Grain Growth Modeling for Additive Manufacturing of Nickel Based Superalloys

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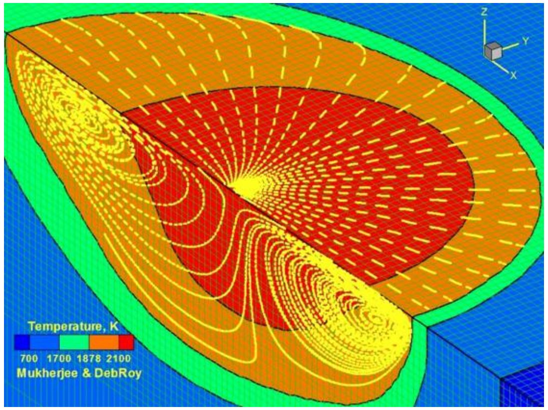
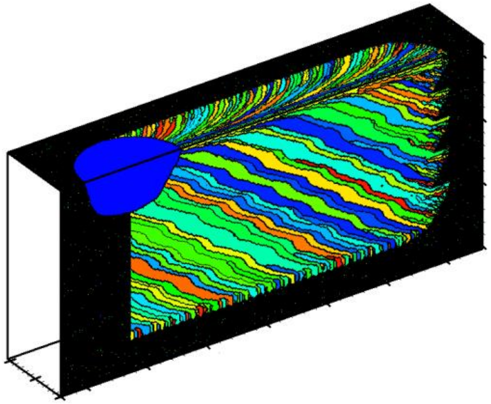
Why grain growth in additive manufacturing ?

Calculation of accurate temperature field

3D accurate grain growth model computationally more efficient than phase field and cellular automata





6th International Conference on Recrystallization and Grain Growth
Pittsburgh, PA, USA, July 17–21, 2016

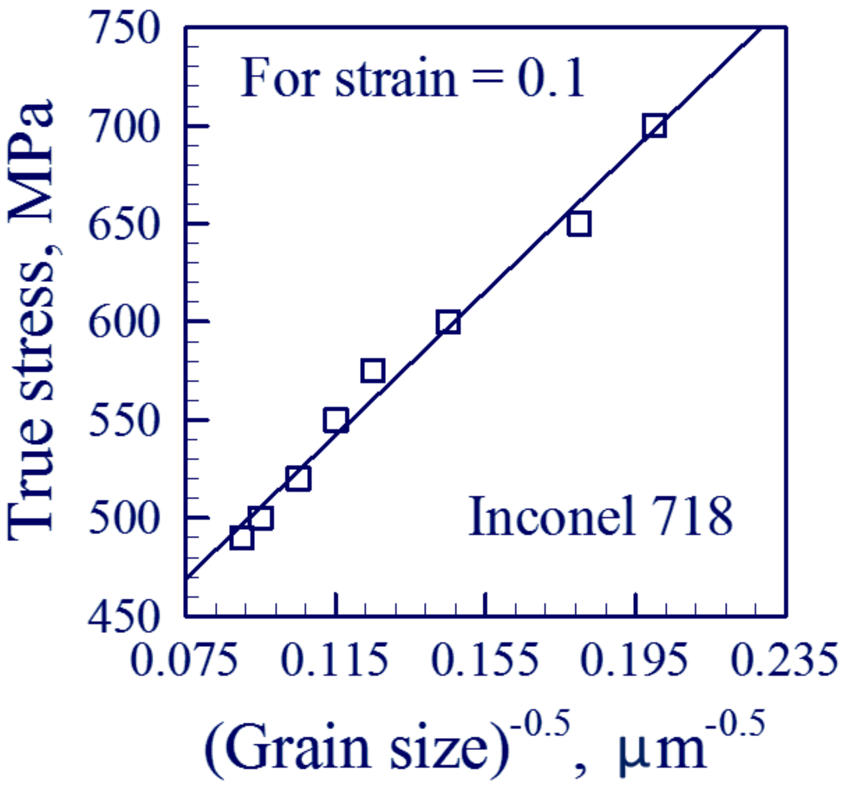
Main objectives

Estimation of accurate temperature field

=> Required for grain growth and microstructure

Prediction of grain growth

=> Affects mechanical properties



Liu et al. High Temp. Mater. Processes. 2016

Approach:

