulation performed in [Sec. 5.2.9](#) is shown in [Fig. 7.13](#). This simulation was performed using five layers of fully fine elements, and [Fig. 7.13](#) shows that this results in a thermal gradient of approximately 110 K. This warrants further investigation as to the most appropriate thermal gradient to be used, and whether this is dependent on the thermal gradient that the hybrid elements would be exposed to in the final simulation.

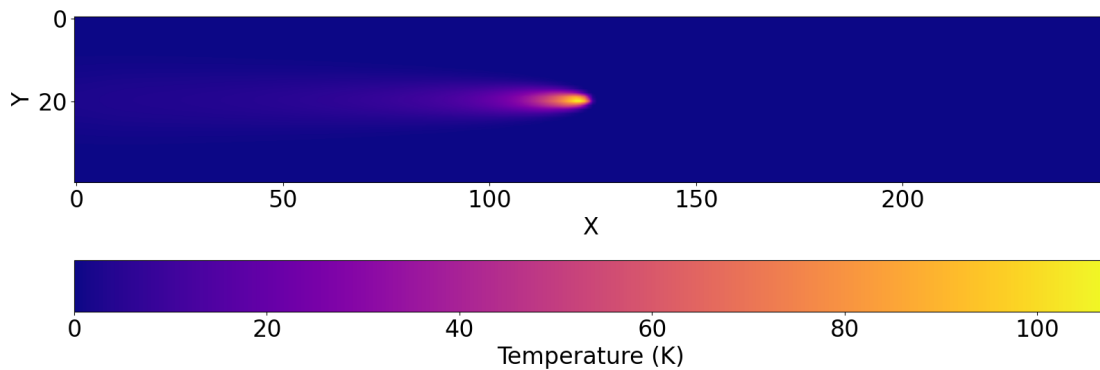


Figure 7.13: Temperature Gradient Across Coarsening Boundary in Coarsening Simulation

[Tab. 7.2](#) shows the comparative computational resources consumed by each simulation. It can be observed that the time taken for the hybrid element simulation, when compared to the fully fine element simulation, experienced a speed-up of approximately 44 times. This results in a ratio of real time to simulation time of 0.24. This significant speed up

makes real-time simulation much more than an attainable goal. Especially when used in conjunction with the adaptive meshing techniques, such as those proposed by Liu *et al.* [186].

7.2.3 Coarsening with Hybrid Elements

As can be seen from [Table 7.3](#) the predicted meltpool measurements for both the fully fine and coarsened simulations were observed to be almost the same. The variation in the measurements for both width and depth is within the expected error of the measurement technique used (as discussed in [Sec. 5.2](#)).

Also shown in [Table 7.3](#) is that through the coarsening of the lower elements a speed-up of factor five was achieved with no observed effect to the accuracy of meltpool prediction. This simulations as performed on a volume of $4.00 \times 250.00 \times 6.25 \text{ mm}^3$. The speed-up achieved through coarsening is expected to only increase as the volume size increases in the z-axis, due to the increase in ratio of coarse to fine elements.

It is also worthy of note that the coarsening strategy employed in this simulation resulted in a fine coarse interface of 25 fine elements neighbouring a single coarse hybrid element. Yet there is no evidence to suggest that this was detrimental to the accuracy of meltpool prediction. This implies that there is a possibility of incredibly aggressive coarsening strategies can be applied to industrial build geometries to achieve faster than real-time simulation. Although, this warrants further investigation in a wider range of scenarios to validate.

7.3 Conclusions

The method of simulation described here shows that an effective resistivity versus temperature curve can be generated for a hybrid solid/powder volume through simulation of a thermal gradient to steady state. Further work is required to investigate the most appropriate thermal gradient to use to reduce error in the volume's implementation in full part simulations. The implemented fixed thermal gradient causes a break down of

the resistivity curve at high temperatures due to the partial melting that occurs in the volume in the areas of increased temperature. However, mesh coarsening should not be implemented close to the incident laser irradiation which should circumvent this limitation.

Due to the relationship between the resistivity of the solid and the powder, a full resistivity curve does not need to be generated. The amount of computation can be reduced due to the near constant value of α (Eqn. 7.5 and 7.6) that allow a full resistivity curve to be calculated from a single value of α calculated from a single steady state simulation. This single simulation takes approximately 34 seconds, and would only be required once per hybrid element composition. This was shown that this could be reduced to 4.50 milliseconds with little to no impact on the accuracy of the calculated α and R values. This process time could be further reduced by dynamically testing the volume to confirm that steady state has been achieved, rather than using a fixed number of time steps and assuming steady state has been achieved.

A further advancement that can be used to generate the α value of each hybrid element can be through machine learning. As the values for α are generated procedurally, once a large enough data set is created, this could potentially be used to train a machine learning model so that α values can be inferred at high speed.

The use of the hybrid elements and associated resistivity curves, when compared to an equivalent volume of fully fine elements, resulted in a maximum error of less than 9% in temperature. This error is reduced to less than 1% after one second of simulated real-time. Thus, use of these hybrid elements should be more than suitable for coarsened elements in the build volume bulk, where the thermal gradients are greatly reduced.

This was then tested through comparison of equivalent volumes using a simulated laser heat source. The predicted meltpool geometries did not vary between the fully fine and coarsened volumes. Thus, this indicates that the performance of these hybrid elements is sufficient that the accuracy of meltpool geometry prediction in a simulated build is maintained whilst computational time is reduced significantly. Further work is required to determine the limits of the application of these hybrid elements.

Chapter 8

Discussion

This work presents a validated novel method of combining multiple phases of material within single mesh elements for finite volume solutions of the heat equation. Specifically with the aim of reducing the overall computing power and time required to perform such simulations on part size volumes within the context of additive manufacture. Thus, overcoming the previous mesh coarsening limitation imposed by complex geometries with a complex powder/solid volume percentages. It is hoped that this work contributes to the establishment of a equal-to or faster-than real-time simulation based method to allow for in-situ dynamic parameter adaption. A summary of the conclusions discussed in Chapters 6 and 7 are given here. Accompanied by suggestions on how this work could be developed and refined.

8.1 Validation

It was shown in Chapter 6 that due to the sparsity of the matrix equation of the heat diffusion equation, the numerical method is well suited to GPU parallelisation. Through utilising the GPU a standard macroscale continuum model for AM was realised, and the benchmark speed of this simulation was only a 3% longer than the proposed Adaptive Mesh Coarsening Strategy model proposed by Liu *et al.*. The benchmark model shown here shows the power of leveraging the GPU, for without any specialised meshing techniques, a sevenfold increase in speed was realised.

One development that can be explored for this parallelised model is the computer science of leveraging the anti-symmetry of enthalpy flow between adjacent elements, and the faster shared memory of GPU blocks. For [Sec. 4.3](#) outlines the discretization and quantisation of the enthalpy flow between elements. Therefore, it is trivial to observe that for adjacent elements, the magnitude of the enthalpy flow with respect to each element is the same but with opposite signs. i.e. from [Fig. 4.2](#), the enthalpy flow from element three to element one is the same as the enthalpy flow from element one to element three but with an opposite sign. Currently, the enthalpy contribution from adjacent elements is calculated every time step. However, due to this shared magnitude, the value need only be calculated once per time step and then added or subtracted from the element as appropriate. If one considers a volume of $3 \times 3 \times 3$ elements, the current method would calculate enthalpy values for each element interface. This is a total of 108 values per time step. If a method is developed in which duplicates are taken in consideration, this value is reduced to 54. This would effectively half the number of calculations per time step. This would allow considerable reduction in the simulation time.

[Chapter 6](#) also showed that the predicted meltpool geometry is heavily dependent on the source term used for simulation. The basic cylindrical volumetric heat source used in [Chapter 6](#) proved sufficient for prediction of meltpool geometries when the parameters used fall within the conduction mode of processing for the alloy used. However, due to the transition of laser/powder/solid interaction that occurs due to keyhole mode processing, this simplified volumetric heat source no longer suffices for meltpool prediction. It is believed that the method used for prediction of heat flow was not the cause of inaccuracy of the meltpool geometries in this case but solely due to the heat source term. this can be corroborated by the agreement of the numerical meltpool geometries and experimental meltpool geometries when the parameter are shown to be operating within the conduction mode processing window. Further development that should be explored is in identifying more developed volumetric source terms that allow for more accurate representation of the heat source which are ambivalent to the processing mode, such as the one presented by Philo *et al.* [191]. An alternative development that would address the same issue,

would be to determine the underlying thermophysical properties that govern the processing mode and identify the threshold at which the conduction to keyhole mode transition occurs. This could then be incorporated into the simulation method so that the threshold is checked before heat input each timestep and the correct processing mode heat source is applied.

8.2 Hybrid Elements

Chapter 7 demonstrates a novel method by which multiple forms of matter can be incorporated into a single cubic element of hybrid properties for advanced mesh coarsening in FVM and FE simulations. This novel method is designed to overcome the limitation imposed in current numerical methods by which material states must remain separate when coarsening, limiting the amount of mesh coarsening that can occur based on the part geometry.

The proposed method is shown to break down at elevated temperatures where there is expected to be partial melting of the hybrid volume during the steady state simulation that is performed in order to gauge the equivalent thermodynamic properties of the hybrid volume. This break down of the method is not considered a limitation of the application of this method, due to the philosophy of mesh coarsening. The areas of the simulated volume that would be considered for mesh coarsening are sufficiently far from the incident heat source that the thermal gradients experienced by the hybrid volume do not approach the gradients at which the steady state simulation breaks down.

The method described also proposes an extension of the steady state method of calculating the equivalent resistivity versus temperature curve for a hybrid volume. The properties of the hybrid volume can be said to be a linear interpolation between the solid and powder properties. The steady state simulation can be used to calculate the coefficient α used in the linear interpolation for a given temperature. If the relationship between the thermodynamic properties of the solid alloy and its powder are fixed, i.e. the ratio between the powder resistivity and the solid resistivity is constant, then the value of α is constant for all temperatures within the valid temperature range. This then means that

the entire resistivity versus temperature curve can be calculated from a single α value generated from a single steady state simulation. This approach was shown to produce excellent agreement with the resistivity versus temperature curve generated through numerous steady state simulations. This approach saves valuable computational time and load by reducing the amount of calculation required when hybrid elements are generated during mesh coarsening.

The proposed method used a large number of steady state time steps to ensure the hybrid volume was at steady state for each resistivity value calculated. This was shown to be able to be reduced by calculating the “worse case” time from the diffusion time of a fully powder volume, thus reducing the number of steady state time steps by three orders of magnitude. Further development of this work could increase this speed-up by querying the hybrid volume at each time step of the steady state simulation to check for steady state, then breaking the simulation loop if the query is returned “true”. This is a common practice in machine learning training for checking convergence of layer weights, and can due to the continual development of machine learning technologies, can be applied here with existing C++/Python libraries.

The value of α calculated for a hybrid volume was found to vary depending on the size of the thermal gradient applied in the steady state simulation, and therefore affected the accuracy of the subsequent simulation using the calculated resistivity versus temperature curve. Further investigation is required to elucidate whether there is an optimum representative thermal gradient to be used or whether the optimum gradient is dependent on the final application. Machine learning would probably also be able to benefit the derivation of the α value for a hybrid element, and would be a further addition to this work worth exploring. As mentioned above, if the solid/powder relationship is constant, the value of alpha versus temperature is constant and is solely dependent on the powder/solid distribution within the hybrid volume with respect to the direction of the thermal gradient. Thus, a neural network can be trained with various hybrid element geometries, material properties, and α values. This network can then be used to infer an α values for various hybrid elements during mesh coarsening without the need for a steady state

simulation. This may greatly reduce the time taken for α value acquisition with inference time optimisation.

Table. 7.2 shows that a hybrid volume of 8,000 elements simulated over 31,551 timesteps takes 4.08 seconds using an NVIDIA RTX 2060 GPU. This corresponds to a total time of 129 microseconds per timestep. In order to achieve real-time simulation speeds this time must be reduced by a factor of 4.07. This can be done through the reduction of number of elements, or increasing the calculation speed of the number of calculations performed per element.

The former would imply that the maximum number of elements that would achieve real-time simulation is 1,965. This would mean that for a build volume of $250 \times 250 \times 30 \text{ mm}^3$ present in the Renishaw 500Q Machine would need to be represented with cubic elements of approximately 21 millimeters. This would be prohibitive in accurately representing the build geometry. This method of reduction of the number of elements assumes that the absolute size of the simulation timestep remains the same. However, as shown in Eqn. 4.31 as element size, h , increases so too does the maximum stable timestep. Therefore, the increase in size of the elements would not need to be as severe as 21 millimeters. In fact, as observed from Eqn. 4.31, the timestep is proportional to the square of the element size. Therefore, a fourfold reduction in number of required timesteps is achieved by doubling element size, which is much more practical.

