Microstructure prediction in additive manufacturing

(TA6V, AlSi10Mg, AlSI M4 materials)

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University campus is up hill in Sart-Tilman



Materials and microstructure



Materials and microstructure & Additive Process

What is the scale of interest?

What are you looking for ?

Static rupture, fatigue rupture?

Where is the weak point?

Santos Macias et al. Scripta Materialia 170 (2019)

Delahaye et al. Acta Materialia (2019)





AM Habraken 6/12/2019 6

Directed Energy Deposition "Easiest" case



Surface tension, Marangoni, Recoil pressure



S. A. Khairallah, A. T. Anderson, A. Rubenchik, and W. E. King. Laser powder-bed fusion additive manufacturing: Physics of complex melt flow and formation mechanisms of pores, spatter, and denudation zones. *Acta Materialia*, 108:36–45, 2016.

 \rightarrow convection-related terms can not be ignored

in calculations of the energy balance in the interaction zone

in calculations of the thermal field in the melt pool in the vicinity of the melt pool

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Challenges about Additive Manufacturing

About Ti6Al4V and phase prediction

What is the goal with AlSi10Mg?

Why is AISI M4 challenging and interesting?



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FROM 1990to 2020

Evolution of the microstructure predictions

PhD (A.M.Habraken, 1989) Coupled thermo mechanical metallurgical analysis during the cooling process of steel pieces (A.M.Habraken, M. Bourdouxhe, Eur.J. Mec A/Solids11(1992)

Microstructure = % phases

Finite element simulations Phenomenological models based on Johnson-Mehl-Avrami-Kolmogorov (JMAK)

Kinetics of Phase transformation explains depth of martensite and curvature during cooling





Evolution of the microstructure predictions

Quite monotonous thermal history still lack of data...

Still effective for some cases

Experiments \rightarrow TTT, often CCT JMAK model = isothermal simulations

Extension towards anisothermal case





Current Evolution of the microstructure predictions

Thermodynamic models and commercial softwares "able" to generate TTT

 \rightarrow Equilibrium diagrams (Calphad,...)

- by minimization of Gibbs energy (each contribution ...)
 - \rightarrow with extended JMAK at anisothermal case \rightarrow kinetics

 \rightarrow Kinetics of phase transformations and phase morphology

by Phase Field approach or Finite elements (slower)
Knowledge of chemical potentials derived from Gibbs energy of the phases,
the nucleation force, phase interface velocity, diffusion equations,
chemical balance... (Tioual PhD 2019 TITAN application ≠ Ti alloy)



Azizi et al. for AlSi10Mg in TMS 2019 Keller et al. For Ni-based superalloys Acta Mat 2017

Finite elements → Tp°(t),
Dictra // Phase Field
→ Microsegregation predictions



learning

??

Machine

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Challenges about Additive Manufacturing (simulations)

Long process

- \rightarrow length of CPU time finite element simulation
- \rightarrow which tricks ?
- ightarrow heterogeneity & complex history of the temperature field

Mixture of liquid and solid state

- \rightarrow CFD + solid FE ?
- \rightarrow PI FEM... (Terrapon Ponthot Bobach PhD ongoing)

High temperature gradient

- ightarrow microstructure mechanisms not well identified
- ightarrow mixture of length scales
- ightarrow lack of material data

High temperature robust camera → big data	Residual stress measurements in depth			
Lack of material data	Multi disciplinary field			
Hard to measure in similar conditions	3D PI FEM liquid- solid thermo mechanic			

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Contents lists available at ScienceDirect

Materials and Design



journal homepage: www.elsevier.com/locate/jmad

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2020 PhD thesis J. Tchuindjang

Laser cladding as repair technology for Ti–6Al–4V alloy: Influence of building strategy on microstructure and hardness



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3D thermal finite element analysis of laser cladding processed Ti-6Al-4V part with microstructural correlations



H.-S. Tran^a, J.T. Tchuindjang^b, H. Paydas^b, A. Mertens^b, R.T. Jardin^a, L. Duchêne^a, R. Carrus^c, J. Lecomte-Beckers^b, A.M. Habraken^{a,*}

2018 Microstru

Microstructure prediction of Ti6Al4V processed by Laser Cladding Master Thesis Elena Esteva Fabrega



1998 Toward a Continuous Cooling Transformations CCT

100 µm

R. Dąbrowski, Archives of Metallurgy and Materials 56 (2011) 703–707.

19



J.Sieniawski et al. Intech Open 2013



Diffusional transformation ($\alpha' \rightarrow \alpha + \beta, \beta \leftrightarrow \alpha$): JMAK Model + additivity rule $f_{\alpha'}(T + dT) = 1 - [1 - \exp[-k(t^f + \Delta t)^n]](1 - f_{\alpha'}{}^{eq})$

f phase fraction

k,*n* JMAK coefficients (depending on T)

 t^{f} = fictious time which would have resulted in fraction f of previous timestep at T + dT



