Building blocks for a digital twin of additive manufacturing

- a path to understand the most important metallurgical variables

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Digital twin of additive manufacturing

Why digital twin of AM?

- Save time and money
- Minimizing trial and error optimization
- Expediting product qualification
- Reducing/alleviating defects

Components developed at Penn State

i. Heat transfer and fluid flow simulation

ii. Solidification, grain structure and texture evolution

iii. Residual stress and distortion simulation considering convective heat transfer

iv. Reduced order modeling - Back of the envelope calculations

DebRoy, Zhang, Turner, Babu. Builiding digital twins…, Scripta Mater. 2016

i. Heat transfer and liquid metal flow

Prediction of deposit geometry

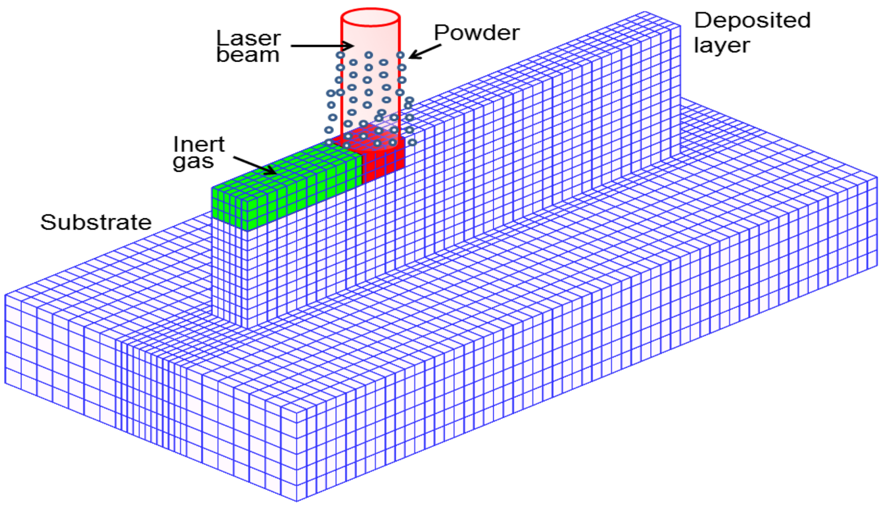
Temperature and velocity distributions

Cooling rates and solidification parameters

Heat transfer and fluid flow model

Solve equations of conservation of mass, momentum and energy

INPUT
Process parameters
Material properties



OUTPUT
Transient temperature & velocity fields, cooling rate, solidification parameters …

Calculation domain: about 250,000 cells

Five main variables: three components of velocities, pressure & enthalpy

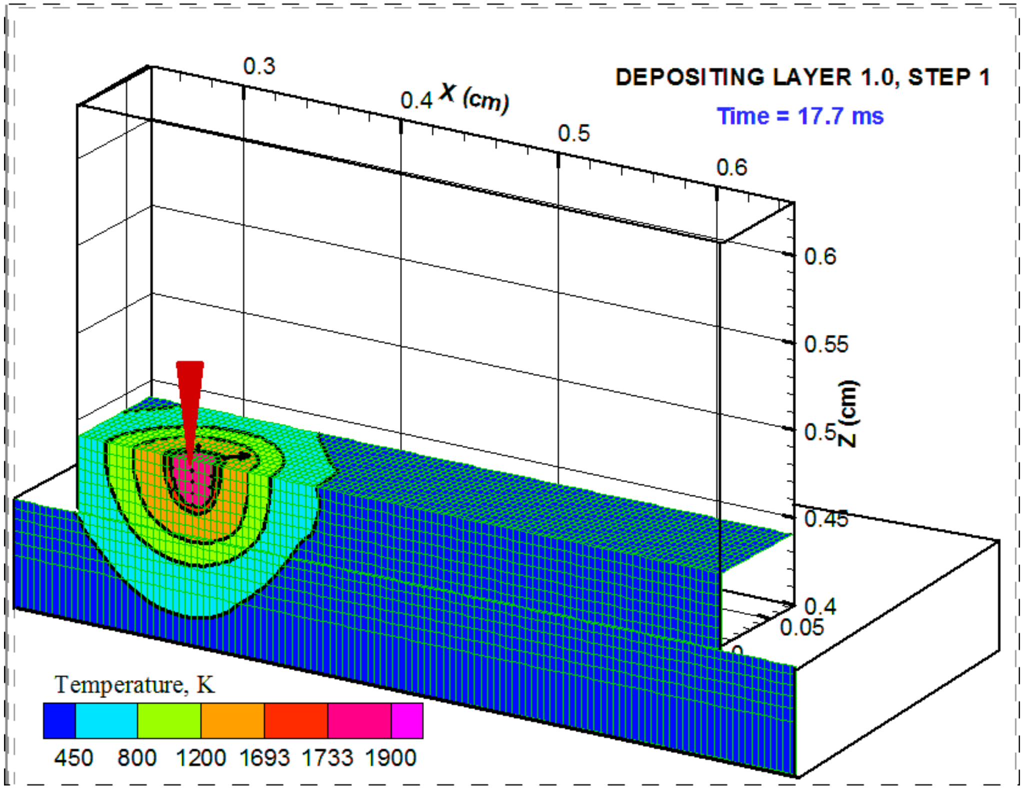
1.25 million algebraic equations (250000 x 5)

100 iteration at any time step => 0.125 billion equations/time step

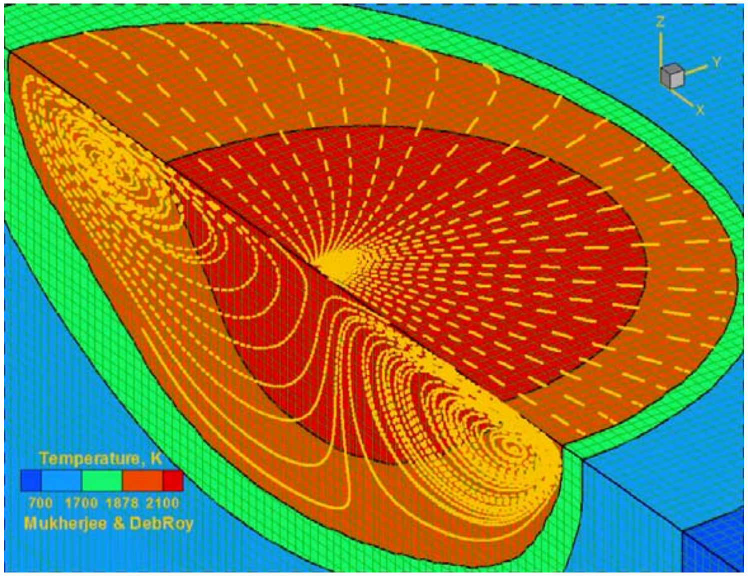
1000 time steps => 125 billion total equations

Manvatkar, De, DebRoy, J. Appl. Phys., 2014

3D transient temperature distribution



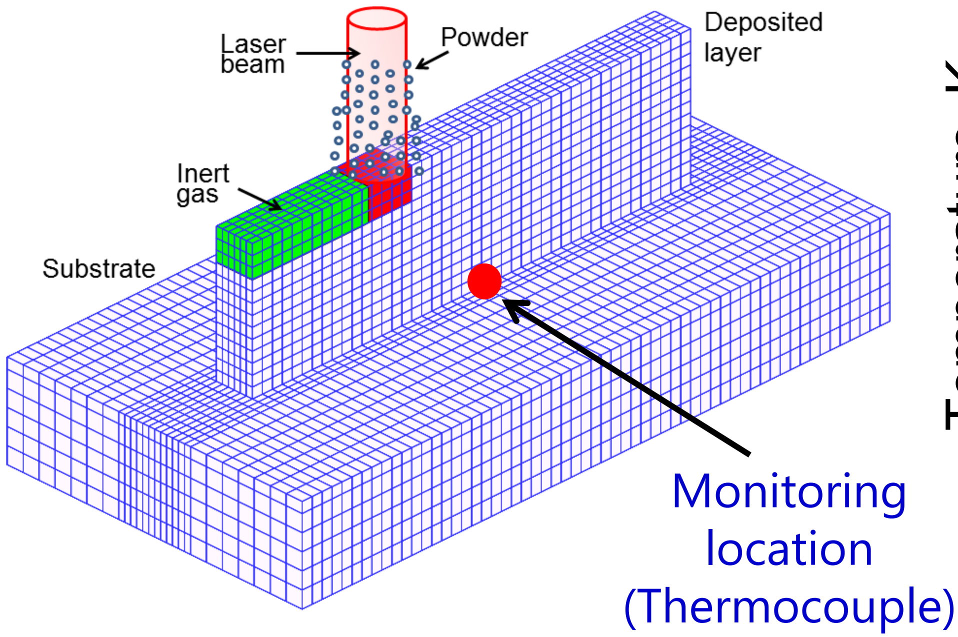
3D velocity field

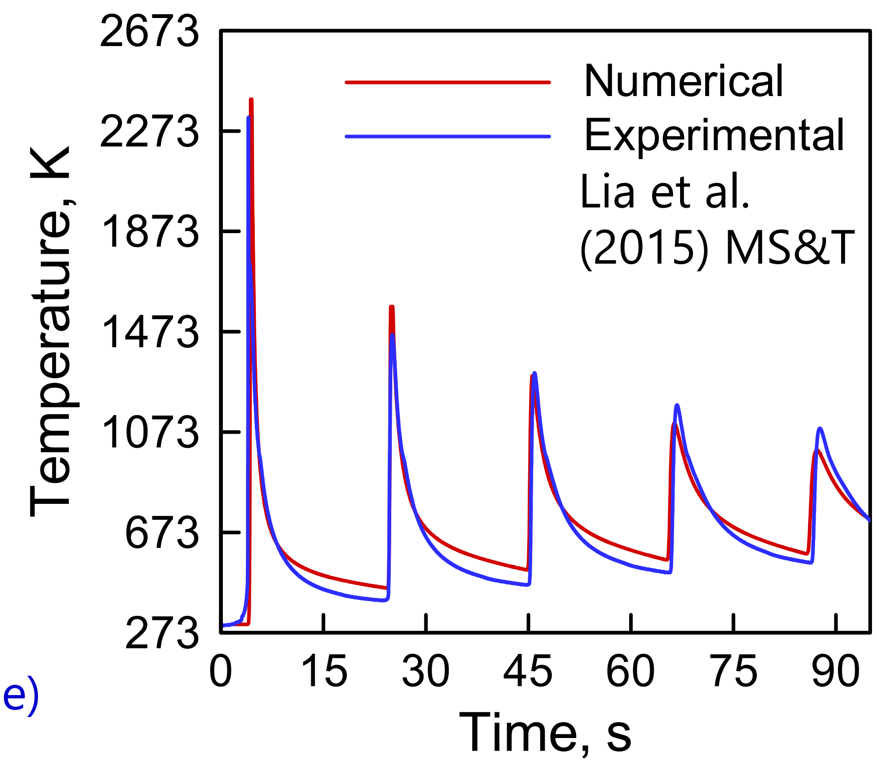


SS 316L

Laser power (W)	Beam radius (mm)	Scanning speed (mm/s)	Layer thickness (mm)	Substrate thickness (mm)
210	0.5	12.5	0.38	4