The latter method is hardware dependent. As discussed in Sec. 2.3.1, the latest flagship device the RTX 4090 has a quoted calculation speed of 82.58 TFLOPS [164]. This is 12.8 times greater than the quoted calculation speed of the RTX 2060 used for the experiments described here. If the memory access time is considered equal on both GPUs, this is theoretically sufficient to perform the simulation experiments in Chap. 7 faster than real-time. At this speed, the full $250 \times 250 \times 300 \text{ mm}^3$ build volume would be able to be simulated in real time if the cubic elements are a minimum of 5.7 millimeters. Hence, with the techniques described here faster than real-time simulation is achievable with the latest consumer hardware.

As shown in Sec. 6.2.1, current state-of-the-art methods displayed by Liu *et al.* using

ABAQUS™ from Dassault Systèmes show a sevenfold increase in simulation speed for $20 \times 40 \times 3 \text{ mm}^3$ volume [186]. Whereas, by utilising the parallelisation techniques outlined in [Sec. 4](#) a similar sevenfold increase in simulation speed is attainable on larger volumes ($80 \times 40 \times 5 \text{ mm}^3$). Additionally, when coarsening is also applied in tandem with parallelisation an additional fifteenfold increase in speed is observed. Reducing the simulation the simulation time of the equivalent volume simulated by Liu *et al.* to a mere 30 minutes. It should also be of note that the Courant-Lewy-Friedrichs condition for maximum time step, discussed in [Sec. 4.3.1](#), that the maximum stable time step for such simulations scales with the square of the element size. Taking this into consideration also, if deployed on a NVIDIA RTX 4090, the full $250 \times 250 \times 300 \text{ mm}^3$ build volume can be simulated in real time using cubic elements just larger than 1 mm^3 . This is sufficient for parts with no geometries smaller than this, but not sufficient for resolving fine details in lattice type structures where struts can measure as small as 0.3 mm. Hence, further work would be required to implement optimisations to this method that have not been deployed here; for example memory read/write optimisation. This would also contribute to real time simulation being achieved in finer detail.

Chapter 9

Conclusions and Further Work

This work demonstrates a novel approach to fast thermal simulation of Laser Powder Bed Fusion via advanced use of parallelisation via GPU technology, and a novel method of meshing for finite volume methods allowing coarsening algorithms to combine different materials into single “hybrid” elements. This chapter provides a summary of the success or failure of each of the research objectives outlined in [Sec. 3.2](#), and provides a general suggestion as to what further work is required to address any shortfalls of the methods proposed in this work.

1. **To produce a base, fully fine resolution simulation method to predict the thermal flow through a macroscale part**

The baseline model was shown to be predominantly successful in simulating macroscale, stainless steel coupons over entire layer time frames, including recoater times. However, a general limitation of a thermal model with no associated fluid flow, means that accuracy is lost when considering processing modes and parameters with significant Marangoni or mass circulation (i.e. keyhole process mode). The model used herein was limited to a single alloy system, preventing validation across multiple materials. Due to the method of simulation, the maximum timestep is limited by the Courant-Lewy-Friedrichs condition. This then makes the number of timesteps required for a specific real time dependent on material.

2. **To validate the performance of this benchmark simulation method through**

utilising it to predict the geometries of meltpools at a range of different processing parameters

It was shown that a conduction only, explicit solver was able to predict the melt-pool geometries of a range of parameters. However, the accuracy in this work was limited to the conduction mode region of the process window. This is due to the change in geometry of the representative volumetric heat source, and significant increase in fluid flow between conduction mode to keyhole mode processing. When the processing parameters are observed in physical experiment to be firmly within the keyhole regime, the model severely under predicts the depth of the meltpool, and over predicts the width. The volumetric heat source doesn't account for the increased material penetration of the laser in keyhole mode.

This indicates that in keyhole mode the predicted temperature distribution around the meltpool is considerably shallower. Therefore, the model would be unable to be used to predict formation of keyhole defects in its current state.

3. To develop a method of overcoming the limitation of current coarsening strategies that cannot coarsen across materials of material states

A method was developed to calculate the combined thermophysical properties of coarsened elements containing both solid metal and metallic powder. Due to the limitation of physically creating these solid/powder volumes these predictions are indirectly validated through comparison to the validated, uncoarsened simulations. It was also shown that the continuous thermal resistivity versus temperature curve could theoretically be derived with reduced amounts of simulation using a single linear interpolation parameter, α . The value of α for 316L Stainless Steel was shown to be consistent ($\pm 2.5\%$) versus temperature within the range of 0.30 to 0.85 of the solidus temperature. Therefore allowing the properties of the resistivity versus temperature curve to be calculated from a single simulation within this temperature range. The accuracy of the thermophysical properties calculated for this hybrid, coarsened element were shown to vary with the thermal gradient used in their derivation. A method to select the optimum thermal gradient for property

derivation, or a “from fundamentals” approach to calculate the correct gradient to use, was not proposed.

4. To validation the performance of these coarsening techniques via comparison to the established, validated, baseline model

The hybrid coarsened elements were successfully used to coarsen a single track simulation. The result of the simulation with coarsening versus the equivalent simulation without coarsening showed no statistically significant error between the two. Due to the reduced number of elements required in the coarsened simulation, CPU RAM usage was reduced by 5%, GPU RAM usage was reduced by 89%, and time taken for equivalent simulations was reduced by almost 98%. This coarsening strategy was limited to the z-axis, further benefits could be recognised with a full adaptive coarsening method in all three axes. Mathematically, there is no limit to directional anisotropic coarsened elements, only the increase complexity of simulatory implementation.

9.1 Further Work

As identified above, the following is believed to be the avenues of study worthy of pursuit:

1. Extend the existing work to other alloy systems with well established, high fidelity thermophysical data.
2. Investigate methods to overcome the Courant-Friedrichs-Lewy condition, or a method to relax this condition in coarsened regions, or during periods of zero heat input (i.e. during recoating).
3. Extend the current model to allow greater faculty in the non-conduction mode processing window. This could be achieved via adding the ability to predict the processing mode and adapting the volumetric heat source as required.

4. Investigate the optimum temperature gradient for generation of hybrid solid/powder elements.
5. Investigate adoption of this hybrid element generation into a dynamic coarsening method to validate and quantify the computational improvement for simulation of macroscale parts of complex geometry.

Appendix A

This is a standard derivation of the parabolic heat equation [193]. Considering an arbitrary volume V bounded by a surface S and let $T(x, y, z, t)$ be the temperature at a point (x, y, z) at time t . There will be flow of heat if the distribution throughout the domain is nonuniform, and a flow will occur between regions of high heat to regions of low heat. According to Fourier's Law, the heat flux $\mathbf{q}(\mathbf{r}, t)$ through a surface element dS is proportional to the gradient of the temperature:

$$\mathbf{q}(\mathbf{r}, t) = -L(\mathbf{r}, t)\nabla T(\mathbf{r}, t) \quad (\text{A.1})$$

Where $\mathbf{r}$ is the position vector and L (a positive quantity) is the thermal conductivity of the material. If $\hat{n}$ is the outward normal to the surface element dS , the rate of outflow of heat (dQ) through dS per unit time can be expressed as:

$$dQ = (\mathbf{q} \bullet \hat{n})dS \quad (\text{A.2})$$

Therefore the amount of heat flowing across the boundary S of V per unit time is:

$$-\int (\mathbf{q} \bullet \hat{n})dS \quad (\text{A.3})$$

The negative shows that this is a net loss of energy from the volume V as heat diffuses away. If e is the specific energy of the volume, and we assume that the body is rigid and at rest, therefore the only energy present is the thermal energy, the rate of change of

thermal energy is given by:

$$\frac{d}{dt} \int \rho e dV = \int \rho \dot{e} dV \quad (\text{A.4})$$

If $F(\mathbf{r}, T, t)$ indicates the generation of heat per unit time per unit volume, the source term becomes:

$$\int F dV \quad (\text{A.5})$$

Generally F is assumed to be a known quantity. The law of conservation of energy gives the relation as:

$$\int \rho \dot{e} dV = - \int (\mathbf{q} \bullet \hat{n}) dS + \int F dV \quad (\text{A.6})$$

Gauss's Divergence theorem gives the identity:

$$\iiint_V (\nabla \bullet \mathbf{F}) dV = \oiint_S (\mathbf{F} \bullet \hat{n}) dS \quad (\text{A.7})$$

This can then be applied to the conservation of energy equation to give all three integrals in terms of dV

$$\int (\rho \dot{e} + \nabla q - F) dV = 0 \quad (\text{A.8})$$

As this is true for any arbitrary volume V , it can be concluded that:

$$\rho \dot{e} = -\nabla q + F \quad (\text{A.9})$$

This is the basic form of heat conduction. To determine an equation for temperature alone an expression must be found for e and q in terms of T . For limited temperature ranges, and for most materials, specific internal energy e varies linearly with T . Thus $\dot{e} = c\dot{T}$. Where c is the specific heat capacity. Similarly, q can be defined as $-K\nabla T(\mathbf{r}, t)$. Thus the heat conduction equation becomes:

$$\dot{T} = \alpha \nabla^2 T + \frac{1}{\rho c} F \quad (\text{A.10})$$

Where $\alpha = Kl\rho c > 0$ is the thermal diffusivity and $\nabla^2 \left(= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$ is called the Laplace operator. If there is no heat source ($F = 0$) the equation reduces to:

$$\dot{T} = \alpha \nabla^2 T \tag{A.11}$$

Appendix B

This is a standard derivation showing how the prototype of the heat equation maintains its parabolic identity when expressed in dimensions higher than two [194]. Consider a second order partial differential equation with n independent variables:

$$\sum_{i=1}^n \sum_{j=1}^n a_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^n b_i \frac{\partial u}{\partial x_i} + cu + d = 0, \quad (\text{B.1})$$

where a_{ij} , b_i , c , d , are functions of $x = (x_1, x_2, \dots, x_n)$, $u = (u_1, u_2, \dots, u_n)$, and n is the number of independent variables. Eqn. B.1 can be written in matrix form:

$$\begin{bmatrix} \frac{\partial}{\partial x_1} & \dots & \frac{\partial}{\partial x_n} \end{bmatrix} \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} \frac{\partial u}{\partial x_1} \\ \vdots \\ \frac{\partial u}{\partial x_n} \end{bmatrix} + \begin{bmatrix} b_1 & \dots & b_n \end{bmatrix} \begin{bmatrix} \frac{\partial u}{\partial x_1} \\ \vdots \\ \frac{\partial u}{\partial x_n} \end{bmatrix} + cu + d = 0. \quad (\text{B.2})$$

If the coefficient matrix $\mathbf{A} = a_{ij}$ is not symmetric, it can be rewritten in the form $\bar{a}_{ij} = \frac{1}{2}(a_{ij} + a_{ji})$, so that Eqn. B.1 becomes:

$$\sum_{i=1}^n \sum_{j=1}^n \bar{a}_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^n b_i \frac{\partial u}{\partial x_i} + cu + d = 0. \quad (\text{B.3})$$

Next, consider the transformation:

$$\xi_i = \sum_{j=1}^n q_{ij} x_j, \quad (\text{B.4})$$

where $\xi = (\xi_1 \cdots \xi_n)$ and $\mathbf{Q} = (q_{ij})$ is an arbitrary $n \times n$ matrix. Chain rule results in the identities:

$$\frac{\partial}{\partial x_i} = \sum_{k=1}^n \frac{\partial}{\partial \xi_k} \frac{\partial \xi_k}{\partial x_i} \quad (\text{B.5})$$

$$\frac{\partial^2}{\partial x_i \partial x_j} = \sum_{k,l=1}^n \frac{\partial^2}{\partial \xi_k \partial \xi_l} \frac{\partial \xi_k}{\partial x_i} \frac{\partial \xi_l}{\partial x_j}. \quad (\text{B.6})$$

This allows the mapping of the derivatives of $u(x_1, x_2, \cdots, x_n)$ with respect to $x_1, x_2, \cdots, x_n$ to the derivatives of $w(\xi_1, \xi_2, \cdots, \xi_n)$ with respect to $\xi_1, \xi_2, \cdots, \xi_n$. Thus, Eqn. B.1 can be expressed as:

$$\sum_{k,l=1}^n \left(\sum_{i,j=1}^n q_{ki} q_{aj} q_{lj} \right) \frac{\partial^2 u}{\partial \xi_k \partial \xi_l} + \mathcal{O}(u) = 0. \quad (\text{B.7})$$

Here, $\mathcal{O}$ represents the lower order terms in the PDE, and the term in brackets represents the coefficient matrix, which upon inspection is of the form $\mathbf{Q}^T \mathbf{A} \mathbf{Q}$. As $\mathbf{A}$ is real and symmetric, it can be decomposed into a form $\mathbf{P}^T \mathbf{A} \mathbf{P} = \mathbf{\Lambda}$. Where $\mathbf{P}$ is an orthogonal matrix of the eigenvectors of $\mathbf{A}$, and $\mathbf{\Lambda}$ is a diagonal matrix of the eigenvalues of $\mathbf{A}$. Also, as $\mathbf{A}$ is real and symmetric, this means that all eigenvalues of $\mathbf{\Lambda}$ will be real. Hence, classification of Second Order PDEs in higher dimensions becomes:

- Elliptic if all eigenvalues of $\mathbf{A}$ contained in $\mathbf{\Lambda}$ are non-zero and have the same sign;
- Hyperbolic if all but one of the eigenvalues of $\mathbf{A}$ contained in $\mathbf{\Lambda}$ are non-zero and have the same sign;
- Parabolic if any of the eigenvalues of $\mathbf{A}$ contained in $\mathbf{\Lambda}$ are zero, this means that that the matrix $\mathbf{A}$ is singular.