Displacive transformation ($\beta \rightarrow \alpha$ '): Koisitinen – Marburger model $f_{\alpha'}(T) = f_{\alpha'}(T_0) + (f_{\beta T_0} - f_{\beta r})[1 - \exp[-\gamma(M_s - T)]]$

 T_0 temperature at which the martensitic transformation starts defining the quantity of parent phase. If the transfo. end tp° known M_f then γ is known

For additive simulations values vary in the literature, for cooling:

- (Tan et al. 2015) $M_s = 1073 \text{ K}$
- (Kelly SM 2004)
- (Charles Murgau C et al. 2012)
- (Crespo A, et al. 2010)
- (Jovanovic et al. 2006)

 $M_{s} = 1073$ K $M_{s} = 848$ K

 $M_{\rm s} = 923 \text{ K}$ $M_{\rm f} = 673 \text{ K}$ $M_{\rm f} = 298 \text{ K}$ Effect of *T Ť* of composition of parent phase → Need of thermodynamics → Difficult in all integration points of a FE mesh



JMAK for diffusional transf.

Experiments

Tran et al.

Materials &

Design 2017

Laser cladding for Ti6Al4V alloy: influence of building strategy on microstructure and hardness.



Decreasing Track Length (DTL) strategy



Paydas, et al. Materials and Design 2015.







Experimental data

Final microstructure in CTL



Results of indentation campaign

(C)

(a) Decrease Track Length (DTL) (b)



Hardness maps and corresponding hardness indentation grids

Paydas et al. Materials and Design 2015.

300

Temperature measurement



FE inverse modelling to identify convection coefficient Sensitivity analysis: T° at thermocouple





Decrease Track Length strategy





2D view of thermal field within HAZ

Validation	Depth	Layer 1	Layer 2	Layer 3	Layer 4	Layer 5
	h _{DL} (μm)	508	688	709	730	793
Simulation result	h _{HAZ} (μm) HAZ _a + HAZ	1618	1864	2174	2377	2605
	·	450				
Measured	n _{DL} (μm)	450	Not accessible, different zones cannot be recovered			
	h _{HAZ} (μm)	1501				
	HAZ_{β} + $HAZ_{\alpha+\beta}$					









Decrease Track Length strategy










Hardness measurement (Hakan et al. 2015)

Tran's Conclusion 2017

Qualitative microstructure prediction with Kelly Ms value// experience $M_s 800^{\circ}$ C and 848° C M_s for α_m HAZ size in substrate validated

Prediction in Constant Track Length:

- Quite Homogeneous T[°] history
- $T_{average} > M_s$ when \dot{T} high
- at the end T < Ms but \dot{T} low

Wi

Basket-weave Widmanstätten structure

Prediction in Decrease Track Length:

- Heterogenous T° history
- At some points :

 $T_{average} < Ms + \dot{T}$ high

Basket-weave Widmanstätten structure + α' Martensite

Crespo vs Esteva Master 2018 thesis (\rightarrow quantitative)

		Crespo	Esteva
	Liquidus	1650 °C	1660 °C
Cooling	Boundaries rates	T < −410°C/s	7 < -410°С/s -410°С/s < Т < -20°С/s Т > -20°С/s
	Ms, Mf	650 °C, 400 °C	655 °C, 355 °C
	$lpha_m$ existance	No	Yes
Heating	Equation $\alpha' \rightarrow \beta$ and α	JMAK	K-M



Experimental data obtained from H.Paydas et al. (2015) Phases hardness values obtained from Pederson (2002) and Crespo (2010).



Obtained Hardness values (Esteva)

Mixture Law:



About Ti6Al4V and phase prediction

Themodynamics approaches must be further developed to get better knowledge about Transformations (start, end, kinetics) for various compositions as well as element diffusion under complex Tp° history (TITAN code T=cte... PhD Tioual Nancy supervised by Benoit Appolaire 2019)... + links with Phase fields

Post processing of T(t), computed by Finite elements, by Crespo type model based on previous results could predict microstructure

 \rightarrow Coupling is important or machine learning....

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Goal= study of static rupture in AlSi10Mg-SLM, (...delaying it...)



Goal= study of static rupture in AlSi10Mg-SLM, (...delaying it...)



Goal= study of static rupture in AlSi10Mg-SLM, (...delaying it...)

Measurements do not dissociate Si in precipitate and Si within the eutectic

Lower value in HAZ → partial decomposition of MPFine eutectic increases Si precipitate size Network of eutectic phase is broken



Goal= study of static rupture in AlSi10Mg-SLM,

(...delaying it...)