3D heat transfer and fluid flow model

=> Transient temperature and the velocity field

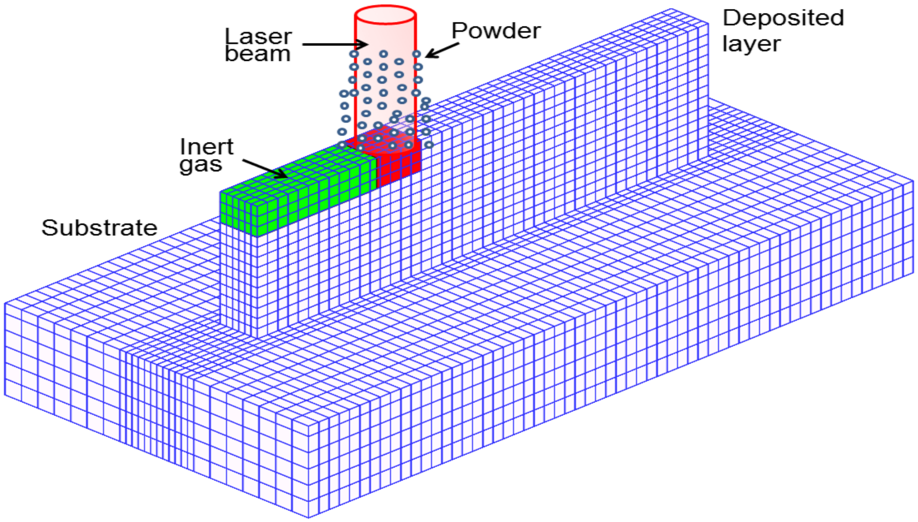
Monte Carlo grain growth model

=> 3D grain growth based on the maximum heat flow direction

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, solidification parameters ...

Calculation domain: about 250,000 cells

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

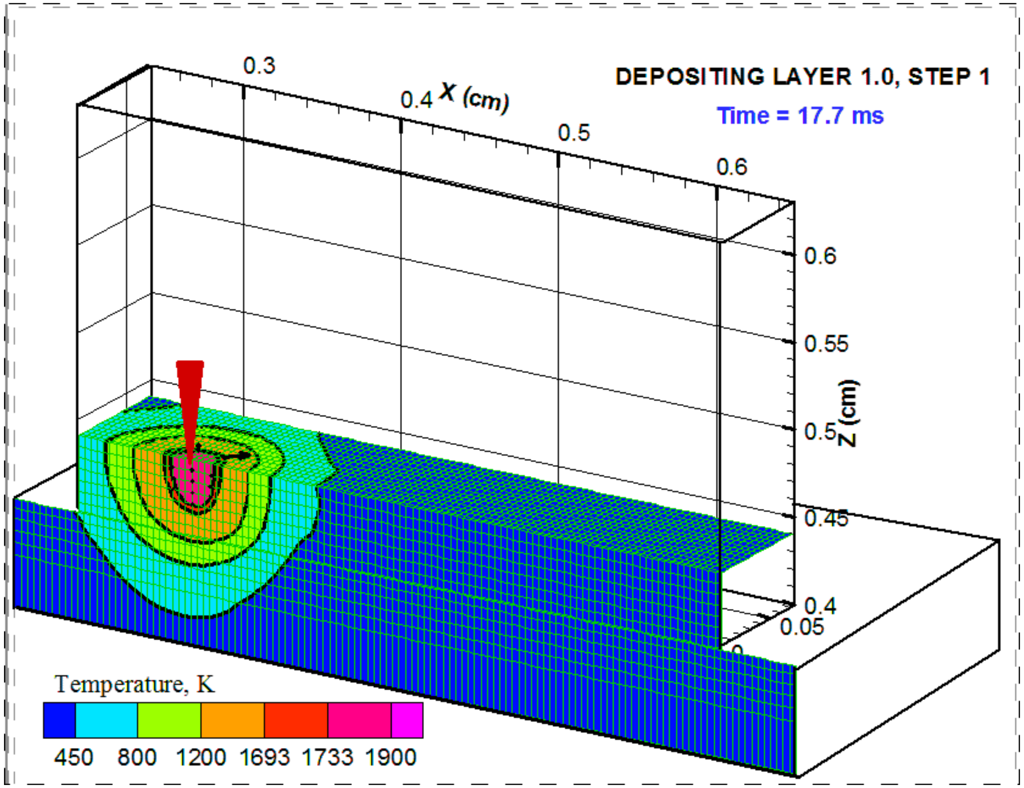
1.25 million algebraic equations (250000 x 5)