The Example of the Three Dimensional Heat Equation The three dimensional heta equation in its longhand form is:

$$\frac{\partial u}{\partial t} - \alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) = 0. \quad (\text{B.8})$$

Thus, by inspection the coefficient matrix $\mathbf{A}$ is:

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & -\alpha & 0 & 0 \\ 0 & 0 & -\alpha & 0 \\ 0 & 0 & 0 & -\alpha \end{bmatrix} \quad (\text{B.9})$$

As the coefficient matrix is already in a diagonalised form, it can be seen that exactly one of the values is zero. Therefore $\mathbf{A}$ is singular, and the three dimensional heat equation maintains its parabolicity in dimensions above the second.

Appendix C

Comparison of optical micrographs to the simulated melt pool geometries. The parameter of each melt pool is given in the figure caption. Images are scaled where appropriate in order to maintain scale between images.

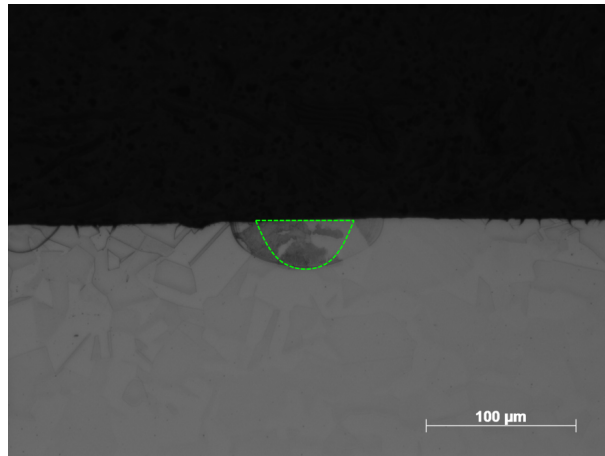


Figure C.1: 40 W 100 mm/s

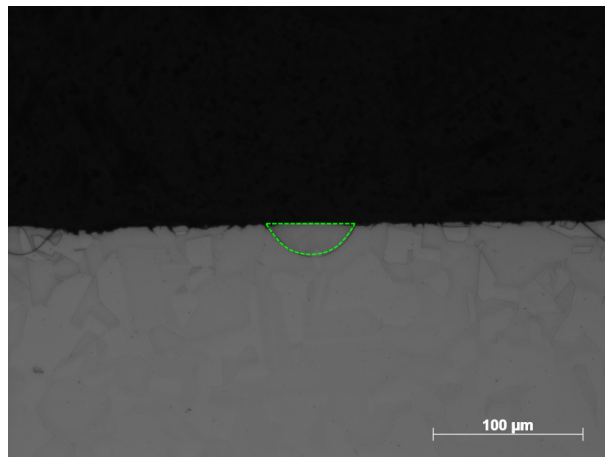


Figure C.2: 40 W 500 mm/s

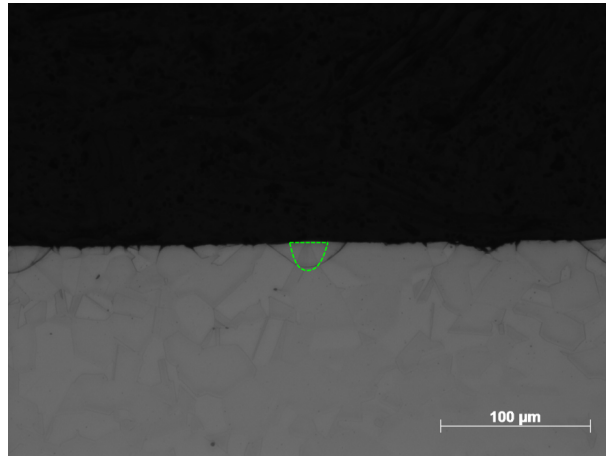


Figure C.3: 40 W 900 mm/s

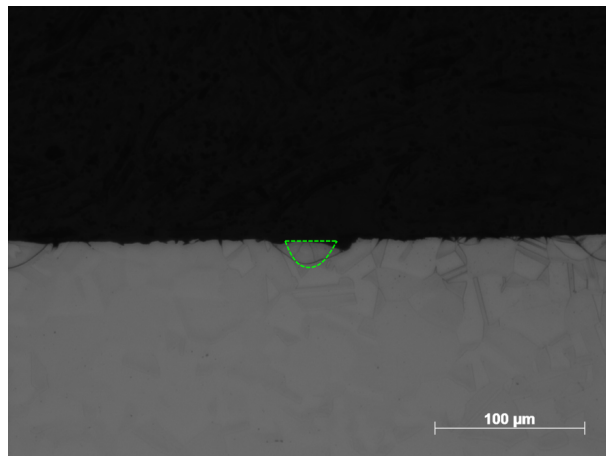


Figure C.4: 40 W 1300 mm/s

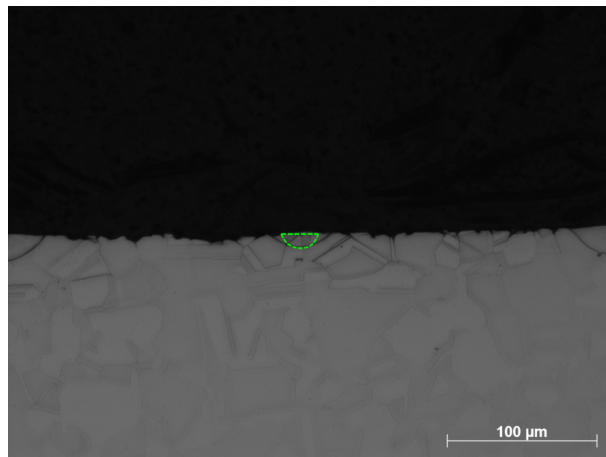


Figure C.5: 40 W 1700 mm/s

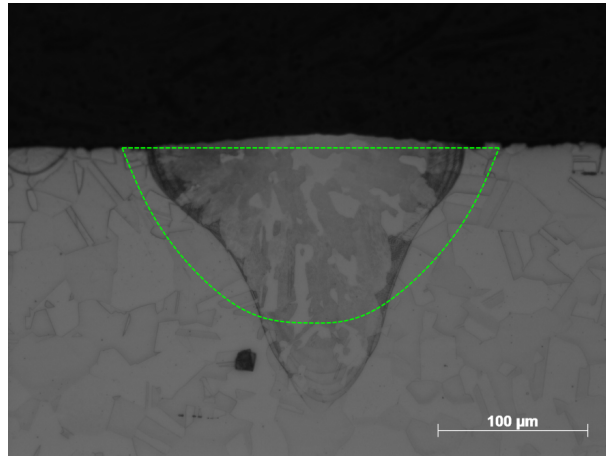


Figure C.6: 90 W 100 mm/s

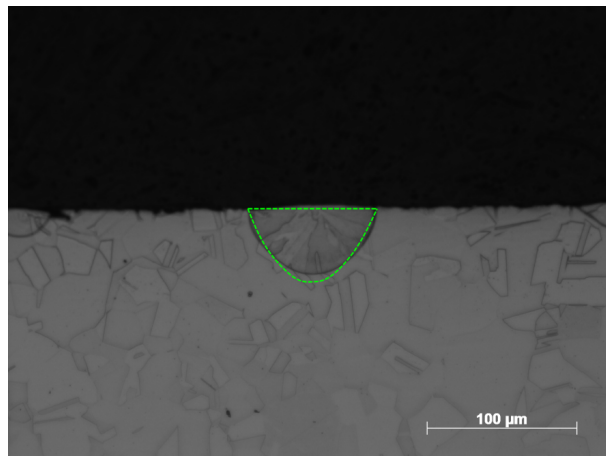


Figure C.7: 90 W 500 mm/s

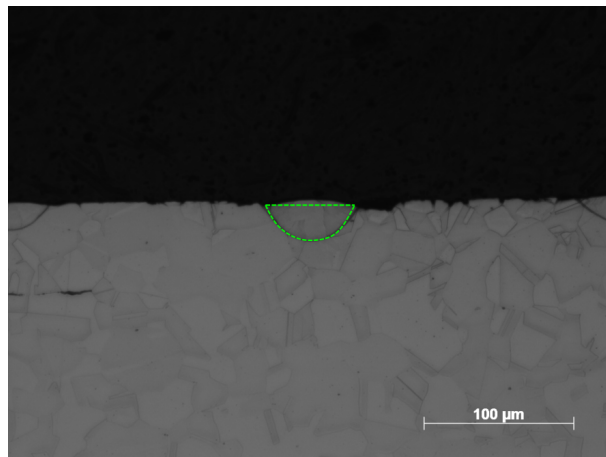


Figure C.8: 90 W 900 mm/s

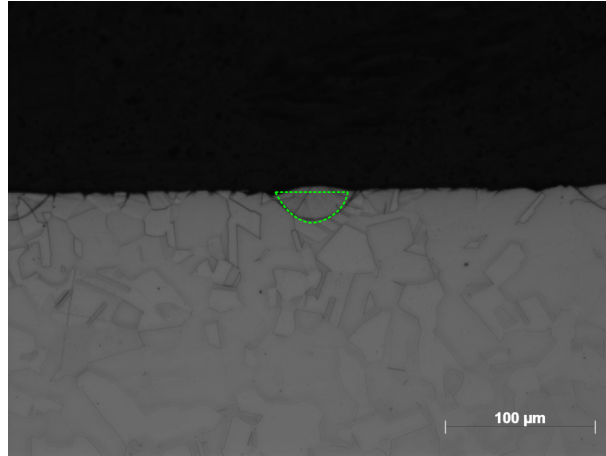


Figure C.9: 90 W 1300 mm/s

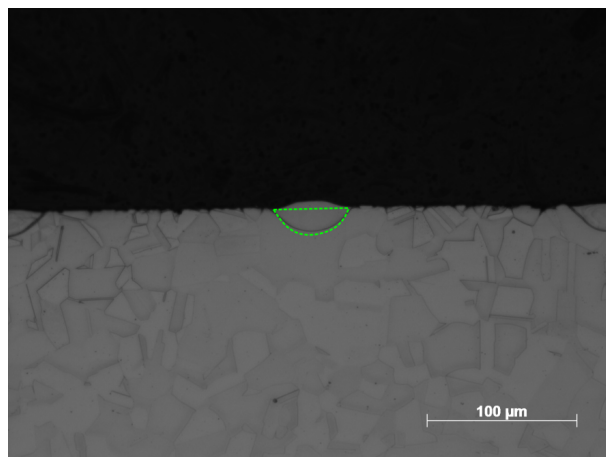


Figure C.10: 90 W 1700 mm/s

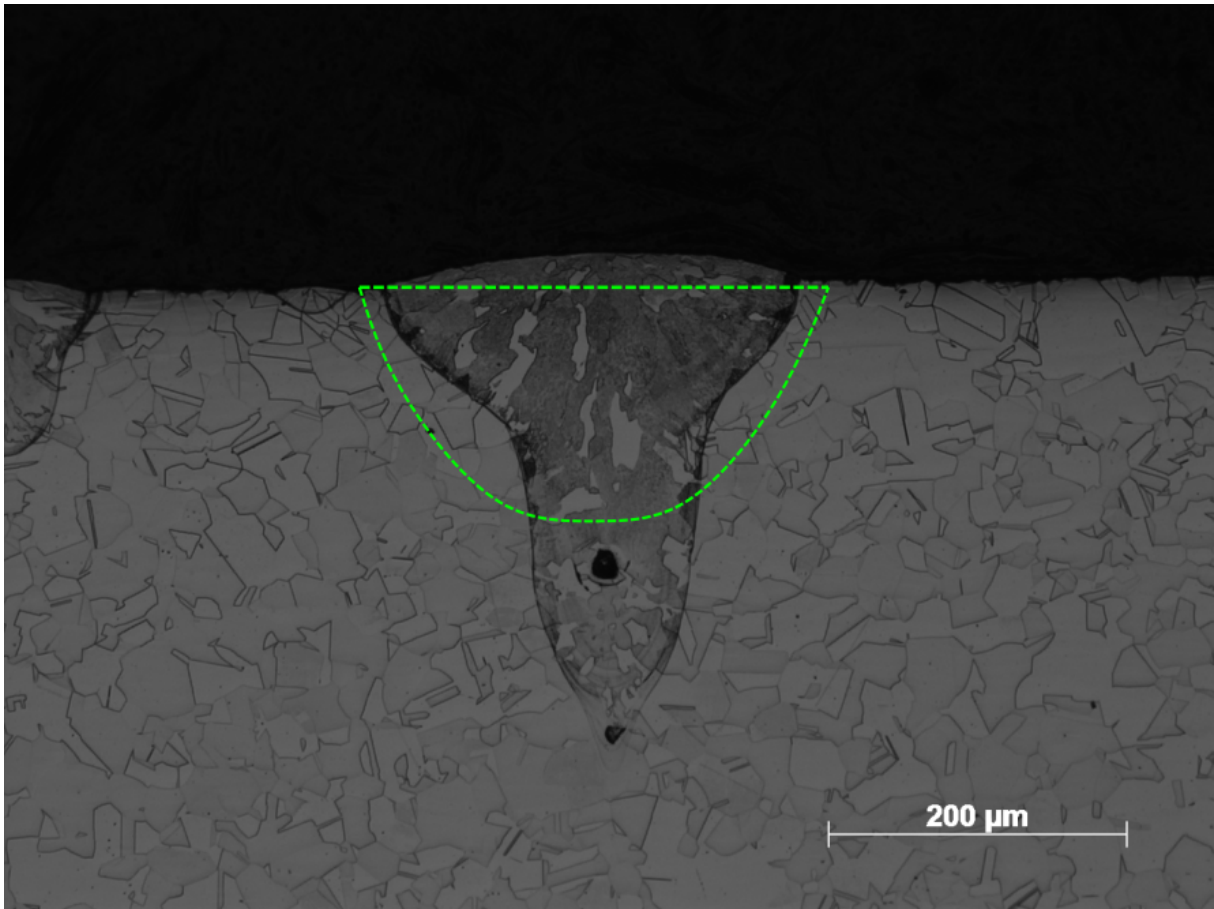


Figure C.11: 140 W 100 mm/s

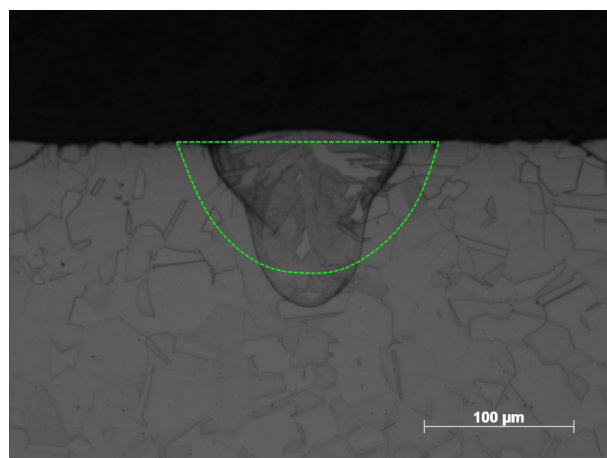


Figure C.12: 140 W 500 mm/s

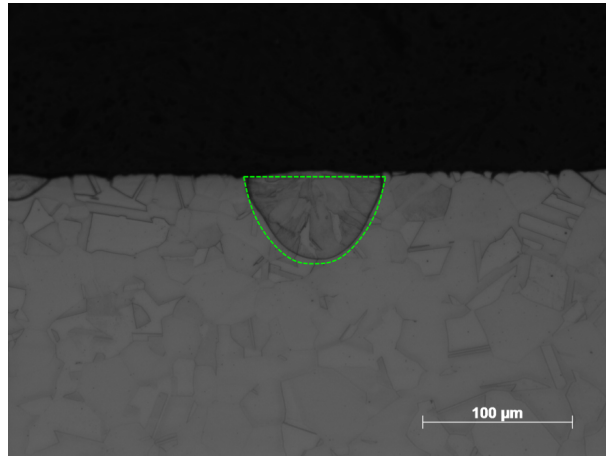


Figure C.13: 140 W 900 mm/s

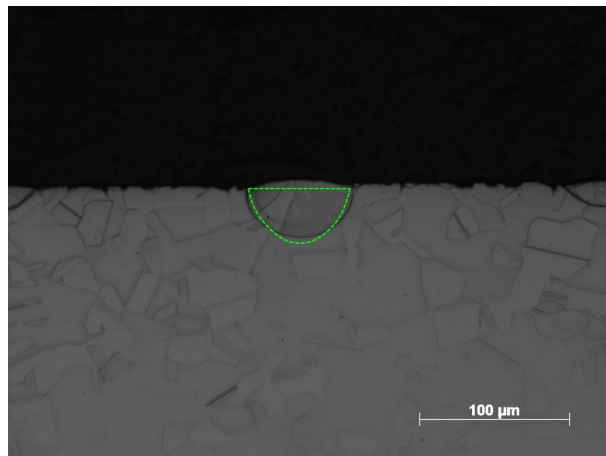


Figure C.14: 140 W 1300 mm/s

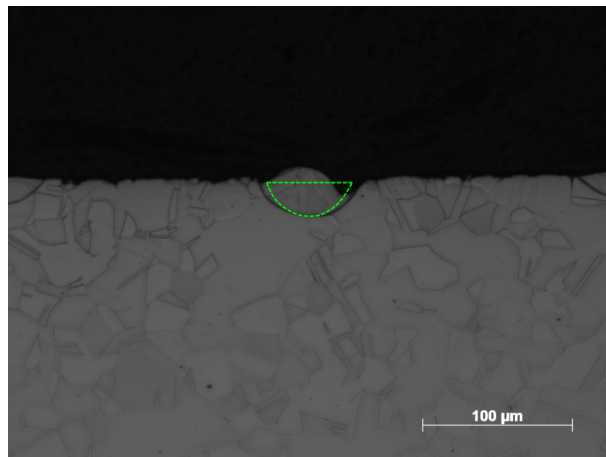


Figure C.15: 140 W 1700 mm/s

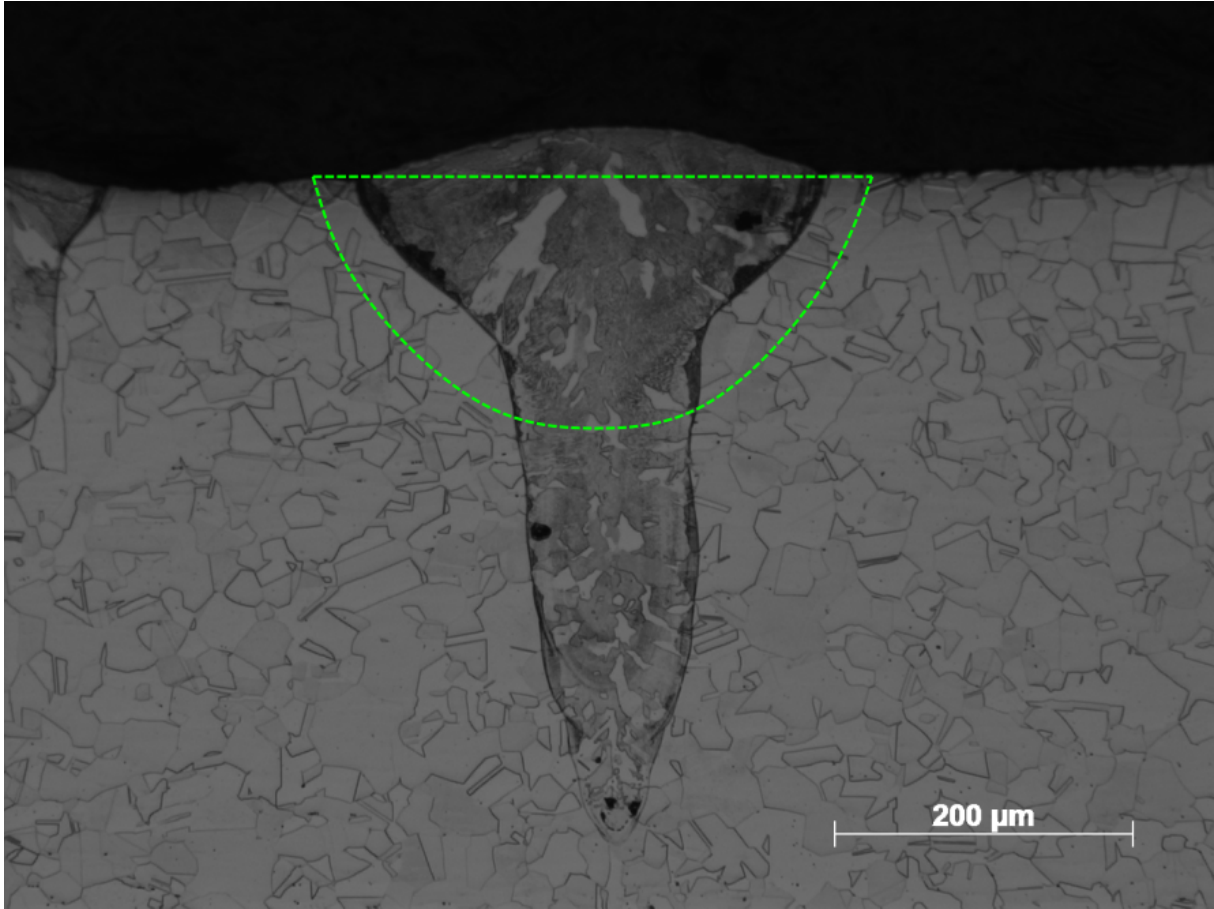


Figure C.16: 190 W 100 mm/s

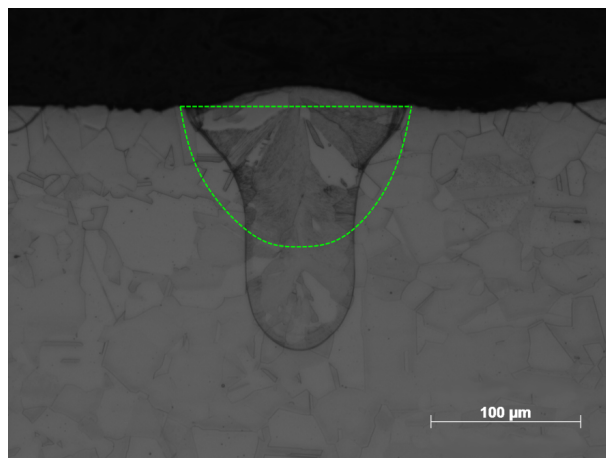


Figure C.17: 190 W 500 mm/s

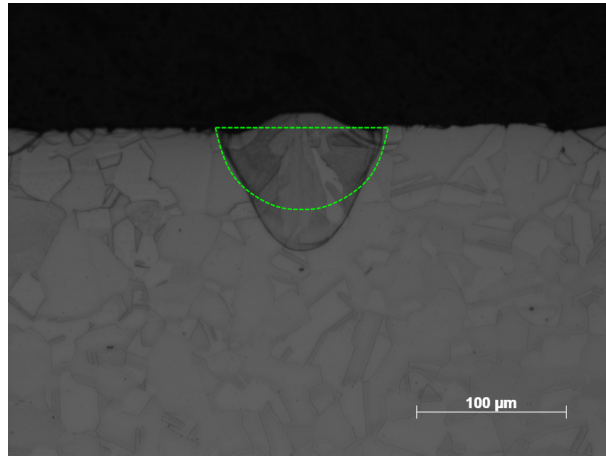


Figure C.18: 190 W 900 mm/s

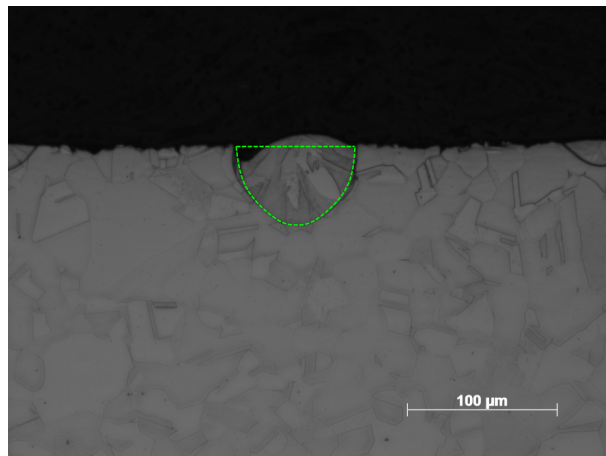


Figure C.19: 190 W 1300 mm/s

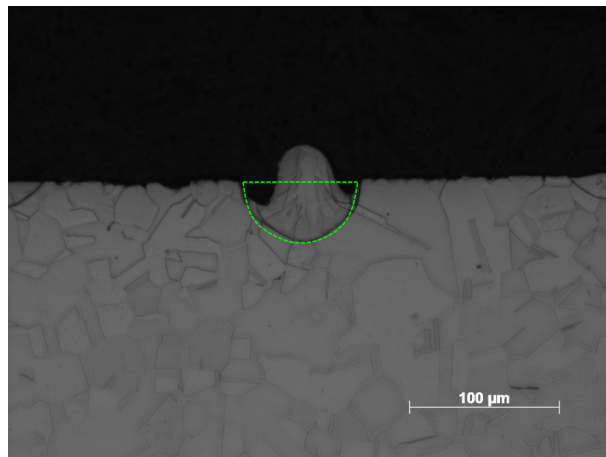


Figure C.20: 190 W 1700 mm/s

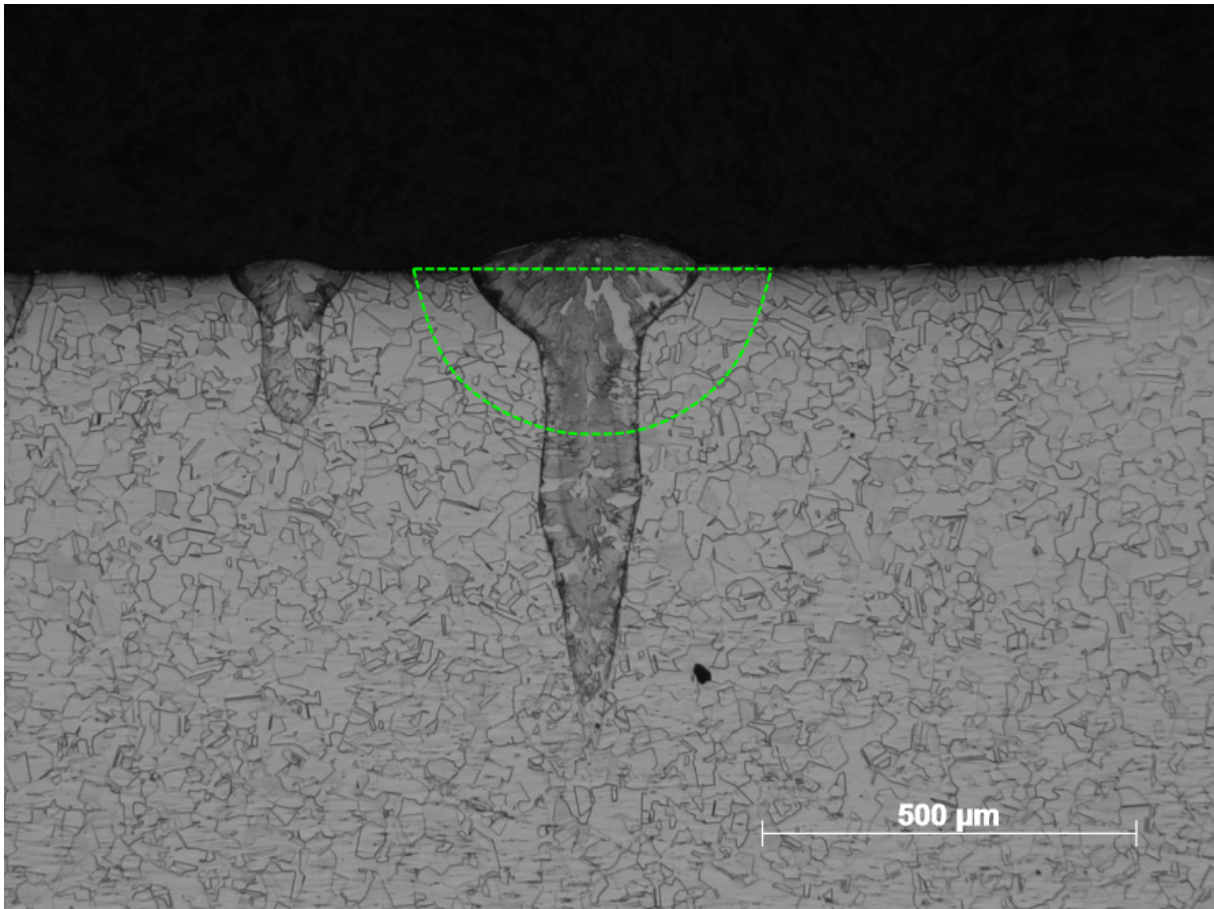


Figure C.21: 240 W 100 mm/s

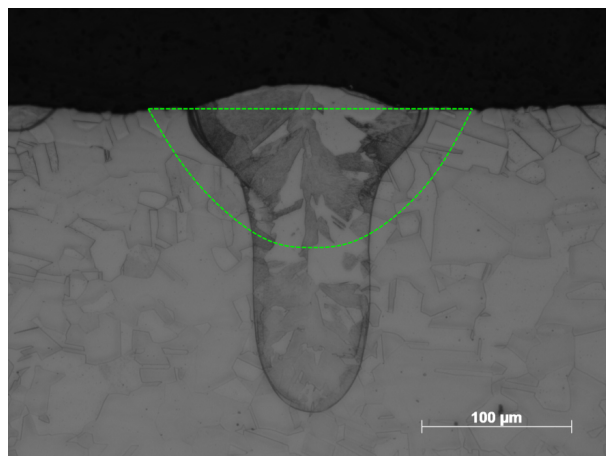


Figure C.22: 240 W 500 mm/s

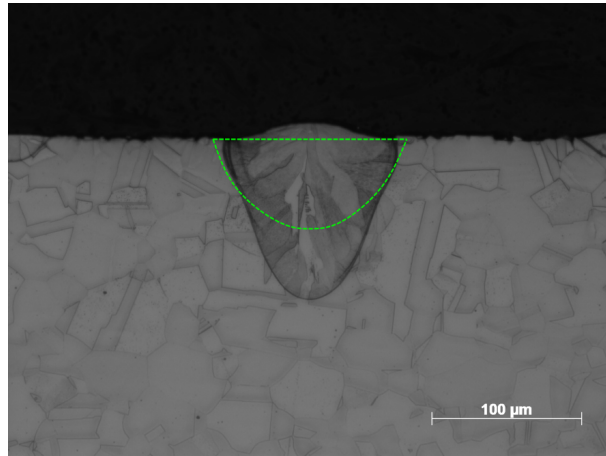