Multiple thermal cycles

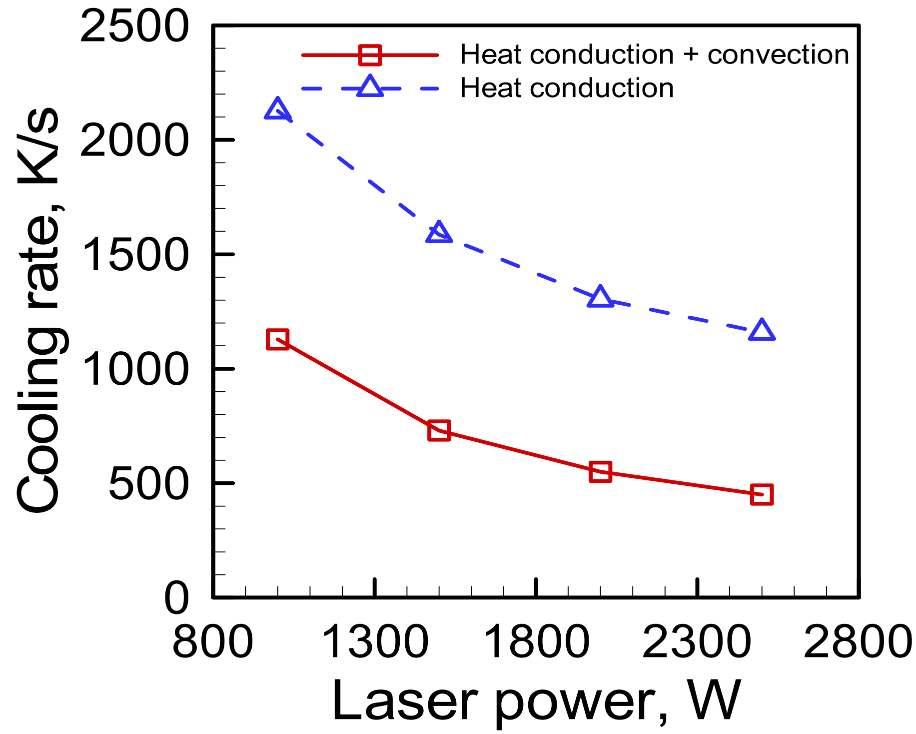




Material	Laser power (W)	Beam radius (mm)	Scanning speed (mm/s)	Powder flow rate (g/s)	Substrate thickness (mm)
Ti-6Al-4V	2000	2.0	10.6	0.4	10

Manvatkar, De, DebRoy, Mater. Sci. Technol., 2015

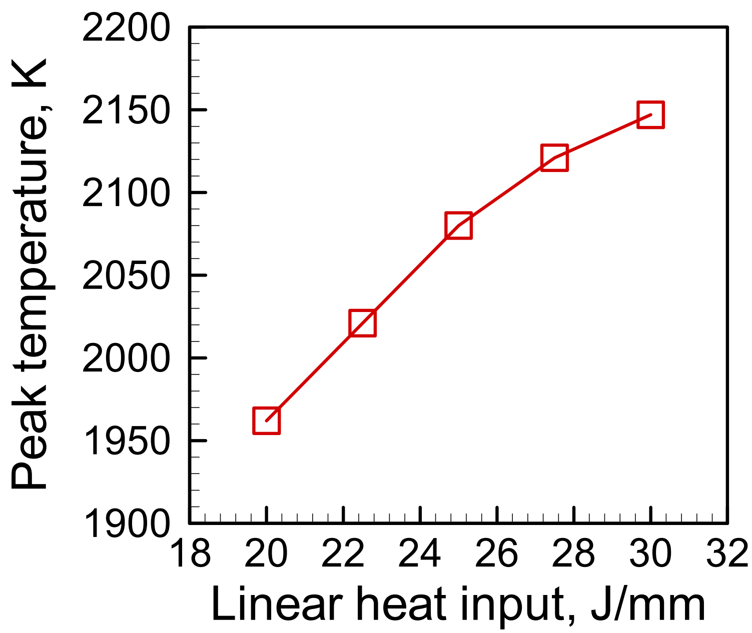
Why considering convective flow?

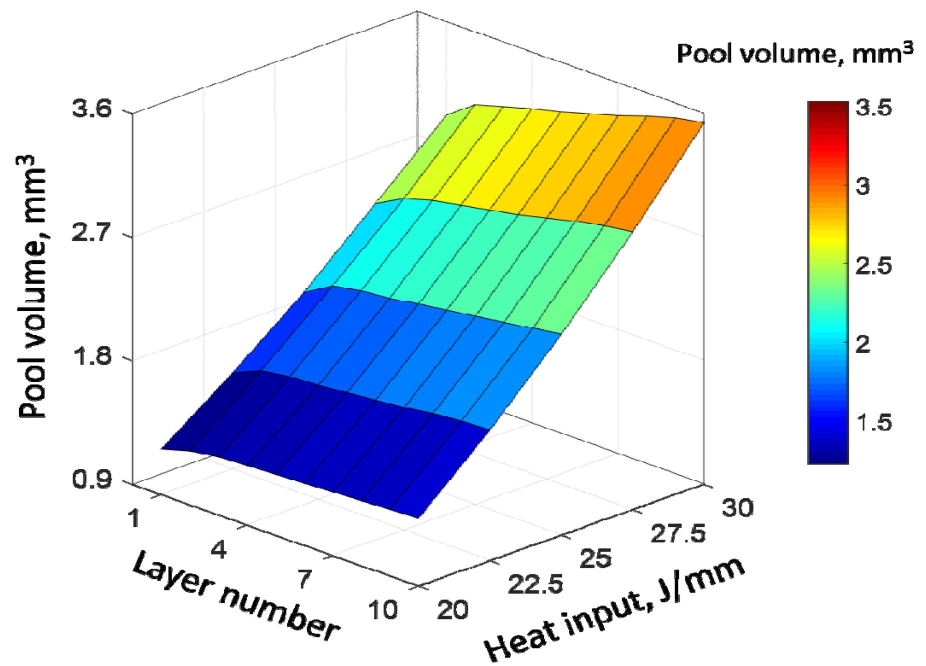


- Heat conduction models neglect the mixing of the hot and the cold liquids.
- Heat conduction models overestimate cooling rates.

Alloy	SS 316L
Beam radius (mm)	2.0
Scanning speed (mm/s)	10
Powder flow rate (g/s)	0.42
Substrate thickness (mm)	10

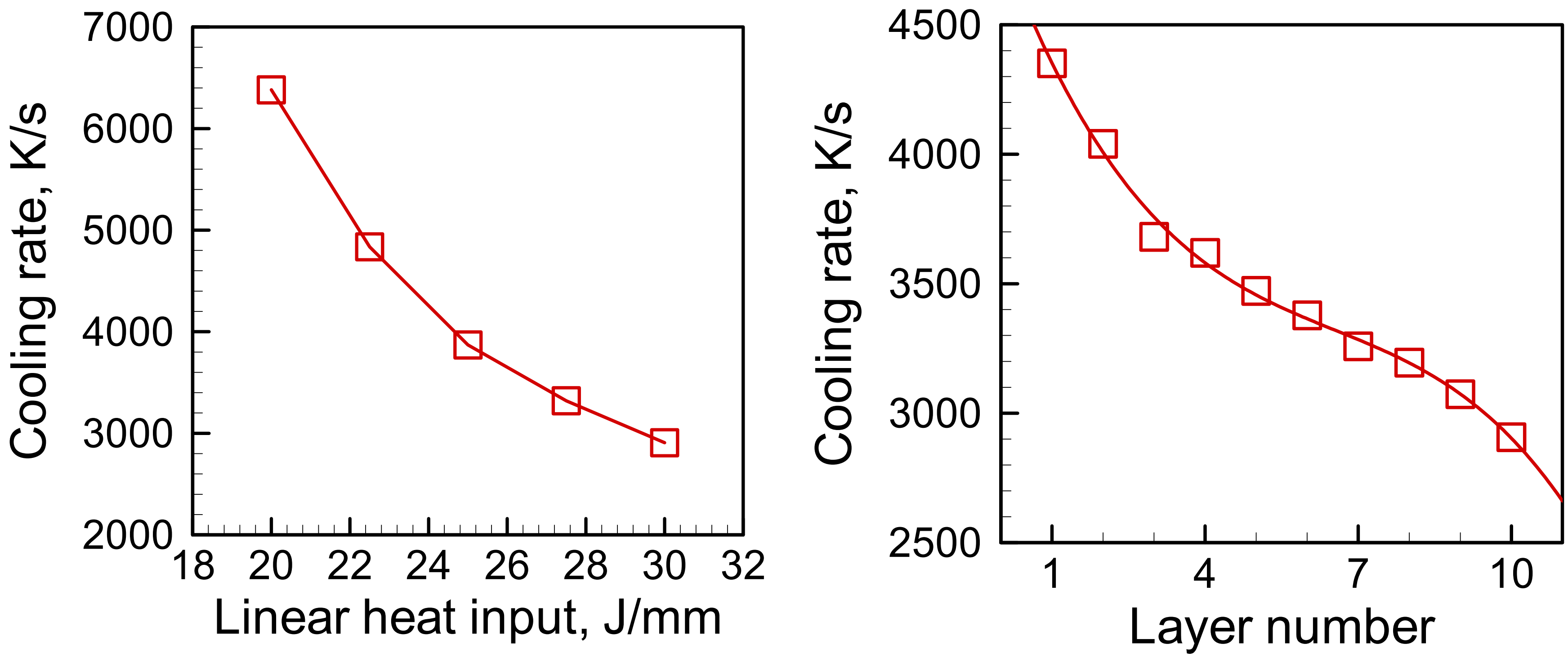
Peak temperature and melt pool volume





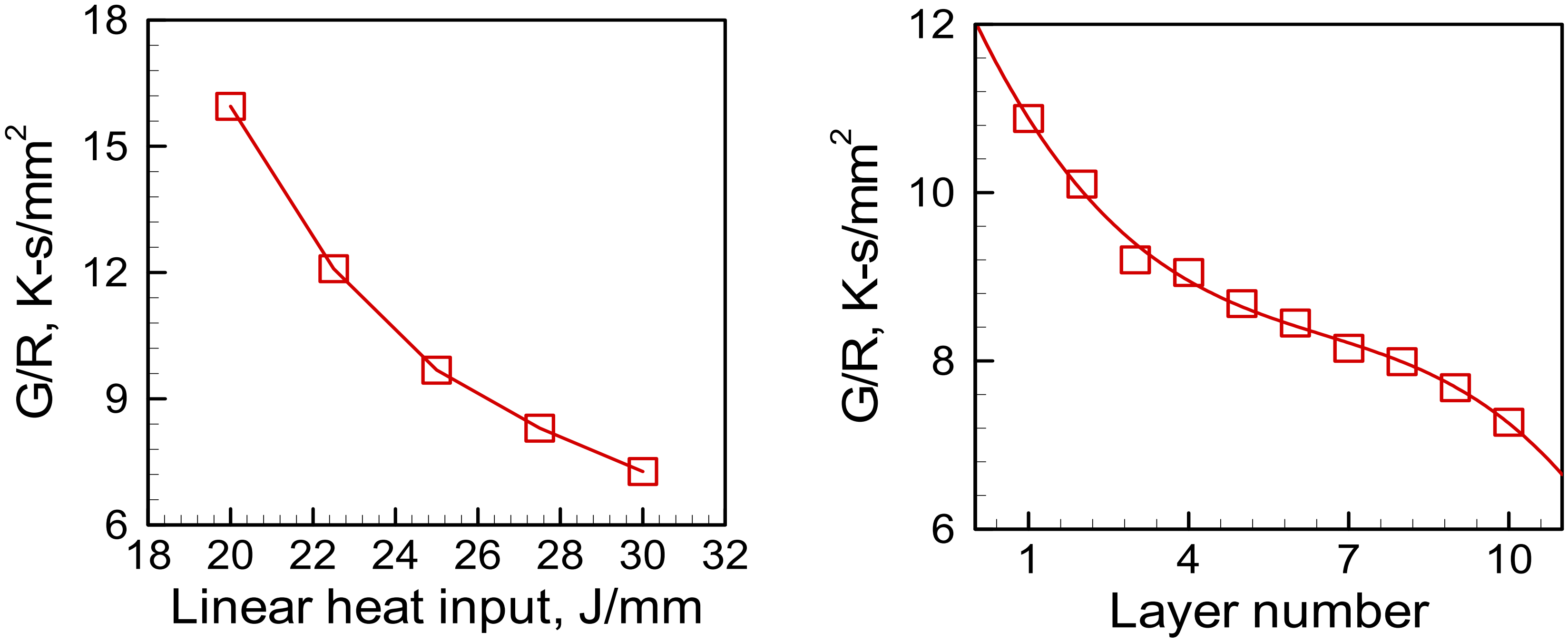
- Peak temperature increases at high power as in welding.
- Pool volume increases with heat input. Pool volume is larger in upper layers due to heat accumulation during the building process.