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

1000 time step => 125 billion total equations

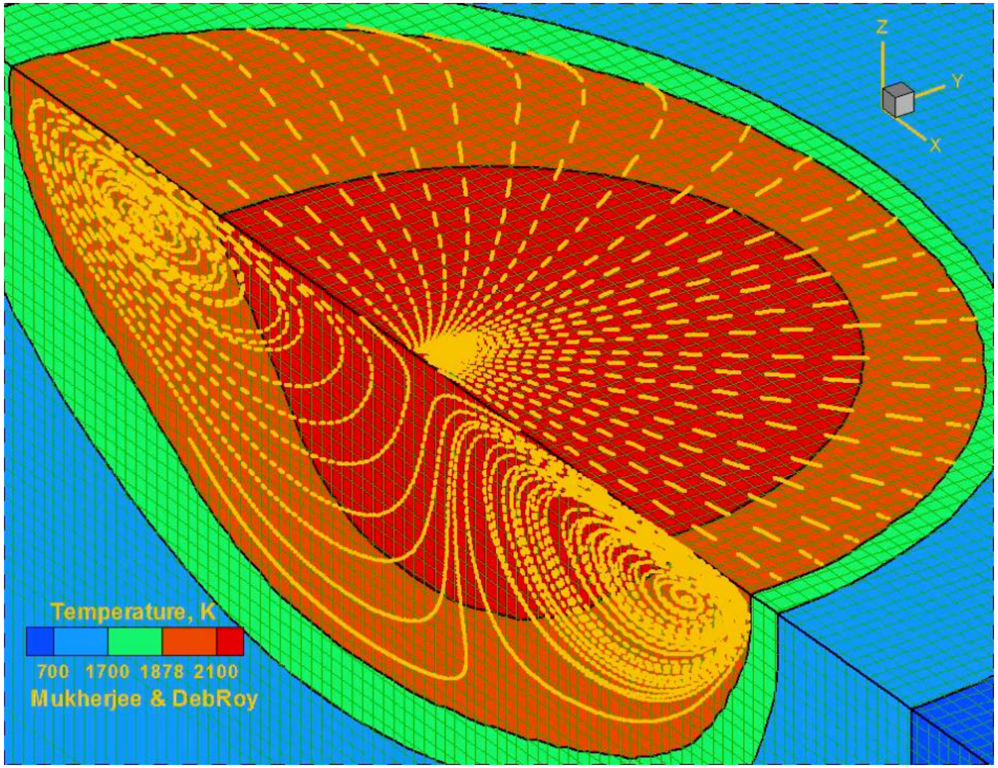
Manvatkar et al. J Appl. Phys. 2014

3D transient temperature distribution



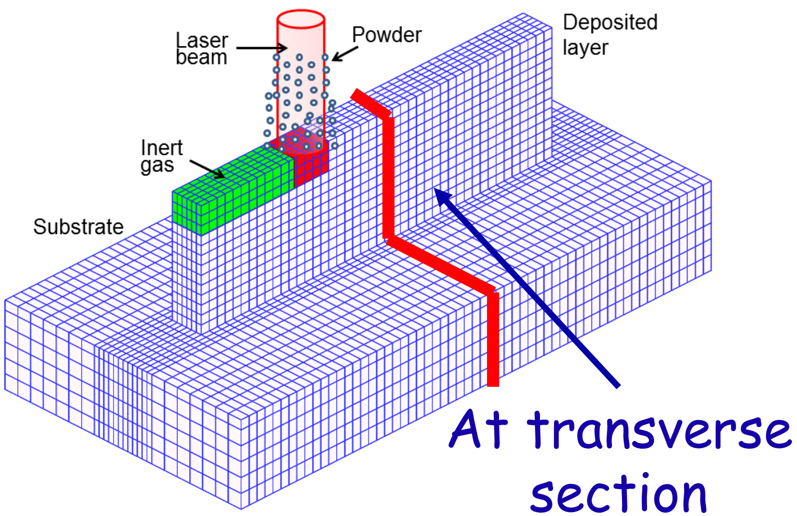
Laser power (W)	Beam radius (mm)	Scanning speed (mm/s)	Layer thickness (mm)	Substrate thickness (mm)
210	0.5	12.5	0.38	4