Figure C.23: 240 W 900 mm/s

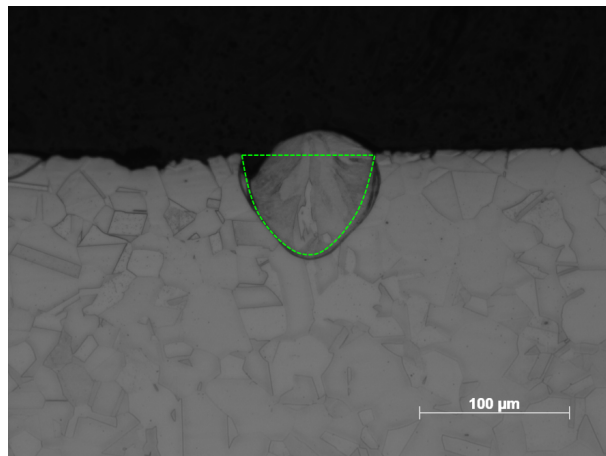


Figure C.24: 240 W 1300 mm/s

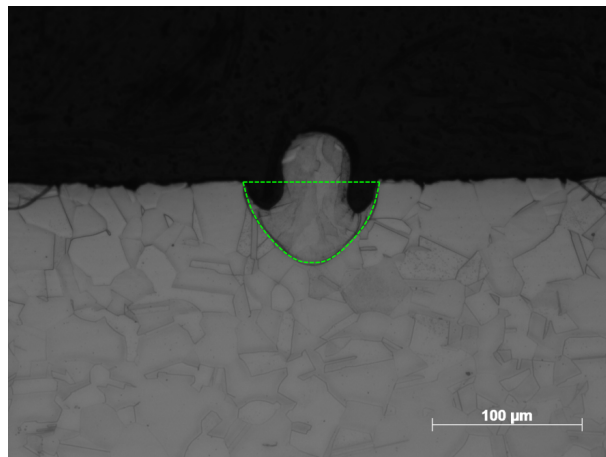


Figure C.25: 240 W 1700 mm/s

References

- [1] L Boltzmann. "Ableitung des Stefan'schen Gesetzes, betreffend die Abhängigkeit der Wärmestrahlung von der Temperatur aus der electromagnetischen Lichttheorie". *Annalen der Physik*, 258(6):291–294, 1884.
- [2] GVR. Additive Manufacturing Market Size, Share & Trends Analysis Report By Component, By Printer Type, By Technology, By Software, By Application, By Vertical, By Material, By Region, And Segment Forecasts, 2024 - 2030. Technical report, GVR, 2023.
- [3] I. Gibson, D. Rosen, B. Stucker, and K. Mahyar. *Additive Manufacturing Technologies*. Springer, Cham, Geneva, Switzerland, 3rd edition, 2020.
- [4] Management Engineering Production Services International. World Stainless Steel Prices, 2024.
- [5] MSE Supplies LLC. MSE Stainless Steel Powder for Additive Manufacturing, 2024.
- [6] Autodesk. Autodesk Netfabb Simulation, 2022.
- [7] Y. Hagedorn. Laser additive manufacturing of ceramic components: Materials, processes, and mechanisms. *Laser Additive Manufacturing: Materials, Design, Technologies, and Applications*, 6608:163–180, 2016.
- [8] J. P. Kruth, G. Levy, F. Klocke, and T. H.C. Childs. Consolidation phenomena in laser and powder-bed based layered manufacturing. *CIRP Annals - Manufacturing Technology*, 56(2):730–759, 2007.

- [9] Peter Heinl, Andreas Rottmair, Carolin Körner, and Robert F. Singer. Cellular titanium by selective electron beam melting. *Advanced Engineering Materials*, 9(5):360–364, 2007.
- [10] Je Kerns. What ’ s the Difference Between Metal 3D Printing Processes ? *Technical Machine Design*, 90(Nov):1–9, 2019.
- [11] Christoph Meier, Ryan W. Penny, Yu Zou, Jonathan S. Gibbs, and A. John Hart. Thermophysical Phenomena in Metal Additive Manufacturing by Selective Laser Melting: Fundamentals, Modeling, Simulation and Experimentation. *Annual Review of Heat Transfer*, 2017.
- [12] Subodh C. Subedi, Ahmad Shahba, Mythili Thevamaran, Dan J. Thoma, and Krishnan Suresh. Towards the optimal design of support structures for laser powder bed fusion-based metal additive manufacturing via thermal equivalent static loads. *Additive Manufacturing*, 57, 2022.
- [13] Matthias Markl and Carolin Körner. Multiscale Modeling of Powder Bed-Based Additive Manufacturing. *Annual Review of Materials Research*, 46(1):93–123, 2016.