Cooling rate



- Cooling rate decreases with linear heat input, as in welding.
- Cooling rate is lower in upper layers, because of significant heat accumulation during the depositing process.

Solidification parameters



- The ratio of temperature gradient to solidification rate, G/R, determines the morphology of the solidification structure.
- G/R decreases in upper layers, due to the decease of temperature gradient G.
- G/R decreases with linear heat input, due to the decease of temperature gradient G or increase of solidification rate.

ii. Microstructure and grain growth

Temporal evolution of grain structure

Spatial distribution of grain shape and size

Effect of scanning strategy on solidification texture

3D Grain growth

INPUT

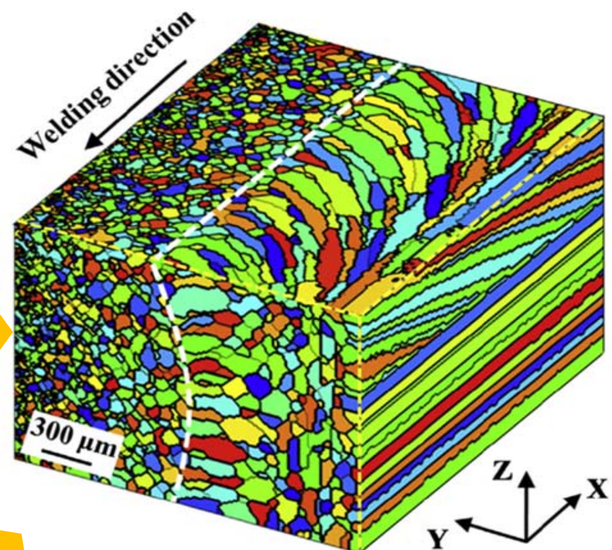
3D Transient heat transfer and fluid flow model

Temperature field, thermal cycles, solidification parameters

+

Material properties

Grain growth model



OUTPUT

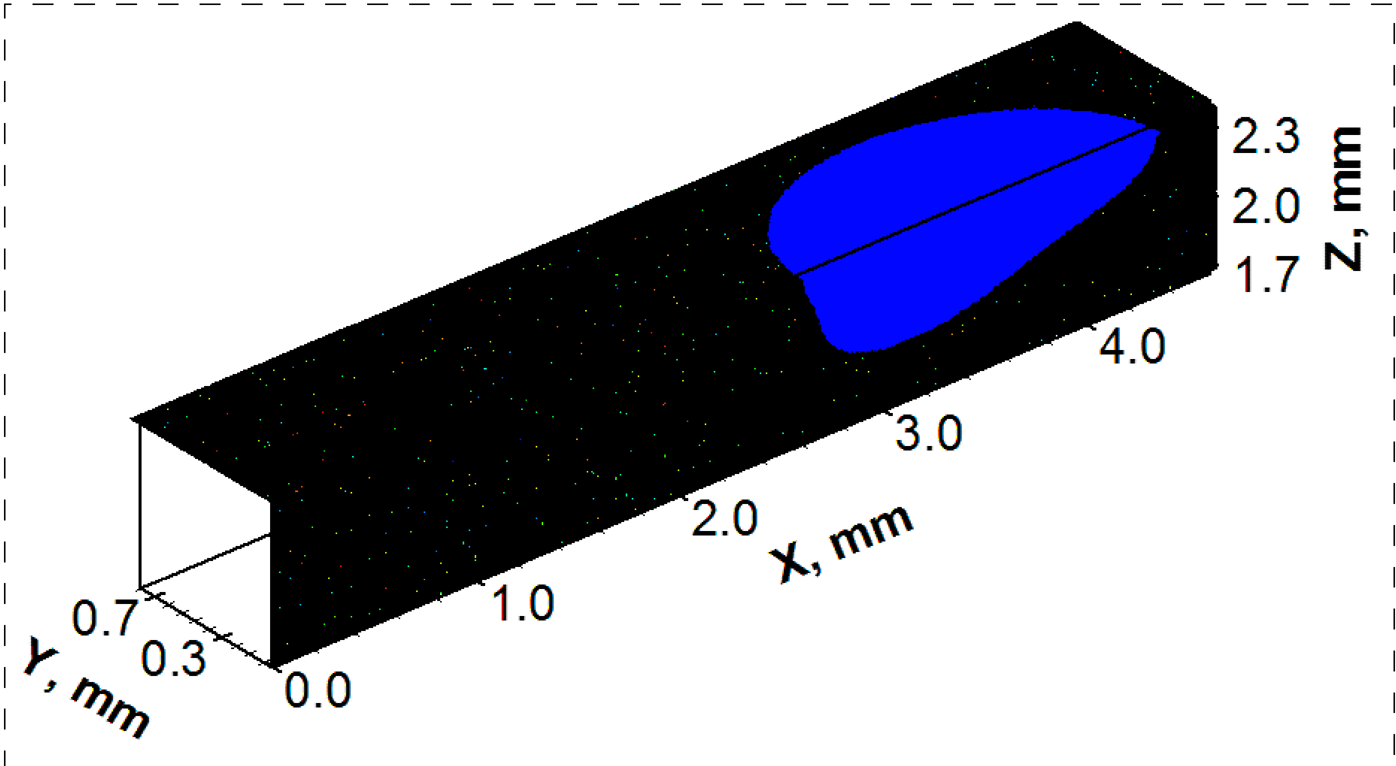
Temporal evolution, spatial distribution of grain structure.

Visualized grain growth process

Grain morphology size, and topology.

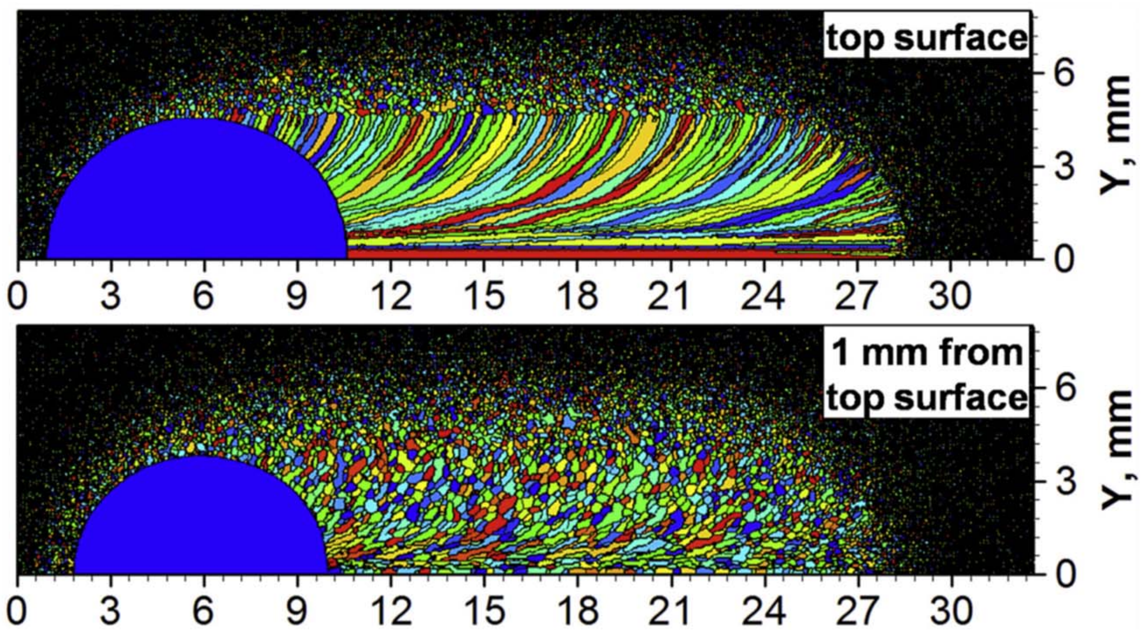
Wei, Elmer, DebRoy, Acta Mater, 2016; Wei, Elmer, DebRoy, Acta Mater (Cu), 2017

Temporal evolution of grain structure

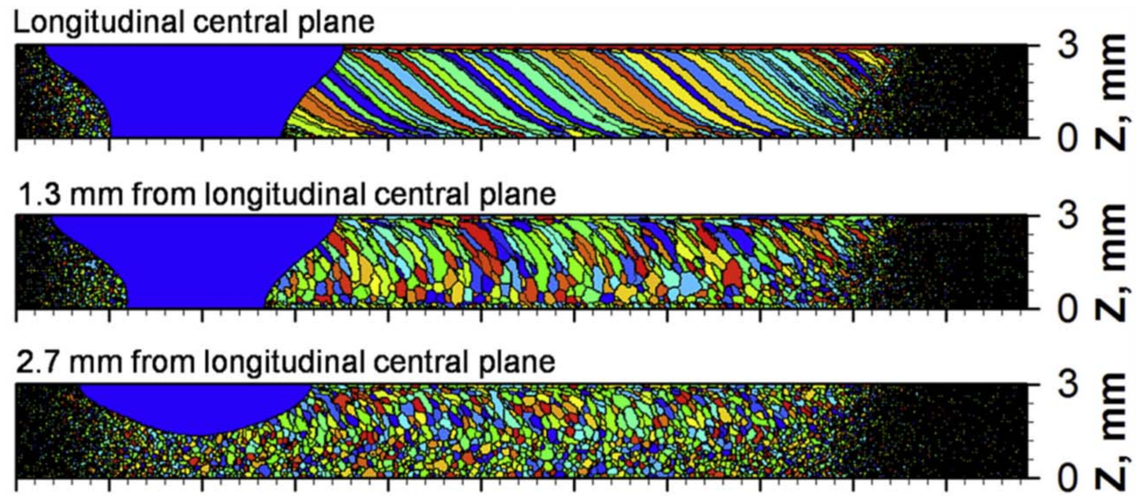


Material	Laser power (W)	Beam radius (mm)	Scanning speed (mm/s)	Layer thickness (mm)	Substrate thickness (mm)
IN 718	250	0.5	15	0.4	4