HAZ is the risky zone \rightarrow optimal parameters should decrease its size

Use of

Rosenthal equation ('direct', a lot of assumptions) \rightarrow temperature history \rightarrow cell parameters

or

Finite element simulations (heavier, more details tp° hstory, need input data)

Process parameters \rightarrow temperature history \rightarrow cell parameters

Thermal field during SLM – Rosenthal's equation

P laser power
c absorbed power coefficient
T0 building plate temperature
k thermal conductivity
α thermal diffusivity

Moving coordinate system : $\xi = x - vt$



$$T = T_0 + \frac{Pc}{2\pi Rk} e^{\frac{-\nu(\xi+R)}{2\alpha}} R = (\xi^2 + y^2 + z^2)^{\frac{1}{2}}$$



Thermal field and link with cell size

Thermal history during SLM – Rosenthal's equation¹:

$$T = T_0 + \frac{Pc}{2\pi Rk} e^{\frac{-\nu(\xi+R)}{2\alpha}} R = (\xi^2 + y^2 + z^2)^{\frac{1}{2}}$$

Cell size vs cooling rate – Matyja's equation²:

$$\lambda = 43.2\dot{T}^{-0.324}$$

Parameter used in Rosenthal's equation:

Parameter	this study	Tang16 ³
Conductivity, $k \ [W/mK]$	150	150
Diffusivity, $\alpha \ [m^2/s]$	6.2^{-5}	6.2^{-5}
Liquidus, T_{liq} [K]	867	867
Solidus, T_{sol} [K]	831	831
Building Plate temperature, T_0 [K]	473	308
Laser Power, P $[W]$	175	370
Beam travel speed, $\nu \ [m/s]$	0.195	1.3
Absorbed power coefficient, $[-]$	0.35	0.35

¹D. Rosenthal, Weld. J. 20 (1941) 220–234.

²H. Matyja, Journal of the Institute of Metals 96 (1968) 30–32.

³M. Tang, P.C. Pistorius, S. Narra, J.L. Beuth, JOM 68 (2016) 960–966.



Results focused on HAZ Simulation // Experiment



Process parameters modifies HAZ width:

5 µm (Delahaye Acta Mat 2019) - fracture strain 1.8%

2 µm (Tang JOM 2017) - fracture strain 12.5%

2 µm (Zhao Mat. Sc. & Eng. A 2019)- fracture strain 11% but different loading direction and mechanism

What about the interest of FE Simulation

Heat conduction equation :

$$\frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) + Q_{x,y,t} = \rho C_p \frac{\partial T}{\partial t}$$

Convection / radiation heat loss :

$$-k\left(\nabla T.n\right) = q_{\text{laser}} - h\left(T - T_0\right) - \epsilon\sigma\left(T^4 - T_0^4\right)$$







What about the interest of FE Simulation?

1. Validation and identification (1 layer) :

Melt pool depth :

Exp. : 90-120 μ m (part supplier)





Thermo-physical properties :

—Bulk : Cp(T), $\rho(T)$ and k(T) measured in MMS

on SLM samples

-Powder : k(T) Sih and Barlow's model¹

-Constant ε

Moving Gaussian heat source :

-Tuning laser absorptivity A to calibrate

—Non-physical meaning of A(\sim 0.02) for 2D thermal model (3D model A \sim 0.35)

¹ Sih et al. Particul. Sci. Technol. 22 (2004)

What about the interest of FE Simulation?

Melt pool depth :

Exp. : 90-120 µm (part supplier)



Thermal history presents different cycles due to multiple layers

 \rightarrow T(t) feeds a Phase Field model

 \rightarrow phases kinetics and Si diffusion can will be studied

 \rightarrow Ongoing PhD

Cooling rate :

 $\dot{T}_{exp} = 10^{6} \text{K.s}^{-1} (\text{microstructure } + \text{Matyja's eq})$ $\dot{T}_{sim} = 0.9 \times 10^{6} \text{K.s}^{-1}$



Common Goal = investigate static rupture and delaying it

Two complementary studies to investigate damage mechanism in SLM as built samples

Zhao et al. Materials Science & Engineering A 2019 minimum HAZ effect: process param. (thin HAZ)

+ tensile load // HAZ



eutectic network with Si precipitates





strain

strain

and crack formation Not in HAZ To increase elongation but dcreasing elastic stress

Si rich network

 \rightarrow voids

nucleation

→Globularization Post treatments (Tp° or FSP) delay crack J. Delahaye et al. Acta Materialia 2019

maximum HAZ effect: process param. (thick HAZ)

+ tensile load \perp HAZ





HAZ

Damage nucleate around Si precipitates in HAZ Crack formation in HAZ

Tang parameters (small HAZ)
→ 12,5 % elongation
Delahaye param (HAZ ↑)
→ 4,5%

What is the goal with AlSi10Mg?