- [14] W. J. Sames, F. A. List, S. Pannala, R. R. Dehoff, and S. S. Babu. The metallurgy and processing science of metal additive manufacturing. *International Materials Reviews*, 61(5):315–360, 2016.
- [15] Timothy W.; Simpson. Additive Manufacturing for Large Parts Powder-bed fusion may not be the answer . *MMS Online*, 1(January):34–35, 2019.
- [16] Matthias Markl, Matthias Lodes, Martin Franke, and Carolin Körner. Additive manufacturing using selective electron beam melting. *Welding and Cutting*, 16(3):177–184, 2017.
- [17] Nikolay K. Tolochko, Yurii V. Khlopkov, Sergei E. Mozzharov, Michail B. Ignatiev, Tahar Laoui, and Victor I. Titov. Absorptance of powder materials suitable for laser sintering. *Rapid Prototyping Journal*, 6(3):155–161, 2000.

- [18] Roland Winston. *Nonimaging optics*. Elsevier Academic Press, Amsterdam ; Boston, Mass., 2005.
- [19] C. D. Boley, S. C. Mitchell, A. M. Rubenchik, and S. S. Q. Wu. Metal powder absorptivity: modeling and experiment. *Applied Optics*, 55(23):6496, 2016.
- [20] A. V. Gusarov and E. P. Kovalev. Model of thermal conductivity in powder beds. *Physical Review B - Condensed Matter and Materials Physics*, 80(2):16–20, 2009.
- [21] A. V. Gusarov and J. P. Kruth. Modelling of radiation transfer in metallic powders at laser treatment. *International Journal of Heat and Mass Transfer*, 48(16):3423–3434, 2005.
- [22] Silvia Vock, Burghardt Klöden, Alexander Kirchner, Thomas Weißgärber, and Bernd Kieback. Powders for powder bed fusion: a review. *Progress in Additive Manufacturing*, 0(0):0, 2019.
- [23] L D (Lev Davidovich) Landau. Electrodynamics of continuous media / by L.D. Landau and E.M. Lifshitz ; translated from the Russian by J.B. Sykes, J.S. Bell and M.J. Kearsley., 1984.
- [24] Johannes Trapp, Alexander M. Rubenchik, Gabe Guss, and Manyalibo J. Matthews. In situ absorptivity measurements of metallic powders during laser powder-bed fusion additive manufacturing. *Applied Materials Today*, 9:341–349, 2017.
- [25] Lien Chin, Lili E Ehrlich, Matthew J Powell-palm, Colt Montgomery, Jack Beuth, and Jonathan A Malen. Thermal conductivity of metal powders for powder bed additive manufacturing. *Additive Manufacturing*, 21(December 2017):201–208, 2018.
- [26] Yu Chen, Guglielmo Vastola, and Yong Wei Zhang. Optimization of Inert Gas Flow Inside Laser Powder Bed Fusion Chamber. In *Solid Freeform Fabrication 2018: Proceedings of the 29th Annual International Solid Freeform Fabrication Symposium - An Additive Manufacturing Conference, SFF 2018*, pages 1931–1939, 2018.