Spatial distribution of grain structure



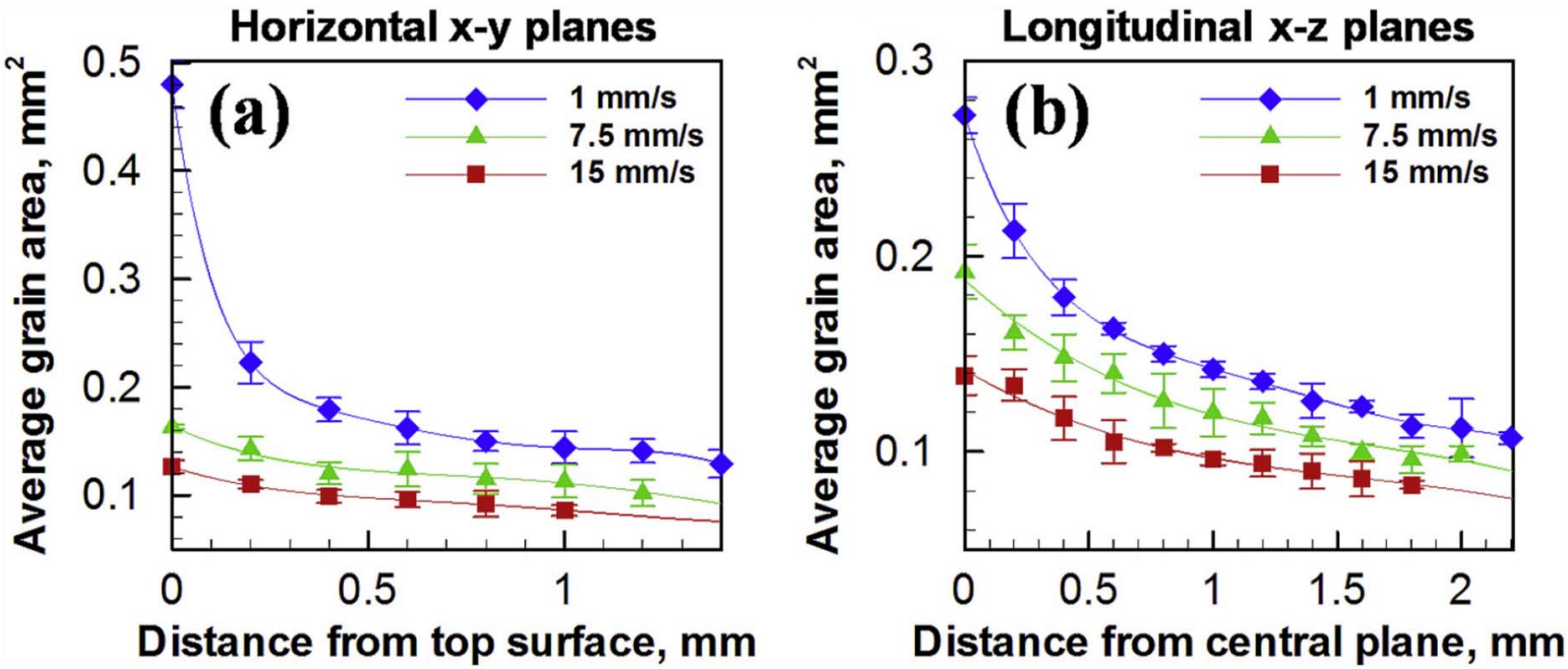
The grain structure varies significantly with the horizontal sectional planes



The morphology and size of the grains varies significantly with the longitudinal sectional planes as well.

Wei, Elmer, DebRoy, Acta Mater (Al), 2017

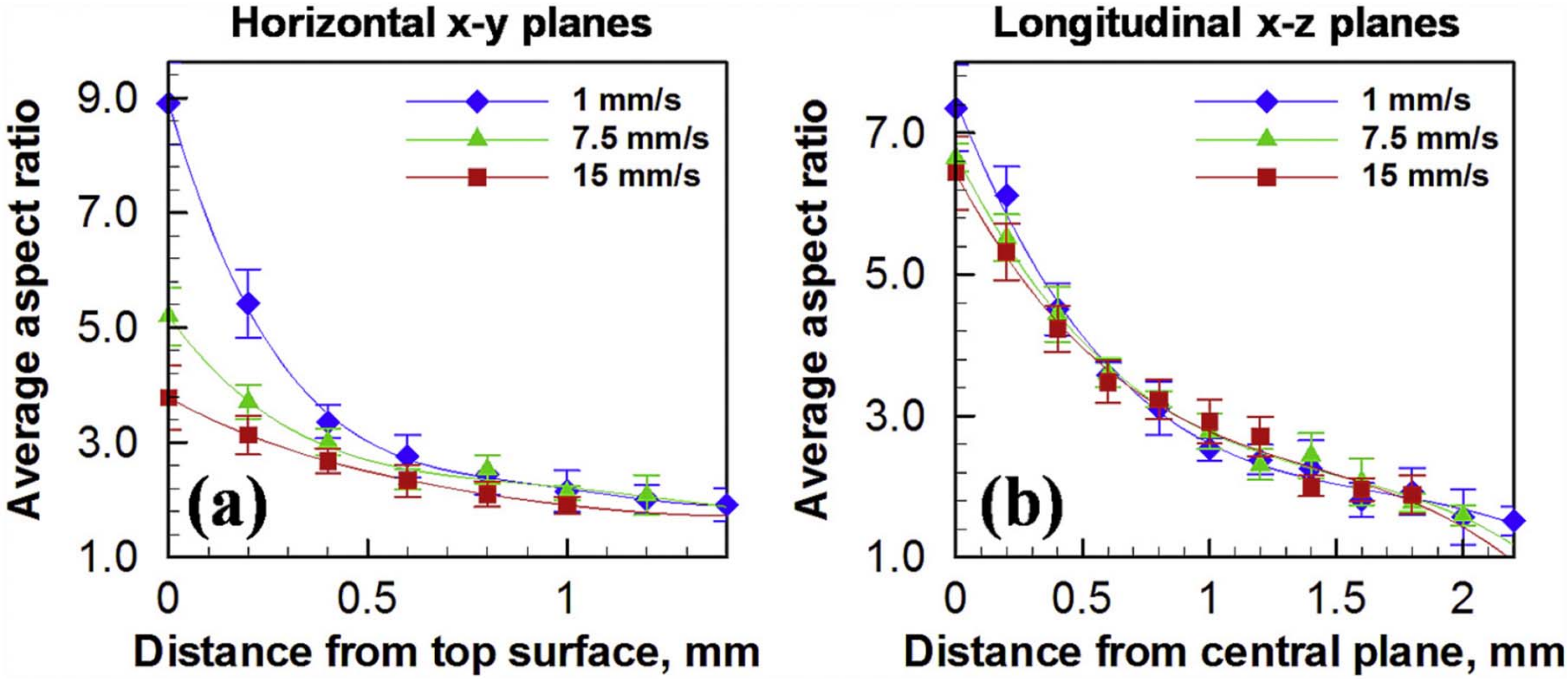
Spatial distribution of grain size



- The cross-sectional area of the grains are larger in the sectional planes near the top surface.
- Grain sizes are smaller at the locations away from the center of the molten pool.

Wei, Elmer, DebRoy, Acta Mater (Al), 2017

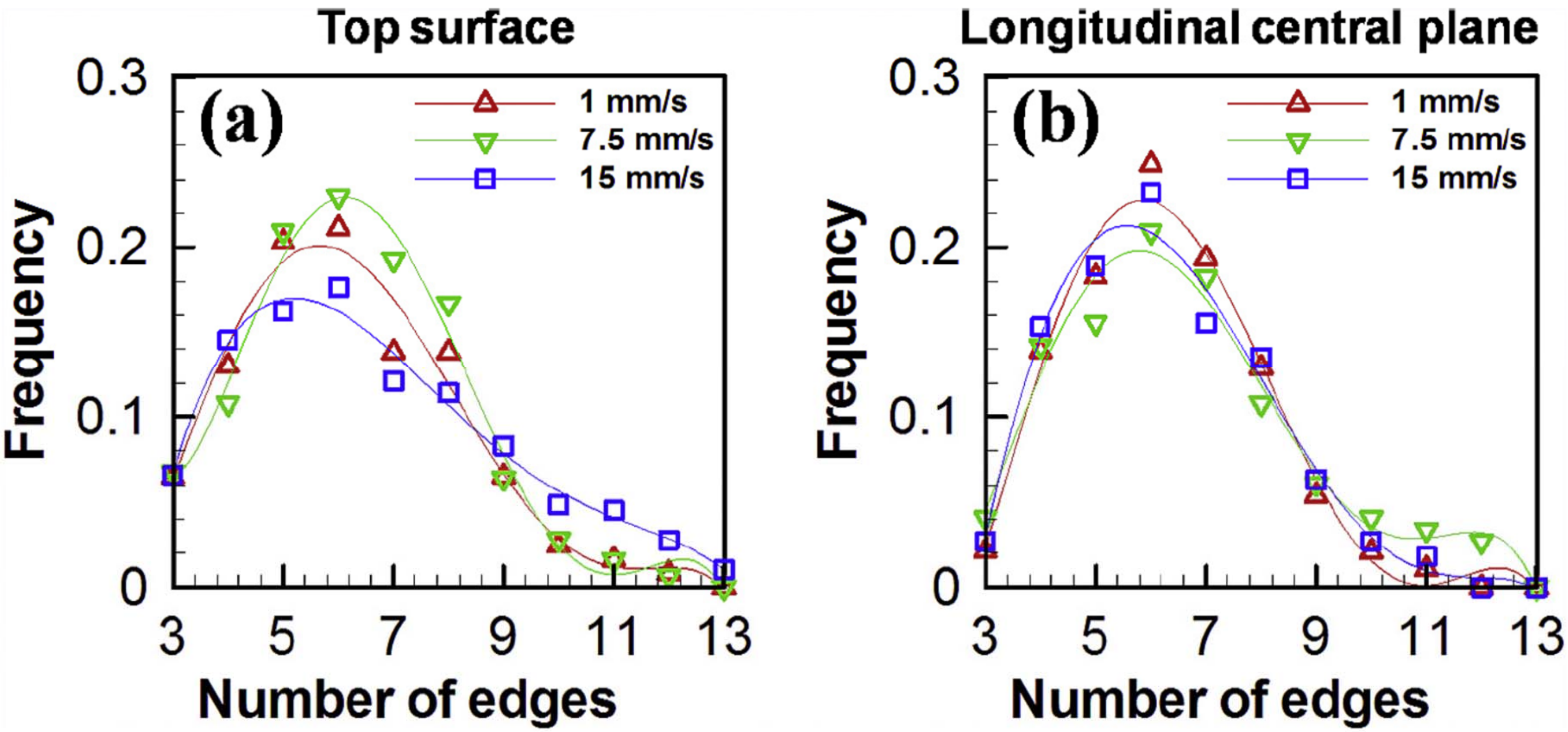
Spatial distribution of grain morphology



- The grains appear in the form of columnar grains near the top surface, and the longitudinal central plane.
- The columnar grains appear in the form of equiaxed grains near the edge of the fusion zone, which may be misleading.