Interest to further investigate thermal history impact

Finite element to get representative T(t)

Phase Field approach

to better understand Si diffusion in typical positions MPF, MPC, HAZ...

Characterize by indentation mechanical behavior of different cells and Si rich eutectic network

Links to fracture behavior

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Material High Speed Steel AISI M4

- Fe-Cr-C-X alloys with X: carbide-forming element
- (i.e. V, Nb, Mo or W)
- Hard carbides \Rightarrow High hardness and wear resistance
- Applications: high speed machining, cutting tools, hot rolling mill rolls, molds...

С	Cr	Mo	V	W	Ni	Si	Fe
1.35	4.30	4.64	4.10	5.60	0.34	0.9	0.33







Finite Element Model - Identification of input data

Material data

conduction, heat capacity, latent heat measured on samples extracted from the clad & the substrate (DSC, Laser flash, dilatometry, quench dilatometer)

Boundary conditions Convection, Radiation, laser absorption fitted by inverse modelling target BOTH Measured Temperature history + Melt pool depth

Laser path (velocity, idle time, tracks scheme) Real one in 3D, simplified but per layer in 2D simulations

Bulk samples

	Bulk Sample
Laser beam speed (mm/s)	6.67
Laser power (W)	1100
Pre-heating (°C)	300
Mass flow (mg/s)	76
Number of tracks per layer	27
Total number of layers	36



40 x 40 x 27.5 mm (972 tracks)



4 Thermocouples Thermal measurement in the substrate

"2D FE" - bulk samples

Tp° in the substrate

Predicted Tp° in the clad



Melt pool depth

Key data for identifying single set of data by inverse simulations (convection, radiation, absorption coefficient)





Thin wall experiments (1) Preheating =150°C



	Substrate pre- heating	Clad deposition
Length of centered laser pass for pre-heating (mm)	40	40
Laser beam speed (mm/s)	41.7	8.3
Laser power (W)	260	(Constant)500
Temperature at thermocouple TC1 at preheating end and at cladding start in °C	217	134
Number of laser passes	20	10

With a thiner substrate: there too much bending \rightarrow risk for laser position With thicker substrate crack situation worst

3D FE thin wall simulations



Measured thermophysical parameters Stress strain curves at 3 tp $^{\circ}$ and strain rate on samples extracted from DED samples

 2D Substrate 42crMo4 ≠ than for bulk sample
 → Impossible to recover temperature measurements with previous values of conductivity and thermal capacity.

→New measurements
 (Previous block for bulk sample in martensite state, current bars in Pearlitic state)

Simulations untill 5th layer Convection f(T) constant value not OK

target measured Tp° history

Thin wall experiments (2) Preheating = 300°C



	Substrate pre- heating	Clad deposition
Length of centered laser pass for pre- heating (mm)	70	40
Laser beam speed (mm/s)	41.7	8.3
Laser power (W)	260	600+500=> 400
Temperature at thermocouple P1 at preheating end and at cladding start in °C	400	310
Number of laser passes	20	10

Pre heating at 300°C

Thin wall experiments (2)

3 Experiments with similar conditions 10 layers without crack



Vertical displacement at the middle



displ.

ZZ

"3D" thin wall thermal simulations

3 Experiments with similar conditions 10 layers without crack







3D FE thin wall thermal simulations

0.1 0 300 100 150 200 250 -0.1 zz (mm) -0.2 -0.3 -0.4 -0.5 t (s) Dia.6 mm 10 mm 2,5 mm

Vertical displacement at the middle

Pre heating curves demonstrated high sensitivity to the right boundary condition TP<500°C so no phase transformation

Cladding process: Low sensitivity to Young modulus Low sensitivity to hardening curve Low sensitivity to elastic limit

High sensitivity to different dilatation coefficient of the substrate and the clad (but clad measurement based on bulk simples with different microstructure→ wrong values)

"3D" thin wall simulations

Idea of dilatation coefficients



High sensitivity to different dilatation coefficients of the substrate and the clad

clad property measured on material from bulk samples (→different microstructures, carbides)

-literature on close composition at higher cooling rate -extrapolation... as first transformation modifies composition

... a nightmare...

3D FE thin wall thermal simulations

Next steps

Shift martensitic transformation to end thermal validation

Work on the stress validation




Why is AISI M4 case so challenging?

Phase transformation define the behavior More fundamental knowledge should be known before trying to model the mechanical behavior

Why is AISI M4 case so interesting?

Good properties + goal for model coupling approaches

Thank you for attendance

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AM Habraken 6/12/2019