- [27] P. Bidare, I. Bitharas, R. M. Ward, M. M. Attallah, and A. J. Moore. Fluid and particle dynamics in laser powder bed fusion. *Acta Materialia*, 142:107–120, 2018.
- [28] C. J. Smith, S. Tammas-Williams, E. Hernandez-Nava, and I. Todd. Tailoring the thermal conductivity of the powder bed in Electron Beam Melting (EBM) Additive Manufacturing. *Scientific Reports*, 7(1):1–8, 2017.
- [29] I. Bitharas, A. Burton, A. J. Ross, and A. J. Moore. Visualisation and numerical analysis of laser powder bed fusion under cross-flow. *Additive Manufacturing*, 37(November 2020):101690, 2021.
- [30] Benedikt Roidl. Continuous Improvement in Gas Flow Design. Technical report, GE Additive, 2020.
- [31] S. N. Bose. Planck ’s Law and Light Quantum Hypothesis . *Zeitschrift für Physik*, 26(Received):1–4, 1924.
- [32] S (Subrahmanyan) Chandrasekhar. *Radiative transfer / by S. Chandrasekhar*. International series of monographs on physics (Oxford, England). Clarendon Press, Oxford, 1st ed. edition, 1950.
- [33] V. K. Bitjukov, Yu I. Khudak, and N. G. Gusein-Zade. Analytical Derivation of the Stefan–Boltzmann Law for Integral Radiance from Planck’s Law for Spectral Radiance. *Bulletin of the Lebedev Physics Institute*, 45(2):46–50, 2018.
- [34] ASTM International. Total Hemispherical Emittance of Surfaces up to 1400°C 1, 2020.
- [35] National Bureau of Standards. Interim report on the thermodynamics of chemical species important in aerospace technology. Technical report, U.S. Department of Commerce, Washington D.C., 2004.
- [36] Ravi K. Enneti, Rick Morgan, and Sundar V. Atre. Effect of process parameters on the Selective Laser Melting (SLM) of tungsten. *International Journal of Refractory Metals and Hard Materials*, 71(October 2017):315–319, 2018.

- [37] L. González-Fernández, E. Risueño, R. B. Pérez-Sáez, and M. J. Tello. Infrared normal spectral emissivity of Ti-6Al-4V alloy in the 500-1150 K temperature range. *Journal of Alloys and Compounds*, 541:144–149, 2012.
- [38] E Hryha, R Shvab, H Gruber, A Leicht, L Nyborg, Eduard Hryha, Ruslan Shvab, Hans Gruber, Alexander Leicht, and Lars Nyborg. Hryha. *La Metallurgica Italiana*, 3:34–39, 2018.
- [39] Chu Lun Alex Leung, Sebastian Marussi, Michael Towrie, Robert C. Atwood, Philip J. Withers, and Peter D. Lee. The effect of powder oxidation on defect formation in laser additive manufacturing. *Acta Materialia*, 166:294–305, 2019.
- [40] Kaihua Zhang, Kun Yu, Yufang Liu, and Yuejin Zhao. Effect of surface oxidation on emissivity properties of pure aluminum in the near infrared region. *Materials Research Express*, 4(8), 2017.
- [41] Hang Jin Jo, Jonathan L. King, Kyle Blomstrand, and Kumar Sridharan. Spectral emissivity of oxidized and roughened metal surfaces. *International Journal of Heat and Mass Transfer*, 115:1065–1071, 2017.
- [42] P. Bidare, I. Bitharas, R. M. Ward, M. M. Attallah, and A. J. Moore. Laser powder bed fusion at sub-atmospheric pressures. *International Journal of Machine Tools and Manufacture*, 130-131(March):65–72, 2018.
- [43] By R S Sagdeyev and V D Shafranov. Absorption of High-frequency Electromagnetic Energy in a High-temperature Plasma. In *2nd International Conference Geneva*, number C, pages 118–124, 1958.
- [44] Zhonghua Li, Bao Qiang Li, Peikang Bai, Bin Liu, and Yu Wang. Research on the thermal behaviour of a selectively laser melted aluminium alloy: Simulation and experiment. *Materials*, 11(7), 2018.
- [45] I. Newton. Scala Graduum Caloris. *Philosophical Transactions*, 22(270):824 – 829, 1701.

- [46] G.W. Richmann. Inquisitio in legen, secundum quam calor fluidi in vase contenti, certo temporis intervallo, in temperie aeris constanter eadem decrescit vel crescit. *Novi Commentarii Academiae Scientiarum Imperialis Petropolitanae*, 1:174 – 197, 1747.
- [47] J.H. Lambert. Tentamen de vi caloris, qua corpora dilatat, eiusdem dimensione. *Acta Helvetica*, 2:172 – 242, 1755.
- [48] P. Dulong and A. Petit. Recherches sur la Mesure des Tempe ratures et sur les Lois de la communication de la chaleur. *Annales de Chemie et de Physique*, 8:113 – 154, 225 – 264, 337 – 367, 1817.
- [49] Leifeng Liu, Qingqing Ding, Yuan Zhong, Ji Zou, Jing Wu, Yu Lung Chiu, Jixue Li, Ze Zhang, Qian Yu, and Zhijian Shen. Dislocation network in additive manufactured steel breaks strength–ductility trade-off. *Materials Today*, 21(4):354–361, 2018.
- [50] Chao Li, Michael F. Gouge, Erik R. Denlinger, Jeff E. Irwin, and Pan Michaleris. Estimation of part-to-powder heat losses as surface convection in laser powder bed fusion. *Additive Manufacturing*, 26(August 2018):258–269, 2019.
- [51] Michael Gouge, Erik Denlinger, Jeff Irwin, Chao Li, and Pan Michaleris. Experimental validation of thermo-mechanical part-scale modeling for laser powder bed fusion processes. *Additive Manufacturing*, 29, 2019.
- [52] Zhe Wu. *The selforganization phenomenon in RayleighBenard convection : a hydrodynamics*. PhD thesis, Cornell University, 2010.
- [53] Anton Kidess, Saša Kenjereš, Bernhard W. Righolt, and Chris R. Kleijn. Marangoni driven turbulence in high energy surface melting processes. *International Journal of Thermal Sciences*, 104:412–422, 2016.
- [54] C Marangoni. *Sull’espansione delle gocce d’un liquido galleggianti sulla superfice di altro liquido*. PhD thesis, University of Pavia, 1865.

- [55] J.C. Maxwell. On the Equilibrium of Heterogenous Substances. In *Proceedings of the Cambridge Philosophical Society Vol. II*, Cambridge, 1876.
- [56] C-L Navier. Sur les lois des mouvements des fluides, en ayant égard à l'adhésion des molecules. *Annales de Chemie et de Physique*, XIX(244), 1821.
- [57] Trong Nhan Le and Yu Lung Lo. Effects of sulfur concentration and Marangoni convection on melt-pool formation in transition mode of selective laser melting process. *Materials and Design*, 179(May):107866, 2019.
- [58] Author K C Mills, B J Keene, R F Brooks, A Shirali, Interfacial Phenomena, and Processing Apr. Marangoni Effects in Welding. *Philosophical Transactions : Mathematical , Physical and Engineering Sciences*, 356(1739):911–925, 2018.
- [59] B J Keene, K C Mills, and R F Brooks. Surface properties of liquid metals and their effects on weldability. *Materials Science and Technology*, 1(7):559–567, 1985.
- [60] Lee Aucott, Hongbiao Dong, Wajira Mirihanage, Robert Atwood, Anton Kidess, Shian Gao, Shuwen Wen, John Marsden, Shuo Feng, Mingming Tong, Thomas Connelly, Michael Drakopoulos, Chris R. Kleijn, Ian M. Richardson, David J. Browne, Ragnvald H. Mathiesen, and Helen V. Atkinson. Revealing internal flow behaviour in arc welding and additive manufacturing of metals. *Nature Communications*, 9(1):1–7, 2018.
- [61] D. K. Aidun and S. A. Martin. Effect of sulfur and oxygen on weld penetration of high-purity austenitic stainless steels. *Journal of Materials Engineering and Performance*, 6(4):496–502, 1997.
- [62] P. D. Lee, P. N. Quested, and M. McLean. Modelling of Marangoni effects in electron beam melting. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 356(1739):1027–1043, 1998.
- [63] Merton Corson Flemings. Solidification processing / (by) Merton C. Flemings., 1974.

- [64] Wilfried Kurz and D.J. Fisher. *Fundamentals of solidification*. Trans Tech Publications Ltd., Baech, Switzerland, fourth rev edition, 1998.
- [65] J.A. Dantzig and M. Rappaz. *Solidification / J.A. Dantzig and M. Rappaz*. Engineering sciences. Materials. EPFL Press, Lausanne, Switzerland, 2nd edition, 2016.
- [66] P-S Laplace and J Lovering. Méchanique Céleste (Translation). In *Proceedings of the American Academy of Arts and Sciences*, volume 24, pages 185–201. American Academy of Arts and Sciences, 1889.
- [67] L. E. Murr, S. A. Quinones, S. M. Gaytan, M. I. Lopez, A. Rodela, E. Y. Martinez, D. H. Hernandez, E. Martinez, F. Medina, and R. B. Wicker. Microstructure and mechanical behavior of Ti-6Al-4V produced by rapid-layer manufacturing, for biomedical applications. *Journal of the Mechanical Behavior of Biomedical Materials*, 2(1):20–32, 2009.
- [68] Lawrence E. Murr, Sara M. Gaytan, Diana A. Ramirez, Edwin Martinez, Jennifer Hernandez, Krista N. Amato, Patrick W. Shindo, Francisco R. Medina, and Ryan B. Wicker. Metal Fabrication by Additive Manufacturing Using Laser and Electron Beam Melting Technologies. *Journal of Materials Science and Technology*, 28(1):1–14, 2012.
- [69] Luke N. Carter, Christopher Martin, Philip J. Withers, and Moataz M. Attallah. The influence of the laser scan strategy on grain structure and cracking behaviour in SLM powder-bed fabricated nickel superalloy. *Journal of Alloys and Compounds*, 615:338–347, 2014.
- [70] L. N. Carter, X. Wang, N. Read, R. Khan, M. Aristizabal, K. Essa, and M. M. Attallah. Process optimisation of selective laser melting using energy density model for nickel based superalloys. *Materials Science and Technology (United Kingdom)*, 32(7):657–661, 2016.
- [71] Hossein Eskandari Sabzi, Suhyun Maeng, Xingzhong Liang, Marco Simonelli, Nesma T. Aboulkhair, and Pedro E.J. Rivera-Díaz-del Castillo. Controlling crack

- formation and porosity in laser powder bed fusion: Alloy design and process optimisation. *Additive Manufacturing*, 34(May):101360, 2020.
- [72] Chaolin Tan, Sheng Li, Khamis Essa, Parastoo Jamshidi, Kesong Zhou, Wenyou Ma, and Moataz M. Attallah. Laser Powder Bed Fusion of Ti-rich TiNi lattice structures: Process optimisation, geometrical integrity, and phase transformations. *International Journal of Machine Tools and Manufacture*, 141(April):19–29, 2019.
- [73] Morgan Letenneur, Alena Kreitchberg, and Vladimir Brailovski. Optimization of laser powder bed fusion processing using a combination of melt pool modeling and design of experiment approaches: Density control. *Journal of Manufacturing and Materials Processing*, 3(1), 2019.
- [74] Luke Nelson Carter. *Selective laser melting of nickel superalloys for high temperature applications*. PhD thesis, University of Birmingham, 2013.
- [75] K. G. Prashanth, S. Scudino, T. Maity, J. Das, and J. Eckert. Is the energy density a reliable parameter for materials synthesis by selective laser melting? *Materials Research Letters*, 5(6):386–390, 2017.
- [76] Shaaz Ghouse, Sarat Babu, Richard J. Van Arkel, Kenneth Nai, Paul A. Hooper, and Jonathan R.T. Jeffers. The influence of laser parameters and scanning strategies on the mechanical properties of a stochastic porous material. *Materials and Design*, 131:498–508, 2017.
- [77] Umberto Scipioni Bertoli, Alexander J. Wolfer, Manyalibo J. Matthews, Jean Pierre R. Delplanque, and Julie M. Schoenung. On the limitations of Volumetric Energy Density as a design parameter for Selective Laser Melting. *Materials and Design*, 113:331–340, 2017.
- [78] D. B. Hann, J. Iammi, and J. Folkes. A simple methodology for predicting laser-weld properties from material and laser parameters. *Journal of Physics D: Applied Physics*, 44(44), 2011.