Wei, Elmer, DebRoy, Acta Mater (Al), 2017

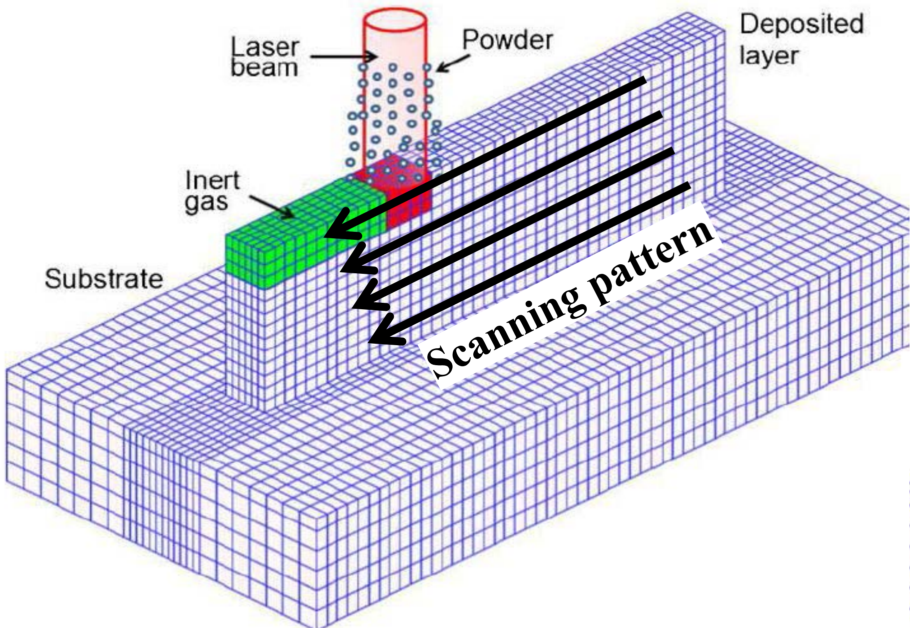
Topological class distribution



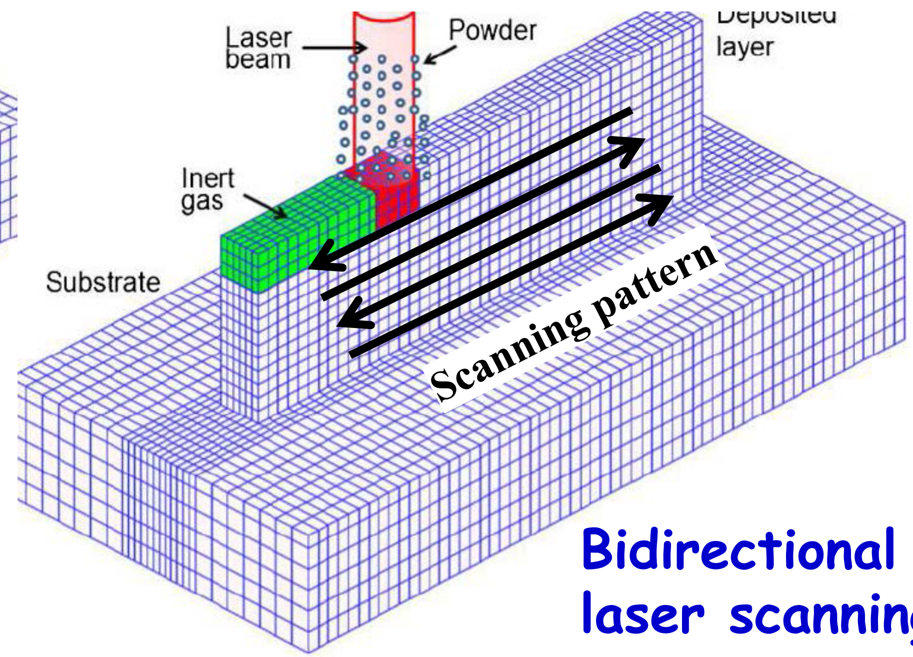
- Grains with six edges have highest frequencies, which is similar to the topological features of grains in isothermal systems.
- The topological class distributions of the grains are unaffected by the pronounced spatial and temporal variations of the temperature in the heat affected zone.

Wei, Elmer, DebRoy, Acta Mater (Al), 2017

Role of laser scanning strategy



Unidirectional laser scanning

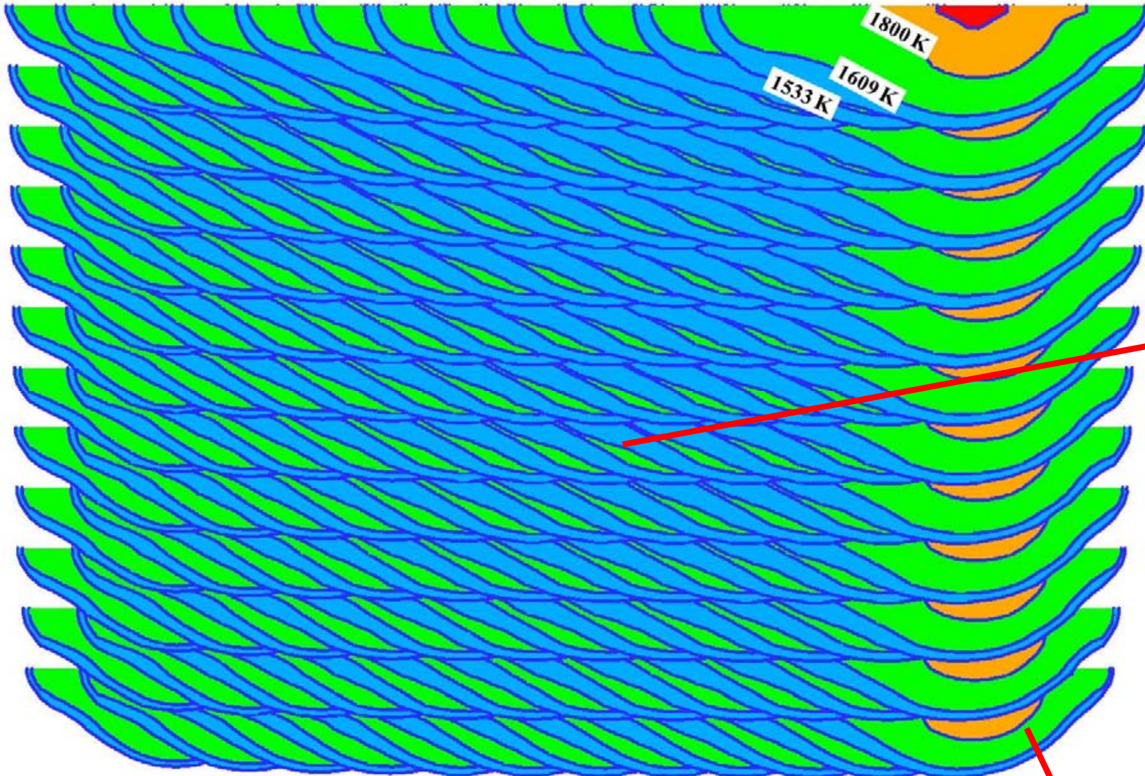


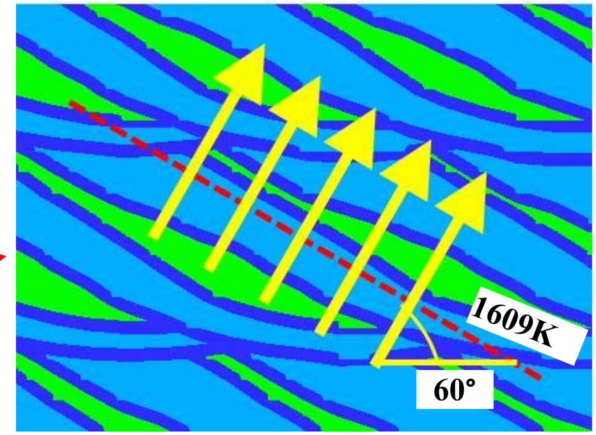
Bidirectional laser scanning

Multiple-layer, single-pass, directed energy deposition of IN718

Manvatkar, De, DebRoy, Mater. Sci. Technol., 2015

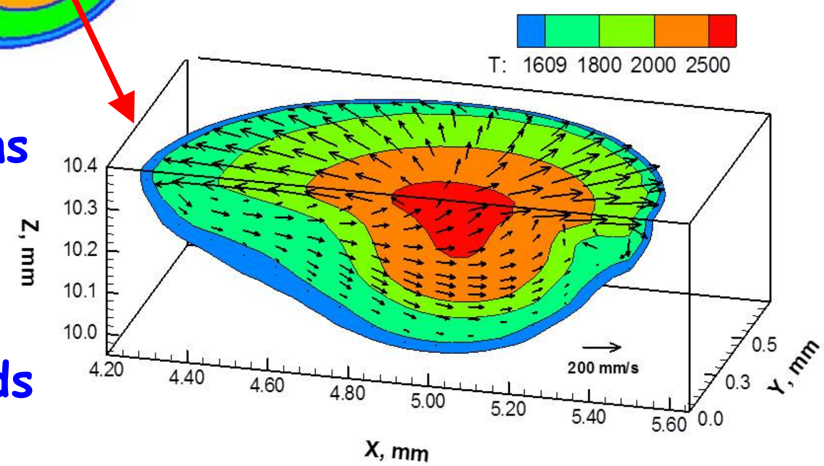
Unidirectional Laser Scanning





Magnification of temperature field with maximum heat flow directions

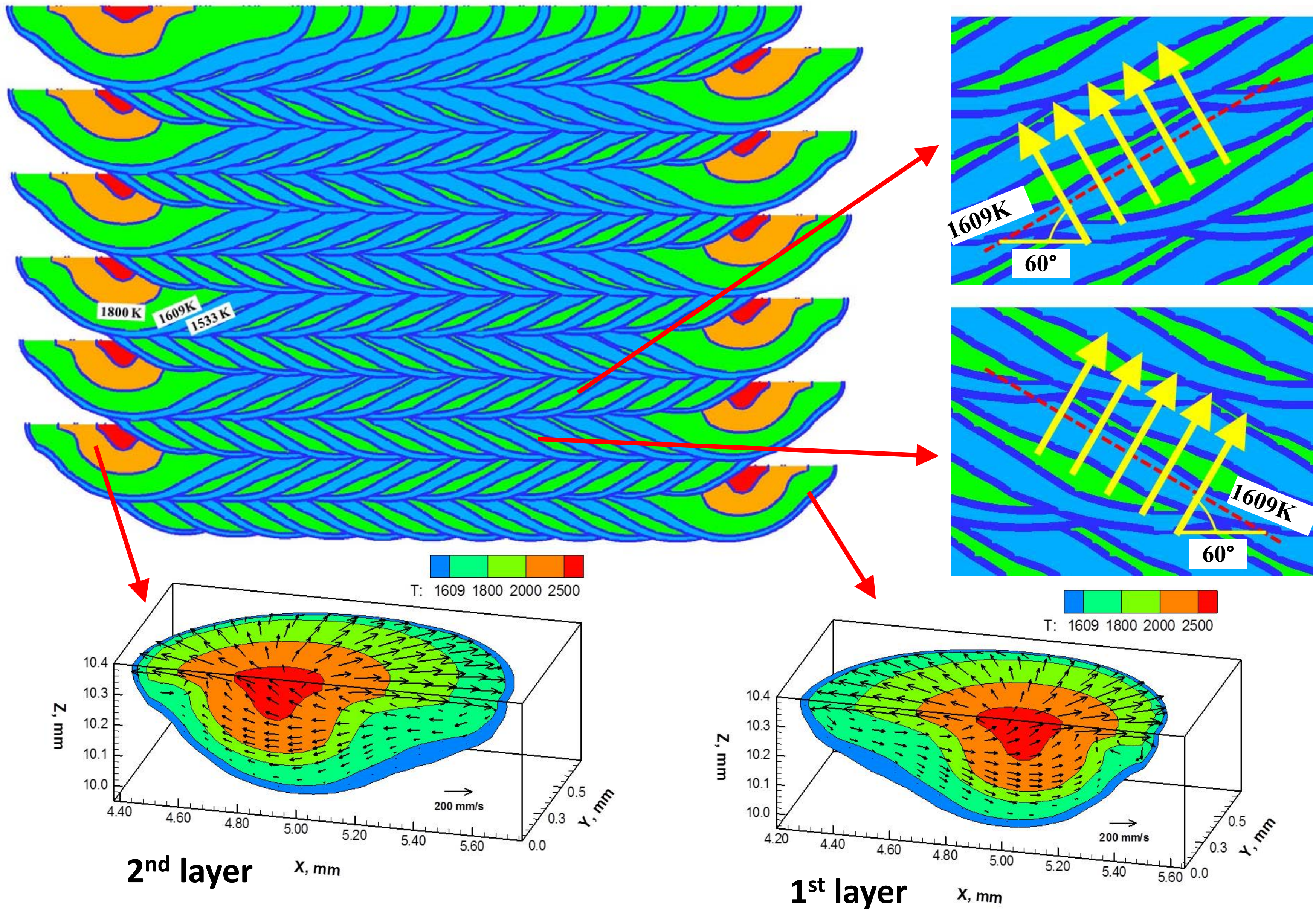
Calculated temperature field of longitudinal sections at various locations