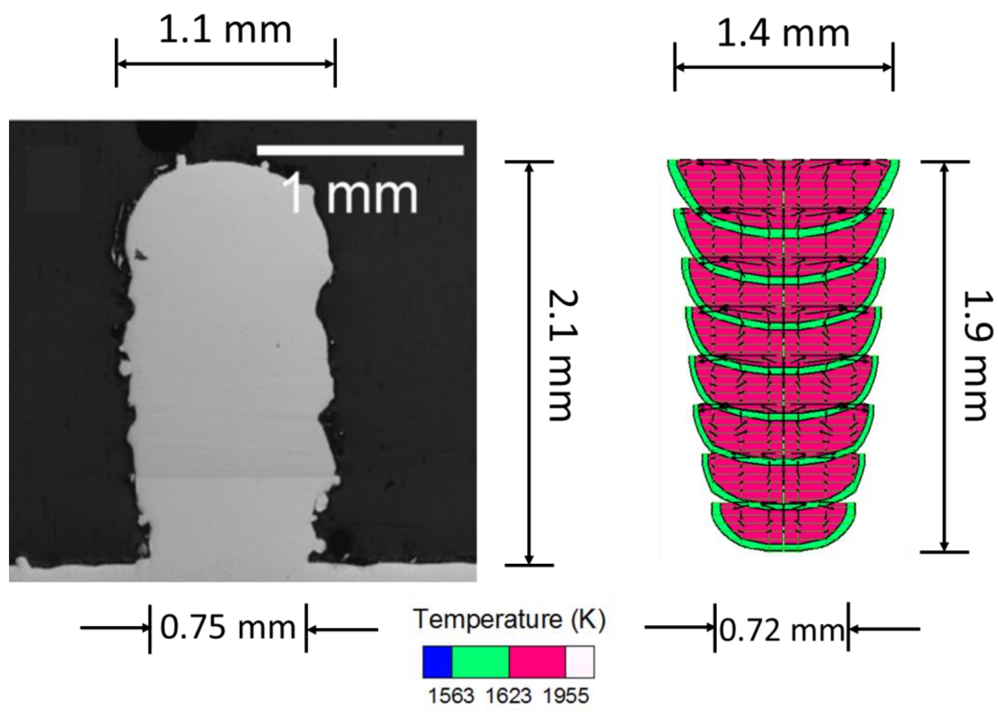
3D transient molten metal velocity field