- [79] Adrian Bejan. *Heat transfer*. Wiley, New York ; Chichester, 1993.
- [80] Y. F. Ternovoi, A. G. Tsipunov, S. B. Kuratchenko, O. M. Kuimova, and K. V. Kondakova. Pore Formation in Atomised Powders. *Poroshkovaya Metallurgiya*, 265(1):10–14, 1985.
- [81] P.V. Ananthapadmanabhan, S. Bhaduri, S.B. Bhaduri, R.W. Cahn, J.S. Colligon, A. Dollet, J.R. Groza, A. Inoue, K.N. Ishihara, H. Jones, K.F. Kobayashi, C.C. Koch, E.J. Lavernia, B. Li, B.X. Liu, C. Suryanarayana, F. Teyssandier, and N. Venkatramani. *Non-equilibrium processing of materials / edited by C. Suryanarayana*. Pergamon materials series ; v. 2. Pergamon, Amsterdam; New York, 1st ed. edition, 1999.
- [82] Iver E. Anderson, Emma M.H. White, and Ryan Dehoff. Feedstock powder processing research needs for additive manufacturing development. *Current Opinion in Solid State and Materials Science*, 22(1):8–15, 2018.
- [83] E.M. Stanciu, A.C. Pâvâlache, G.M. Dumitru, O.G. Dontu, D. Besnea, and I.M. Vasile. Mechanism of keyhole formation in laser welding. *The Romanian Review Precision Mathematics, Optics & Mechatronics*, 20(38):171–176, 2010.
- [84] R. Rai, J. W. Elmer, T. A. Palmer, and T. Debroy. Heat transfer and fluid flow during keyhole mode laser welding of tantalum, Ti-6Al-4V, 304L stainless steel and vanadium. *Journal of Physics D: Applied Physics*, 40(18):5753–5766, 2007.
- [85] Ross Cunningham, Cang Zhao, Niranjana Parab, Christopher Kantzos, Joseph Pauza, Kamel Fezzaa, Tao Sun, and Anthony D. Rollett. Keyhole threshold and morphology in laser melting revealed by ultrahigh-speed x-ray imaging. *Science*, 363(6429):849–852, 2019.
- [86] Patcharapit Promoppatum, Shi Chune Yao, P. Chris Pistorius, and Anthony D. Rollett. A Comprehensive Comparison of the Analytical and Numerical Prediction of the Thermal History and Solidification Microstructure of Inconel 718 Products Made by Laser Powder-Bed Fusion. *Engineering*, 3(5):685–694, 2017.

- [87] Rongxuan Wang, Benjamin Standfield, Chaoran Dou, Andrew Chung Chee Law, and Zhenyu Kong. Real-Time Process Monitoring and Closed-Loop Control on Laser Power Via a Customized Laser Powder Bed Fusion Platform. *SSRN Electronic Journal*, 66(August 2022):103449, 2022.
- [88] Qingsong Wei, Yin Xie, Qing Teng, Muyu Shen, Shanshan Sun, and Chao Cai. Crack Types, Mechanisms, and Suppression Methods during High-energy Beam Additive Manufacturing of Nickel-based Superalloys: A Review. *Chinese Journal of Mechanical Engineering: Additive Manufacturing Frontiers*, 1(4):100055, 2022.
- [89] Thomas Böllinghaus and Horst Herold. *Hot Cracking Phenomena in Welds*. Springer Berlin, Heidelberg, 3 2005.
- [90] Yuanbo T. Tang, Chinnapat Panwisawas, Joseph N. Ghousoub, Yilun Gong, John W.G. Clark, André A.N. Németh, D. Graham McCartney, and Roger C. Reed. Alloys-by-design: Application to new superalloys for additive manufacturing. *Acta Materialia*, 202:417–436, 2021.
- [91] Chuan Guo, Gan Li, Sheng Li, Xiaogang Hu, Hongxing Lu, Xinggang Li, Zhen Xu, Yuhan Chen, Qingqing Li, Jian Lu, and Qiang Zhu. Additive manufacturing of Ni-based superalloys: Residual stress, mechanisms of crack formation and strategies for crack inhibition. *Nano Materials Science*, 5(1):53–77, 2023.
- [92] M. G. Collins and J. C. Lippold. An investigation of ductility dip cracking in nickel-based filler materials - Part I. *Welding Journal (Miami, Fla)*, 82(10), 2003.
- [93] Xiaoqiang Zhang, Huabin Chen, Luming Xu, J. Xu, X. Ren, and Xiaoqi Chen. Cracking mechanism and susceptibility of laser melting deposited Inconel 738 superalloy. *Materials and Design*, 183:108105, 2019.
- [94] Luke N. Carter, Moataz M. Attallah, and Roger C. Reed. Laser Powder Bed Fabrication of Nickel-Base Superalloys: Influence of Parameters; Characterisation, Quantification and Mitigation of Cracking. In *Superalloys 2012*, pages 577–586. The Minerals, Metals & Materials Society (TMS), 2012.

- [95] P R Newswire. Stainless Steel Industry to Exceed \$182 Billion in Value by 2027 - Increasing Modern Construction of Buildings & Structures that Require Aesthetic Appeal and Extended Life, 2 2020.
- [96] Research and Markets. Global Stainless Steel (200 Series, 300 Series, 400 Series, Duplex) Market 2016-2024: POSCO, Acerinox, Baosteel, Aperam, and Outokumpu Dominate the \$127 Billion Industry - Research and Markets, 12 2016.
- [97] The united Nations. The Paris Agreement, 2015.
- [98] GE Additive. Shell and GE Additive metal 3D print oxygen hydrogen micromixer at Energy Transition Campus Amsterdam, 2022.
- [99] Thaddeus B Massalski, Hiroaki Okamoto, PRnbsp Subramanian, Linda Kacprzak, and William W Scott. *Binary alloy phase diagrams*, volume 1. American society for metals Metals Park, OH, 2nd edition, 1986.
- [100] J W Elmer, Todd A Palmer, Sudarsanam S Babu, W. Zhang, and Tarasankar Debroy. Direct Observations of Austenite , Bainite , and Martensite Formation during Arc Welding of 1045 Steel Using Time-Resolved X-ray Diffraction. *Welding Research*, 83(9), 2004.
- [101] aalco. Specification of 1.4404/316L, 2023.
- [102] K. C. Mills and M. J. Richardson. The Heat Capacity of $\text{Cu}_2\text{Te}(\text{c})$, $\text{CuTe}(\text{c})$, $\text{Ag}_2\text{Te}(\text{c})$ and $\text{Ag}_{1.64}\text{Te}(\text{c})$. *Thermochimica Acta*, 6:427–438, 1973.
- [103] K. D. Maglic, A. Cezairliyan, and V. E. Peletsky, editors. *Compendium of Thermophysical Property Measurement Methods, Volume 2*. Springer US, New York, 1992.
- [104] E. Griffiths and G.W.C. Kaye. The Measurement of Thermal Conductivity (Communication No. 1). *Royal Society Communications*, 52(2):71 – 98, 1923.

- [105] L A Chapman, A T Fry, and S J Roberts. Thermal Diffusivity and Thermal Conductivity Measurements on Oxide Scales. Technical Report July, National Physical Laboratory, Teddington, 2005.
- [106] H S (Horatio Scott) Carslaw and J C Jaeger. *Conduction of heat in solids*. Clarendon Press, Oxford, 2nd ed. edition, 1959.
- [107] W J Parker, R J Jenkins, C P Butler, and G L Abbott. Flash Method of Determining Thermal Diffusivity, Heat Capacity, and Thermal Conductivity. *Journal of Applied Physics*, 32:1967–1684, 1961.
- [108] Emilios Leonidas, Sabino Ayvar-Soberanis, Hatim Laalej, Stephen Fitzpatrick, and Jon R. Willmott. A Comparative Review of Thermocouple and Infrared Radiation Temperature Measurement Methods during the Machining of Metals. *Sensors*, 22(13):1–23, 2022.
- [109] Metal Powder Report. EOS GmbH - Taking the laser lead. *Metal Powder Report*, 69(3):24–27, 2014.
- [110] F Klocke, H Wirtz, and W Meiners. Direct manufacturing of metal prototypes and prototype tools. In *Proceedings of the SFF Symposium*, pages 141–148, 1996.
- [111] David Keicher. Beyond Rapid Prototyping to Direct Fabrication: Forming Metallic Hardware Directly from a CAD Solid Model. *Materials Technology*, 13:5–7, 1998.
- [112] J. P. Kruth, L. Froyen, J. Van Vaerenbergh, P. Mercelis, M. Rombouts, and B. Lauwers. Selective laser melting of iron-based powder. *Journal of Materials Processing Technology*, 149(1-3):616–622, 2004.
- [113] H. Meier and Ch Haberland. Experimentelle Untersuchungen zum Laserstrahlgenerieren Metallischer Bauteile. *Materialwissenschaft und Werkstofftechnik*, 39(9):665–670, 2008.
- [114] I. Yadroitsev, Ph Bertrand, and I. Smurov. Parametric analysis of the selective laser melting process. *Applied Surface Science*, 253(19):8064–8069, 2007.

- [115] K. Saeidi, X. Gao, Y. Zhong, and Z. J. Shen. Hardened austenite steel with columnar sub-grain structure formed by laser melting. *Materials Science and Engineering A*, 625:221–229, 2015.
- [116] Zhongji Sun, Xipeng Tan, Shu Beng Tor, and Wai Yee Yeong. Selective laser melting of stainless steel 316L with low porosity and high build rates. *Materials and Design*, 104:197–204, 2016.
- [117] K. Saeidi, X. Gao, F. Lofaj, L. Kvetková, and Z. J. Shen. Transformation of austenite to duplex austenite-ferrite assembly in annealed stainless steel 316L consolidated by laser melting. *Journal of Alloys and Compounds*, 633:463–469, 2015.
- [118] Y. Jin, M. Bernacki, G. S. Rohrer, A. D. Rollett, B. Lin, and N. Bozzolo. Formation of annealing twins during recrystallization and grain growth in 304L austenitic stainless steel. *Materials Science Forum*, 753:113–116, 2013.
- [119] Azdiar A. Gazder, Ahmed A. Saleh, and Elena V. Pereloma. Microtexture analysis of cold-rolled and annealed twinning-induced plasticity steel. *Scripta Materialia*, 65(6):560–563, 2011.
- [120] K. M. Bertsch, G. Meric de Bellefon, B. Kuehl, and D. J. Thoma. Origin of dislocation structures in an additively manufactured austenitic stainless steel 316L. *Acta Materialia*, 199:19–33, 2020.
- [121] John von Neumann. The general and logical theory of automata. *Systems Research for Behavioral Science: A Sourcebook*, v:97–107, 1963.
- [122] Jacob T. Schwartz, John von Neumann, and Arthur W. Burks. Theory of Self-Reproducing Automata, 1966.
- [123] H. W. Hesselbarth and I. R. Göbel. Simulation of recrystallization by cellular automata. *Acta Metallurgica Et Materialia*, 39(9):2135–2143, 1991.
- [124] R S Qin and H K D H Bhadeshia. Phase Field Method. *Materials Science and Technology*, 26(7):803–811, 2010.

- [125] David W. Hoffman and John W. Cahn. A vector thermodynamics for anisotropic surfaces. I. Fundamentals and application to plane surface junctions. *Surface Science*, 31(C):368–388, 1972.
- [126] R. S. Qin and H. K.D.H. Bhadeshia. Phase-field model study of the effect of interface anisotropy on the crystal morphological evolution of cubic metals. *Acta Materialia*, 57(7):2210–2216, 2009.
- [127] R. S. Qin and H. K.D.H. Bhadeshia. Phase-field model study of the crystal morphological evolution of hcp metals. *Acta Materialia*, 57(11):3382–3390, 2009.
- [128] Oliver Penrose and Paul C. Fife. Thermodynamically consistent models of phase-field type for the kinetic of phase transitions. *Physica D: Nonlinear Phenomena*, 43(1):44–62, 1990.
- [129] A. A. Wheeler, G. B. McFadden, and W. J. Boettinger. Phase-field Model for Solidification of a Eutectic Alloy, 1996.
- [130] N. Moelans, B. Blanpain, and P. Wollants. Quantitative analysis of grain boundary properties in a generalized phase field model for grain growth in anisotropic systems. *Physical Review B - Condensed Matter and Materials Physics*, 78(2), 2008.
- [131] Z Li, M Greenwood, and A Phillion. A phase field methodology for simulating the microstructure evolution during laser powder bed fusion in-situ alloying process. *IOP Conference Series: Materials Science and Engineering*, 1281(1):012017, 2023.
- [132] Z. Zhang, Z. J. Tan, X. X. Yao, C. P. Hu, P. Ge, Z. Y. Wan, J. Y. Li, and Q. Wu. Numerical methods for microstructural evolutions in laser additive manufacturing. *Computers and Mathematics with Applications*, 78(7):2296–2307, 2019.
- [133] Lu Li, Ji Qin Li, and Tai Hsi Fan. Phase-field modeling of wetting and balling dynamics in powder bed fusion process. *Physics of Fluids*, 33(4), 2021.