Three dimensional melt pool – Temperature and velocity fields

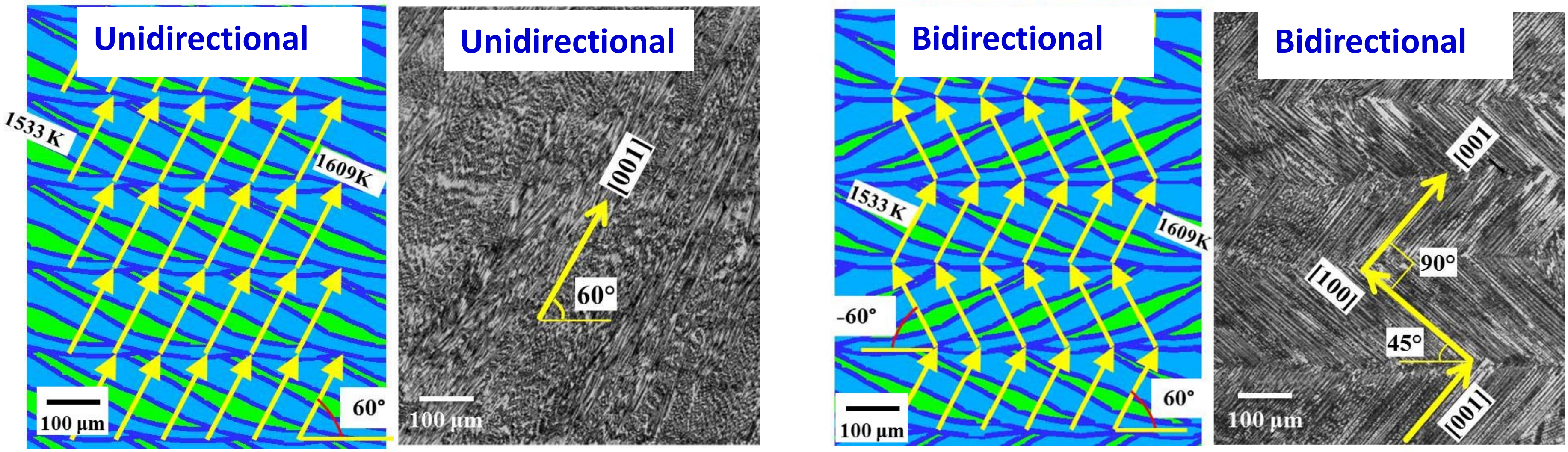
Wei, Mazumder, DebRoy, Nature Sci. Rep., 2015

Bidirectional laser scanning



Wei, Mazumder, DebRoy. Nature Sci. Rep. 2015

Solidification Texture from Different Laser Scanning



- For unidirectional scanning, the angle of the primary dendrites is about 60° to the horizontal line.
- For bidirectional scanning, there is 15° deviation of between the primary dendrites and the maximum heat flow direction. The angle between primary dendrites of neighboring layers is 90°.

Wei, Mazumder, DebRoy, Nature Sci. Rep., 2015

iii. Residual stresses and distortion considering convective heat transfer

Thermo-mechanical model based on accurate temperature calculations considering flow of liquid metal

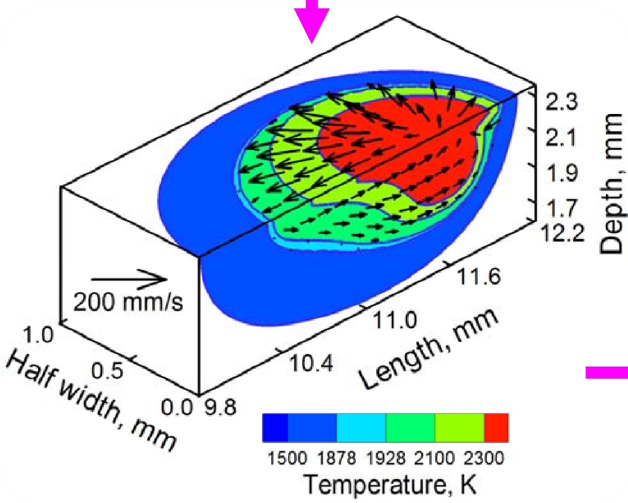
Calculation of residual stresses and distortion