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

Experimental validation: Shape and size of deposition

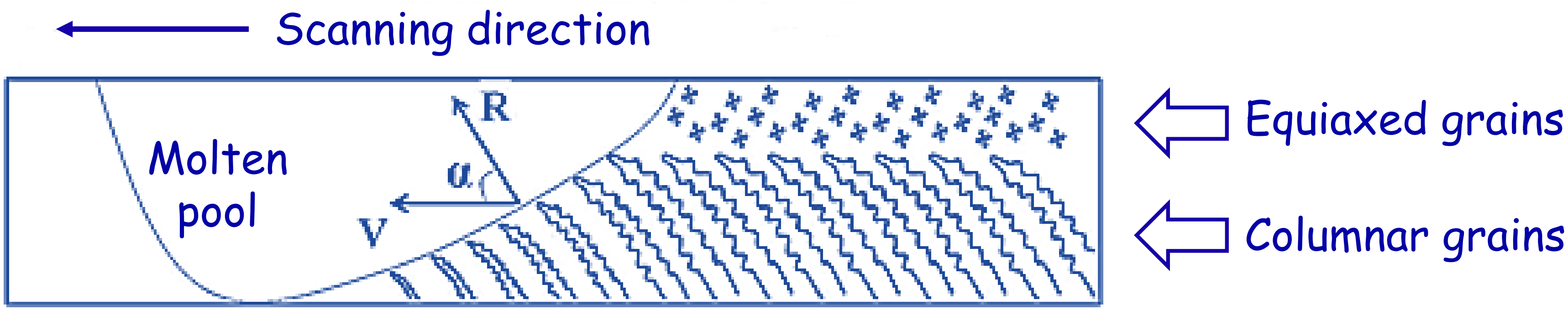




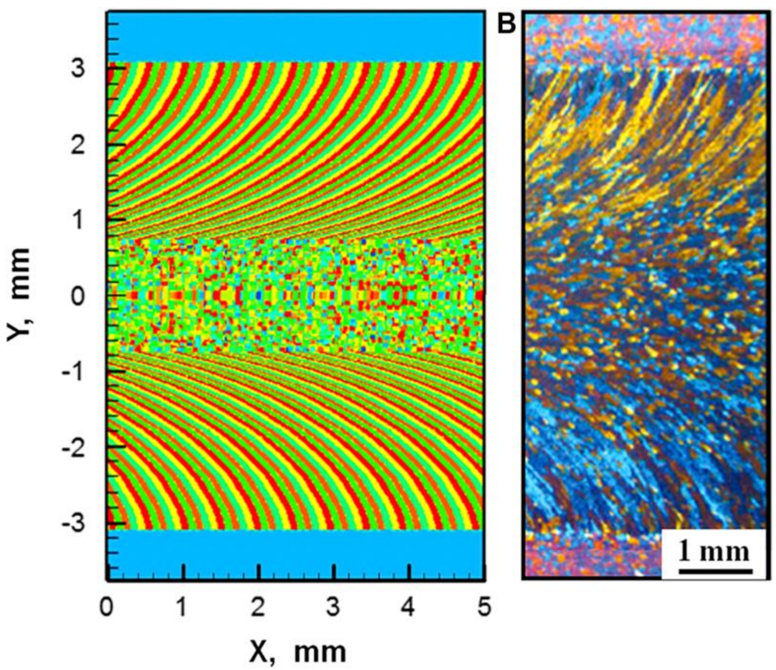
Material	Laser power (W)	Beam radius (mm)	Scanning speed (mm/s)	Layer thickness (mm)	Substrate thickness (mm)
IN 625	600	0.5	7.5	0.25	7

Mukherjee, Zuback, De & DebRoy. Sci. Rep. (2016)
www.nature.com/articles/srep19717

Solidification morphology



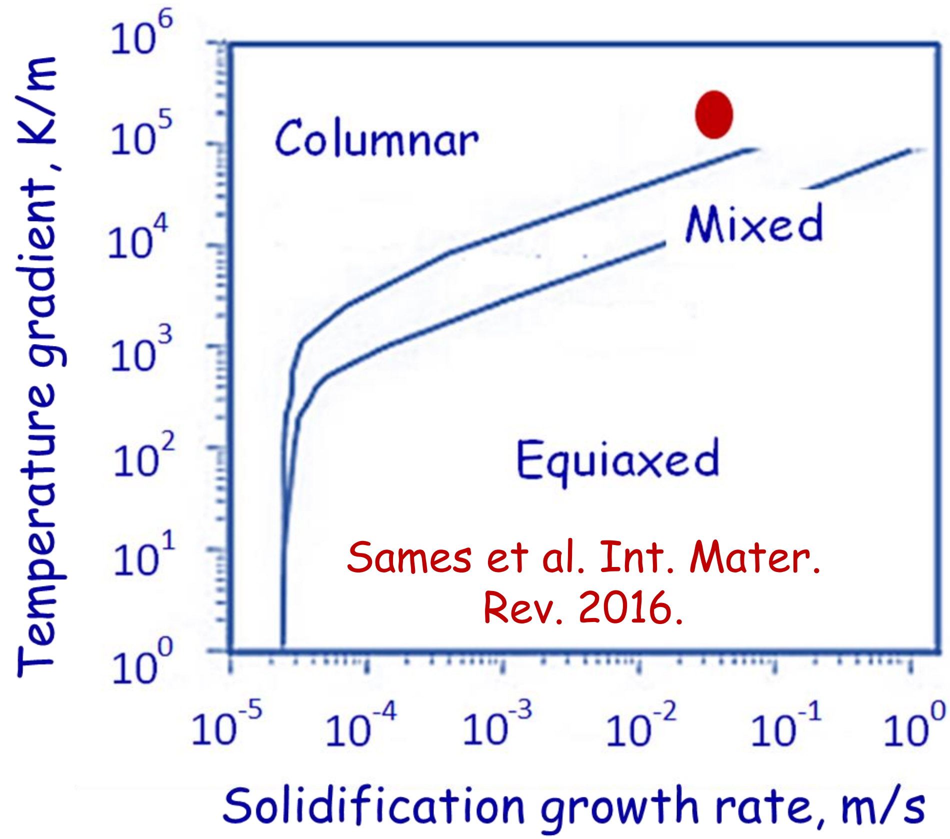
Solidification morphology depends on => $\frac{\text{Temperature gradient (G)}}{\text{Growth rate (R)}}$