- [134] Cunyi Li, Jianguang Fang, Yuheng Wan, Na Qiu, Grant Steven, and Qing Li. Phase field fracture model for additively manufactured metallic materials. *International Journal of Mechanical Sciences*, 251(January):108324, 2023.
- [135] Mohammad Hossein Mosallanejad, Behzad Niroumand, Alberta Aversa, and Abdollah Saboori. In-situ alloying in laser-based additive manufacturing processes: A critical review. *Journal of Alloys and Compounds*, 872:159567, 2021.
- [136] Shahed Rezaei, Ali Harandi, Tim Brepols, and Stefanie Reese. An anisotropic cohesive fracture model: Advantages and limitations of length-scale insensitive phase-field damage models. *Engineering Fracture Mechanics*, 261(December 2021):108177, 2022.
- [137] Paul Meakin and R Jullien. Restructuring effects in the rain model for random deposition. *Journal De Physique*, 48:1651–1662, 1987.
- [138] Carolin Körner, Elham Attar, and Peter Heinl. Mesoscopic simulation of selective beam melting processes. *Journal of Materials Processing Technology*, 211(6):978–987, 2011.
- [139] Pooja Bhalode and Marianthi Ierapetritou. Discrete element modeling for continuous powder feeding operation: Calibration and system analysis. *International Journal of Pharmaceutics*, 585(February):119427, 2020.
- [140] Y. Lee. *Simulation of Laser Additive Manufacturing and its Applications*. PhD thesis, Ohio State University, 2015.
- [141] Atul Dubey, Avik Sarkar, Marianthi Ierapetritou, Carl R. Wassgren, and Fernando J. Muzzio. Computational approaches for studying the granular dynamics of continuous blending processes, 1 - DEM based methods. *Macromolecular Materials and Engineering*, 296(3-4):290–307, 2011.
- [142] Bruno Chareyre and Pascal Villard. Dynamic Spar Elements and Discrete Element Methods in Two Dimensions for the Modeling of Soil-Inclusion Problems. *Journal of Engineering Mechanics*, 131(7):689–698, 2005.

- [143] Yunafang Cheng, Shijiun Guo, and Heyi Lai. Computer simulation of random packing of spherical particles. *Beijing Keji Daxue Xuebao/Journal of University of Science and Technology Beijing*, 21(4):387–391, 1999.
- [144] Frédéric Victor Donzé. Impacts on cohesive frictional geomaterials. A DEM analysis applied to concrete. *Revue européenne de génie civil*, 12(7-8):967–985, 2008.
- [145] Benjamin Thomas Stegman, Jack Lopez, William Jarosinski, Haiyan Wang, and Xinghang Zhang. The Influence of Powder Particle Size Distributions on Mechanical Properties of Alloy 718 by Laser Powder Bed Fusion. *Metals*, 13(8):1–11, 2023.
- [146] M. Rombouts, L. Froyen, A. V. Gusarov, E. H. Bentefour, and C. Glorieux. Photopyroelectric measurement of thermal conductivity of metallic powders. *Journal of Applied Physics*, 97(2), 2005.
- [147] A. V. Gusarov, T. Laoui, L. Froyen, and V. I. Titov. Contact thermal conductivity of a powder bed in selective laser sintering. *International Journal of Heat and Mass Transfer*, 46(6):1103–1109, 2003.
- [148] Loong Ee Loh, Chee Kai Chua, Wai Yee Yeong, Jie Song, Mahta Mapar, Swee Leong Sing, Zhong Hong Liu, and Dan Qing Zhang. Numerical investigation and an effective modelling on the Selective Laser Melting (SLM) process with aluminium alloy 6061. *International Journal of Heat and Mass Transfer*, 80:288–300, 2015.
- [149] M. F. Zäh and S. Lutzmann. Modelling and simulation of electron beam melting. *Production Engineering*, 4(1):15–23, 2010.
- [150] N. Contuzzi, S. L. Campanelli, and A. D. Ludovico. 3D finite element analysis in the Selective Laser Melting process. *International Journal of Simulation Modelling*, 10(3):113–121, 2011.
- [151] Peter Mercelis and Jean Pierre Kruth. Residual stresses in selective laser sintering and selective laser melting. *Rapid Prototyping Journal*, 12(5):254–265, 2006.

- [152] Itziar Serrano-Munoz, Tatiana Mishurova, Tobias Thiede, Maximilian Sprengel, Arne Kromm, Naresh Nadammal, Gert Nolze, Romeo Saliwan-Neumann, Alexander Evans, and Giovanni Bruno. The residual stress in as-built Laser Powder Bed Fusion IN718 alloy as a consequence of the scanning strategy induced microstructure. *Scientific Reports*, 10(1):1–15, 2020.
- [153] Yukio Ueda, Keiji Fukuda, Keiji Nakacho, and Setsuo Endo. A New Measuring Method of Residual Stresses with the Aid of Finite Element Method and Reliability of Estimated Values. *Journal of the Society of Naval Architects of Japan*, 1975(138):499–507, 1975.
- [154] Nils Keller and Vasily Ploshikhin. New method for fast predictions of residual stress and distortion of AM parts. *25th Annual International Solid Freeform Fabrication Symposium & Additive Manufacturing Conference, SFF 2014*, pages 1229–1237, 2014.
- [155] Pedro Alvarez, Joseba Ecenarro, Iñaki Setien, Maria San Sebastian, Alberto Echeverria, and Luka Eciolaza. Computationally efficient distortion prediction in Powder Bed Fusion Additive Manufacturing. *International Journal of Engineering Research & Science*, 2(10):39–46, 2016.
- [156] J. Gil, M. Pires, F. Fiorentin, M. Vaz, A. Castanhola, M. Parente, and A. de Jesus. Numerical modeling and prediction of residual stresses in AISI 316L and 18Ni300 steels produced by selective laser melting. *Procedia Structural Integrity*, 34(2019):6–12, 2021.
- [157] Erik R Denlinger, Michael Gouge, Pan Michaleris, Erik R Denlinger, Jeff Irwin, Jarred C Heigel, Michael Gouge, Erik R Denlinger, Michael Gouge, Erik R Denlinger, Allison M Beese, Long-Qing Lei Chen, Long-Qing Lei Chen, Erik R Denlinger, Alexander J Dunbar, Michael Gouge, Jarred C Heigel, Jeff Irwin, Yanzhou Ji, Pan Michaleris, Michael Gouge, Pan Michaleris, Allison M Beese, Yanzhou Ji, Long-Qing Lei Chen, Long-Qing Lei Chen, and Jeff Irwin. *Thermo-Mechanical Modeling of Additive Manufacturing*. Butterworth-Heinemann, 2018.

- [158] Chigusa Kita. Events and Sightings. *IEEE Annals of the History of Computing*, 34(2):60–69, 2012.
- [159] J.A. Weisbecker. Build the PIXIE Graphic Display. *Popular Electronics*, page 41, 1977.
- [160] DOS Days. 3Dfx Interactive, Inc., 2024.
- [161] Nvidia. Nvidia Ada Gpu Architecture. Technical report, NVIDIA, 2022.
- [162] AMD. AMD Radeon RX 7900 XTX, 2023.
- [163] Tech Power Up. Nvidia GeForce 256, 2004.
- [164] Nvidia. Nvidia RTX 40 Series, 2024.
- [165] Farid Pazhoohi and Alan Kingstone. The Effect of Movie Frame Rate on Viewer Preference: An Eye Tracking Study. *Augmented Human Research*, 6(1):1–5, 2021.
- [166] Amazon Web Services. CPU vs GPU, 2024.
- [167] J.Z. Czech. *Introduction to Parallel Computing*. Cambridge University Press, Cambridge, U.K., 1st edition, 2016.
- [168] Amazon Web Services. AWS Pricing, 2024.
- [169] R. Courant, H. Lewy, and K. Friedrichs. Über die partiellen Differenzengleichungen der mathematischen Physik. *Mathematische Annalen*, 100(43):32–74, 1928.
- [170] R. Clausius. Ueber die bewegende Kraft der Wärme und die Gesetze, welche sich daraus für die Wärmelehre selbst ableiten lassen. *Annalen der Physik*, 155(3):368–397, 1850.
- [171] J.B.J Fourier. *Théorie analytique de la chaleur*, par M . Fourier. Fermin Didot, Paris, 1822.
- [172] William F. Trench. On the eigenvalue problem for Toeplitz band matrices. *Linear Algebra and Its Applications*, 64(C):199–214, 1985.

- [173] S. E. Ekström and S. Serra-Capizzano. Eigenvalues and eigenvectors of banded Toeplitz matrices and the related symbols. *Numerical Linear Algebra with Applications*, 25(5):1–17, 2018.
- [174] G. Kirchhoff. On the relationship between the emissivity and absorptivity of a body for heat and light. *Annalen de Physik*, 109:275–301, 1860.
- [175] Komron J. Shayegan, Souvik Biswas, Bo Zhao, Shanhui Fan, and Harry A. Atwater. Direct observation of the violation of Kirchhoff’s law of thermal radiation. *Nature Photonics*, 17(10):891–896, 2023.
- [176] J. Goldak, A. Chakravarti, and M. Bibby. A New Finite Element Model for Welding Heat Sources. *Metallurgical Transactions B*, 15B:305, 1984.
- [177] V.D. Fachinotti, A.A. Ancar, and A. Cadona. Analytical solutions of the thermal field induced by moving double-ellipsoidal and double-elliptical heat sources in a semi-infinite body. *International Journal for Numerical Methods in Biomedical Engineering*, 27(4):595–607, 2011.
- [178] N. T. Nguyen, A. Ohta, K. Matsuoka, N. Suzuki, and Y. Maeda. Analytical Solutions for Transient Temperature of Semi-Infinite Body Subjected to 3-D Moving Heat Sources. *Welding Journal (Miami, Fla)*, 78(8), 1999.
- [179] Zhidong Zhang, Yuze Huang, Adhitan Rani Kasinathan, Shahriar Imani Shahabad, Usman Ali, Yahya Mahmoodkhani, and Ehsan Toyserkani. 3-Dimensional heat transfer modeling for laser powder-bed fusion additive manufacturing with volumetric heat sources based on varied thermal conductivity and absorptivity. *Optics and Laser Technology*, 109:297–312, 1 2019.
- [180] Erik R. Denlinger, Jeff Irwin, and Pan Michaleris. Thermomechanical modeling of additive manufacturing large parts. *Journal of Manufacturing Science and Engineering, Transactions of the ASME*, 136(6):1–8, 2014.

- [181] Dominik Schötzau and Christoph Schwab. Time discretization of parabolic problems by the hp-version of the discontinuous Galerkin finite element method. *SIAM Journal on Numerical Analysis*, 38(3):837–875, 2001.
- [182] nTop. Guide to lattice structures in additive manufacturing, 2022.
- [183] ASTM. ASTM D7896-19 - Standard Test Method for Thermal Conductivity, Thermal Diffusivity, and Volumetric Heat Capacity of Engine Coolants and Related Fluids by Transient Hot Wire Liquid Thermal Conductivity Method, 2019.
- [184] P. Bidare, R. R.J. Maier, R. J. Beck, J. D. Shephard, and A. J. Moore. An open-architecture metal powder bed fusion system for in-situ process measurements. *Additive Manufacturing*, 16:177–185, 2017.
- [185] Kenneth C Mills. *Recommended Values of Thermophysical Properties for Selected Commercial Alloys*. Woodhead Publishing, Sawston, 1st edition, 2002.
- [186] Ming Liu, Louis N S Chiu, Dedao Liu, Aijun Huang, Chris Davies, Xinhua Wu, and Wenyi Yan. A macroscale thermal simulation strategy with track-scale resolution for laser powder bed fusion. *Materials & Design*, 226, 2023.
- [187] Manyalibo Matthews, Johannes Trapp, Gabe Guss, and Alexander Rubenchik. Direct measurements of laser absorptivity during metal melt pool formation associated with powder bed fusion additive manufacturing processes. *Journal of Laser Applications*, 30(3):032302, 2018.
- [188] I. Bitharas, N. Parab, C. Zhao, T. Sun, A. D. Rollett, and A. J. Moore. The interplay between vapour, liquid, and solid phases in laser powder bed fusion. *Nature Communications*, 13(1):1–12, 2022.
- [189] A J Ross, I Bitharas, K G Perkins, and A J Moore. Volumetric heat source calibration for laser powder bed fusion. *Additive Manufacturing*, 60, 2022.

-
- [190] A. V. Gusarov and I. Smurov. Radiation transfer in metallic powder beds used in laser processing. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 111(17-18):2517–2527, 2010.
- [191] A. M. Philo, S. Mehraban, M. Holmes, S. Sillars, C. J. Sutcliffe, J. Sienz, S. G.R. Brown, and N. P. Lavery. A pragmatic continuum level model for the prediction of the onset of keyholing in laser powder bed fusion. *International Journal of Advanced Manufacturing Technology*, 101(1-4):697–714, 2019.
- [192] Wayne E. King, Holly D. Barth, Victor M. Castillo, Gilbert F. Gallegos, John W. Gibbs, Douglas E. Hahn, Chandrika Kamath, and Alexander M. Rubenchik. Observation of keyhole-mode laser melting in laser powder-bed fusion additive manufacturing. *Journal of Materials Processing Technology*, 214(12):2915–2925, 2014.
- [193] David V (David Vernon) Widder. The heat equation / D.V. Widder., 1975.
- [194] A Salih. Classification of Partial Differential Equations and Canonical Forms 1 Second-Order Partial Differential Equations, 2014.