Effects of layer thickness and heat input

Thermo-mechanical model

3D Transient heat transfer and fluid flow model

Temperature and velocity distribution for the domain

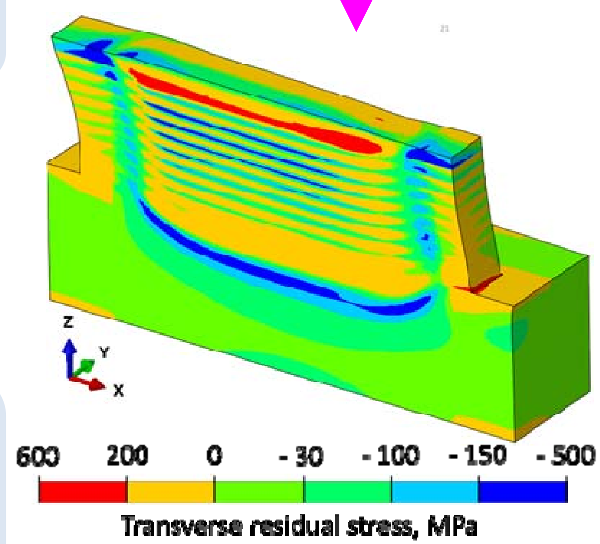


Geometry, mesh and temperature field

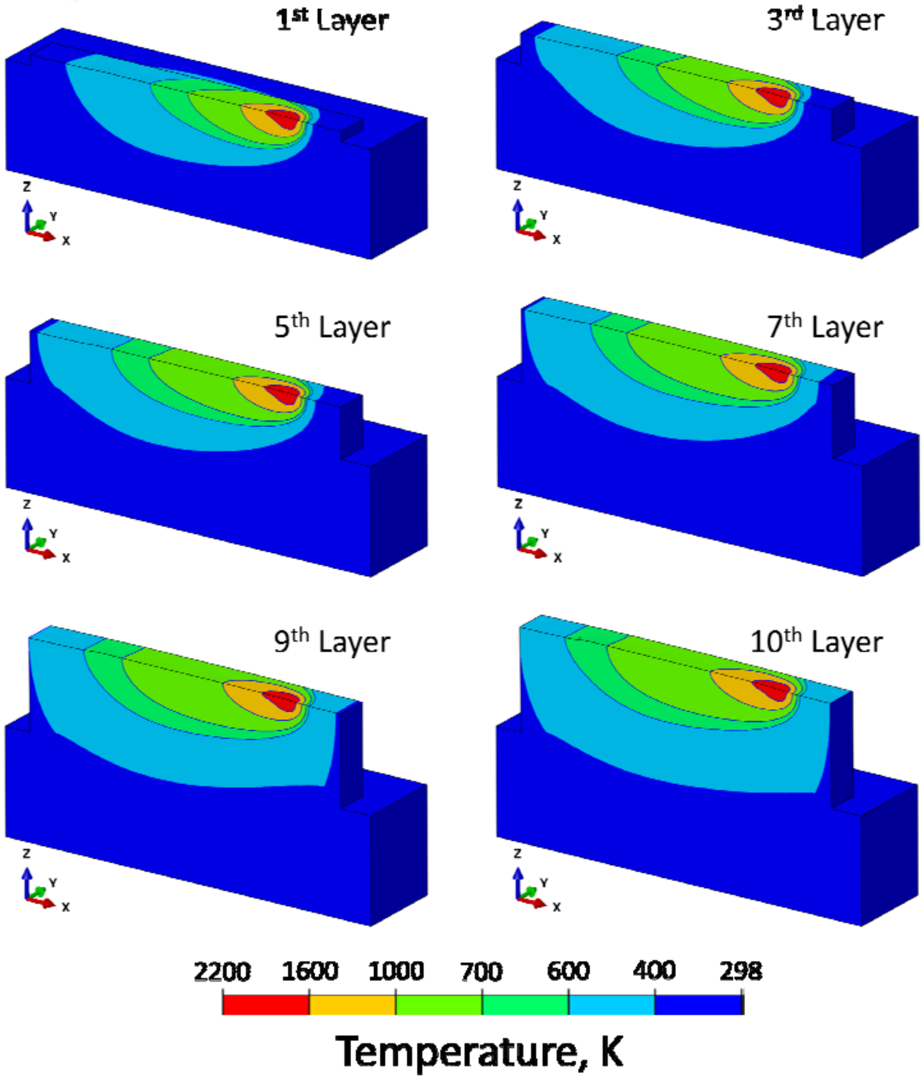
Python script

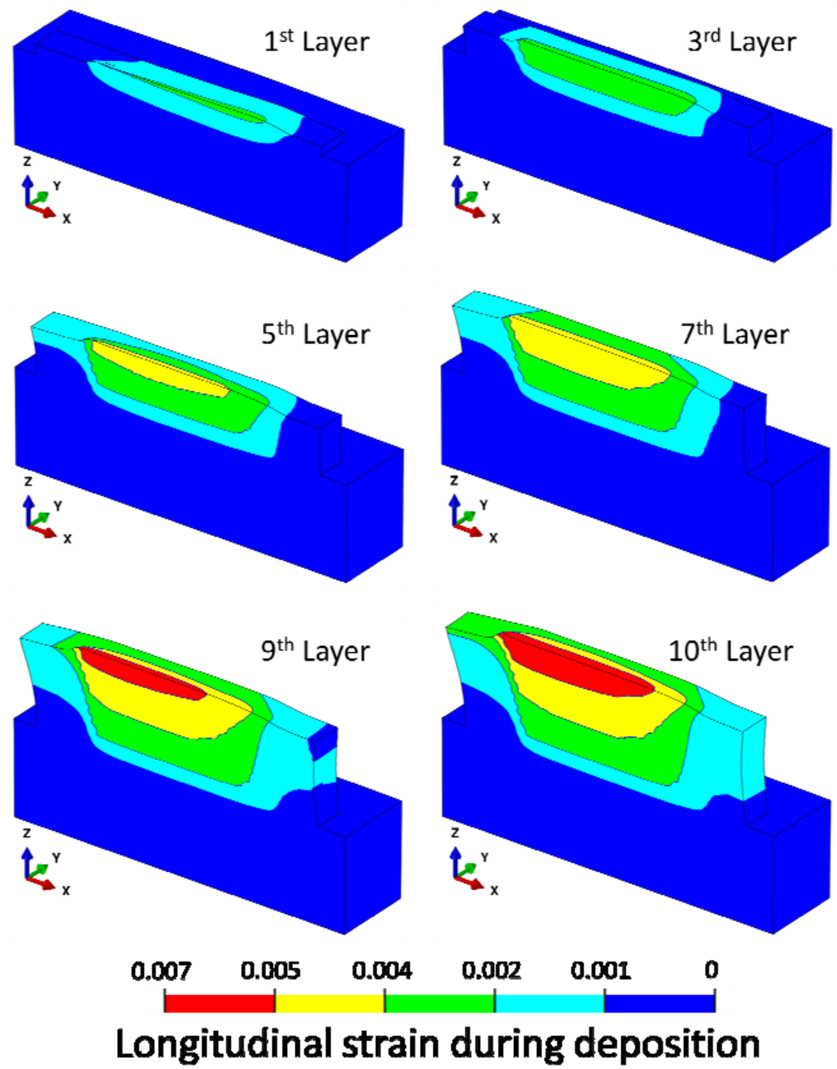
Abaqus database (.odb) file

Residual stress, strain, deformation for the domain



Calculated strain from temperature field





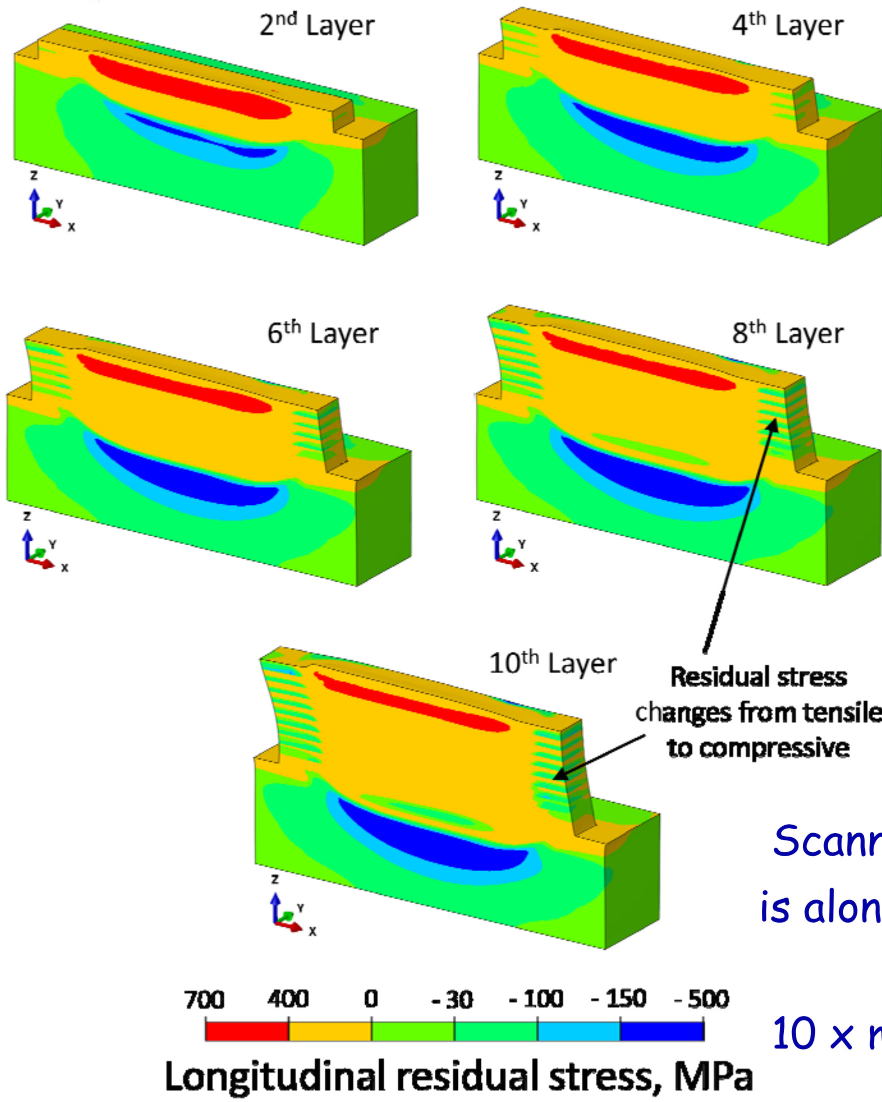
Alloy: Inconel 718, Laser power: 300 W, Speed: 15 mm/s

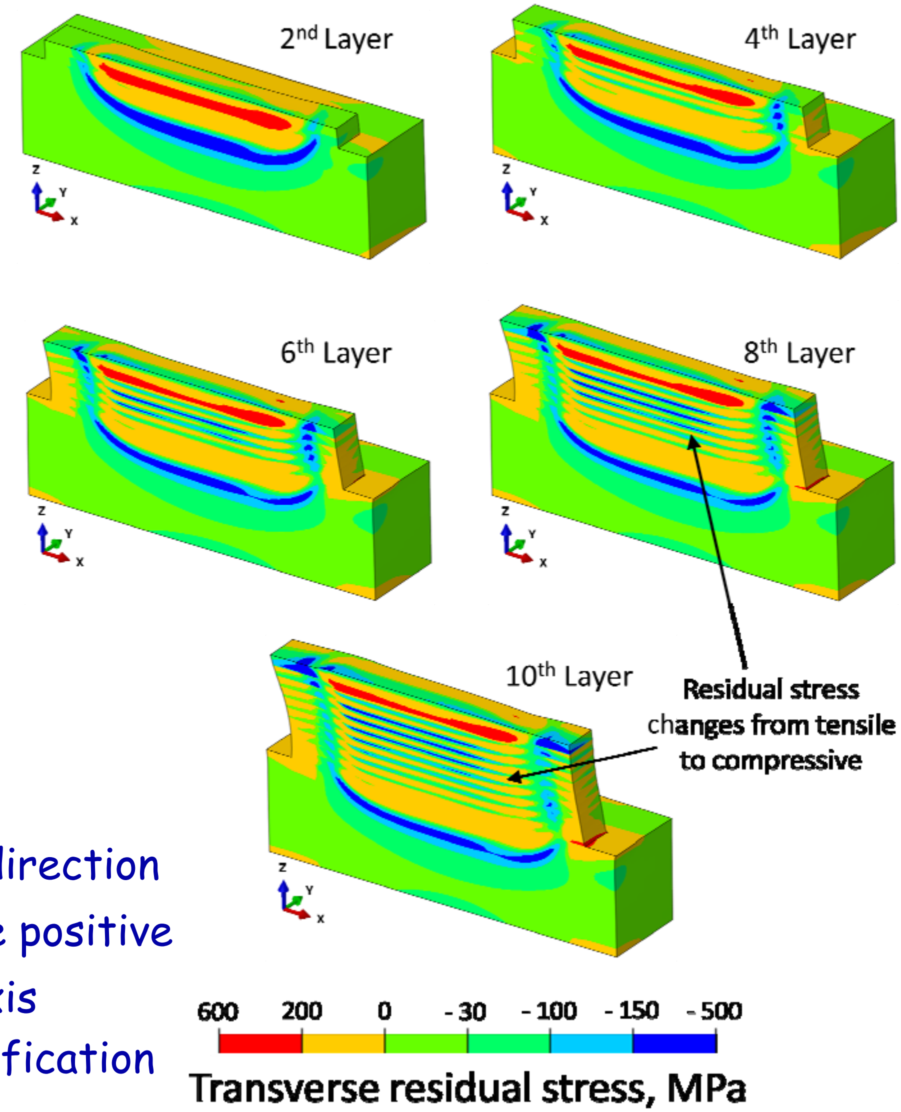
Scanning direction is along the positive x-axis

10 x magnification

Mukherjee, Zhang, DebRoy. Comput. Mater. Sci. 2017

Calculation of residual stresses





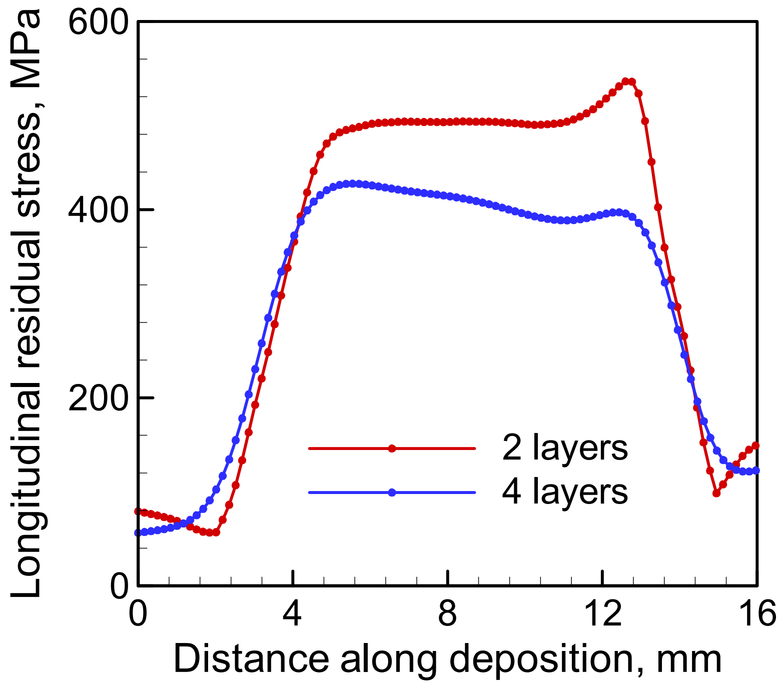
Scanning direction is along the positive x-axis

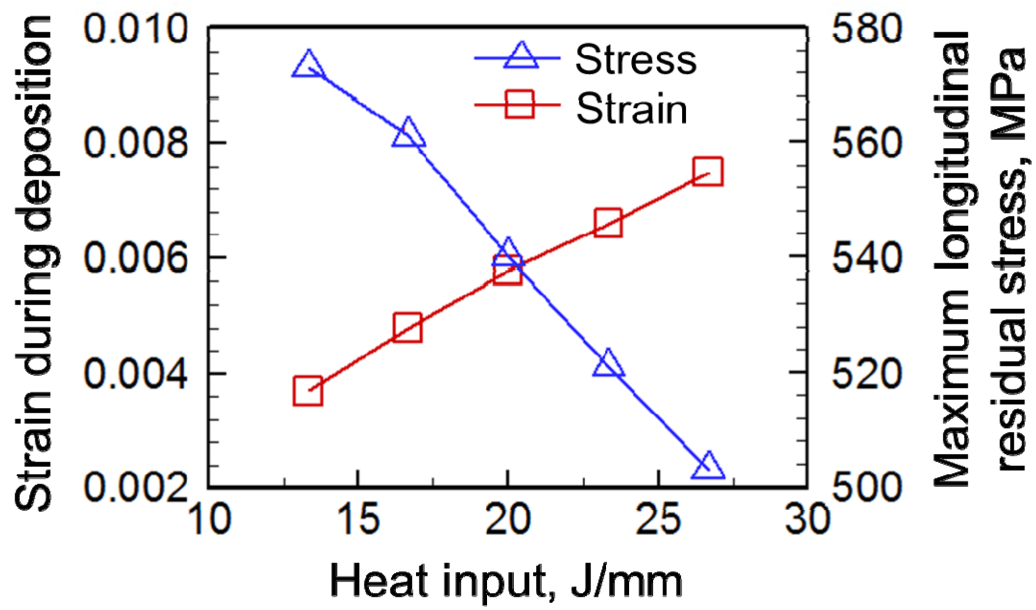
10 x magnification

Alloy: Inconel 718, Laser power: 300 W, Speed: 15 mm/s

Mukherjee, Zhang, DebRoy. Comput. Mater. Sci. 2017

Effects of layer thickness and heat input





⇒ Thinner layer thickness and lower heat input are helpful.

⇒ Residual stresses can be decreased as much as 30% by doubling the number of layers to build the same height.

⇒ Doubling the heat input reduces the residual stresses by about 20% and enhances the distortion by about 2.5 times.

Mukherjee, Zhang, DebRoy. Comput. Mater. Sci. 2017

iv. Reduced order modeling - Back of the envelope calculations

Dimensionless numbers to explain transport phenomena

Why dimensionless numbers?

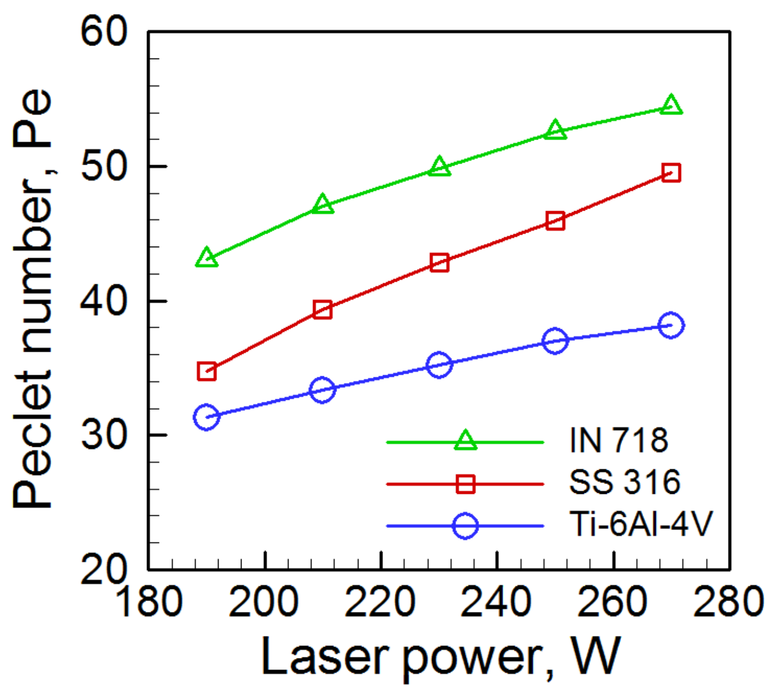
- Reduce the number of parameters that need to be investigated
- Groups of variables provide important insights unlike individual variables
- Calculated using the heat transfer fluid flow model

Peclet number

$$Pe = \frac{U\,L}{\alpha}$$

Thermal diffusivity	α
Pool length	L
Characteristics velocity	U

Relative importance of
heat transfer
by convection and conduction



Scanning speed: 15 mm/s

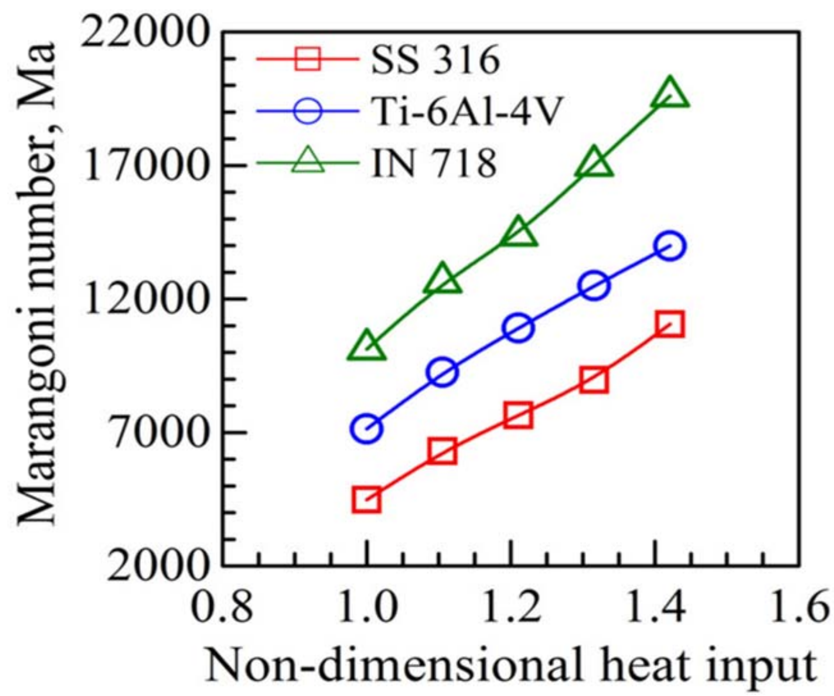
Mukherjee, Manvatkar, De, DebRoy, J. Appl. Phys., 2017

Dimensionless numbers to explain transport phenomena

Marangoni number

$$Ma = -\frac{d\gamma}{dT}\frac{w\Delta T}{\eta\,\alpha}$$

Surface tension gradient	$d\gamma/dT$
Pool width	w
Temperature difference	ΔT
Viscosity	η
Thermal diffusivity	α



- Represents the effects of Marangoni stress on molten metal velocity
- High Marangoni no. => Active circulation => Wider molten pool
- Higher Marangoni no. => more efficient convective heat transfer

Mukherjee, Manvatkar, De, DebRoy, Scripta Mater., 2017

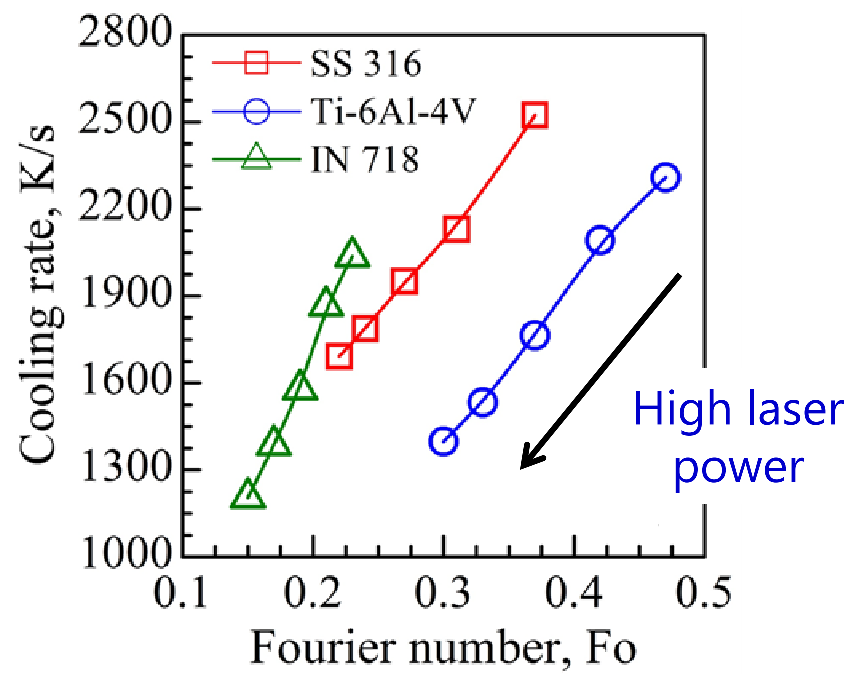
Dimensionless numbers to explain transport phenomena

Fourier number

$$\frac{\text{Heat dissipation rate}}{\text{Heat storage rate}}$$

$$F_o = \alpha / V\,L$$

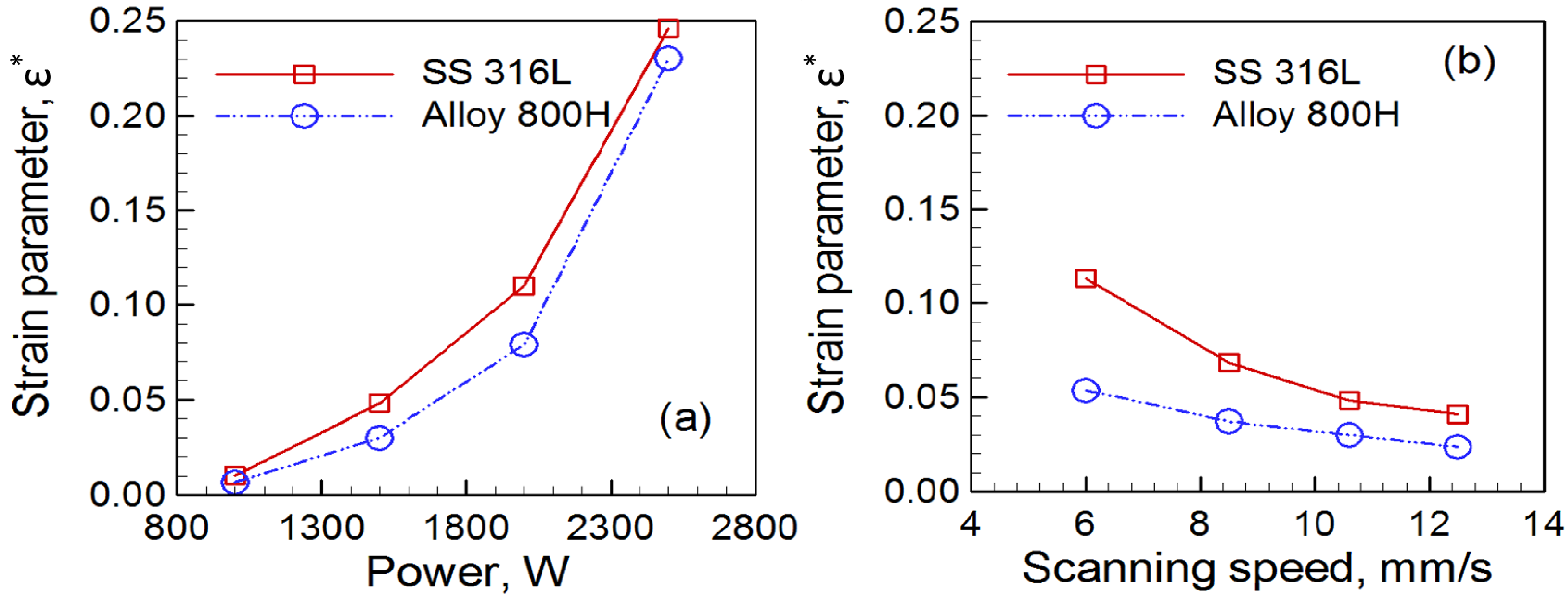
Thermal diffusivity	α
Pool length	L
Scanning speed	V



- Laser power: 190-270 W, scanning speed: 15 mm/s
- High Fourier no. => Fast heat dissipation => Rapid cooling
- Ti-6Al-4V has the highest thermal diffusivity among 3 alloys

Mukherjee, Manvatkar, De, DebRoy, J. Appl. Phys., 2017

Prediction of thermal strain



$$\varepsilon^* = \frac{\beta \Delta T}{EI} \frac{t}{F\sqrt{\rho}} H^{3/2}$$

High Power and low speed

↓

High peak temperature and large pool

↓

More solidification shrinkage

↓

High thermal strain and distortion

Variables	Symbols
Thermal expansion coefficient	β
Temperature difference	ΔT
Fourier number	F
Heat input per unit length	H
Total time	t
Flexural rigidity of substrate	EI
Density	ρ

Mukherjee, Zuback, De, DebRoy, Nature Sci. Rep., 2016

Research needs for building a digital twin

- More rigorous validation of component models
- Including convective heat transfer to make models more realistic
- Scale-up of models for real life components
- Solid state transformations for common engineering alloys
- Reverse modeling

Thank you !

http://www.matse.psu.edu/modeling