- In a big molten pool for GTAW, G/R can vary significantly
- A mixture of columnar and Equiaxed grains can be observed

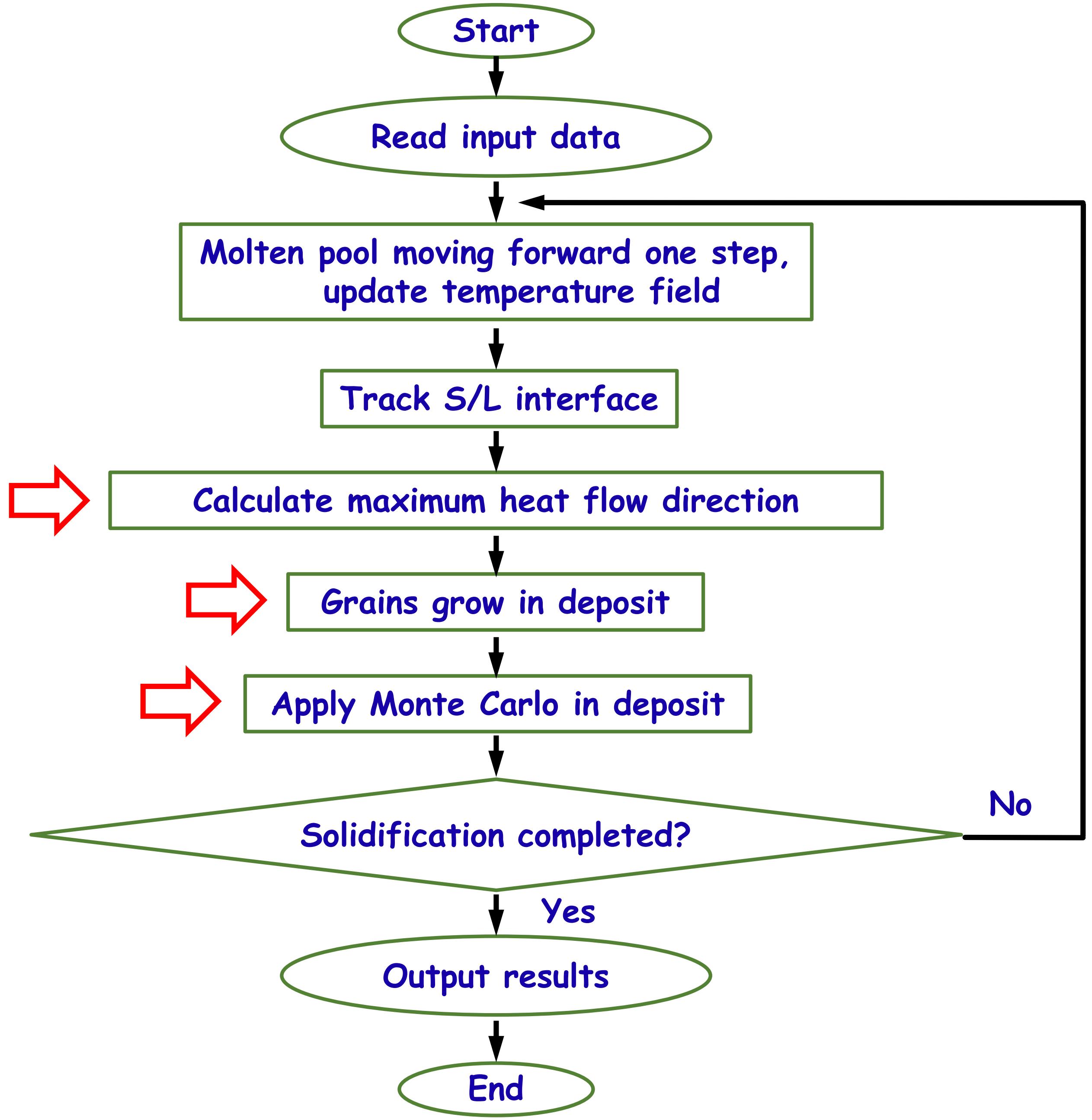
Wei et al. Acta Mater. 2016.

Solidification morphology during AM of IN 718

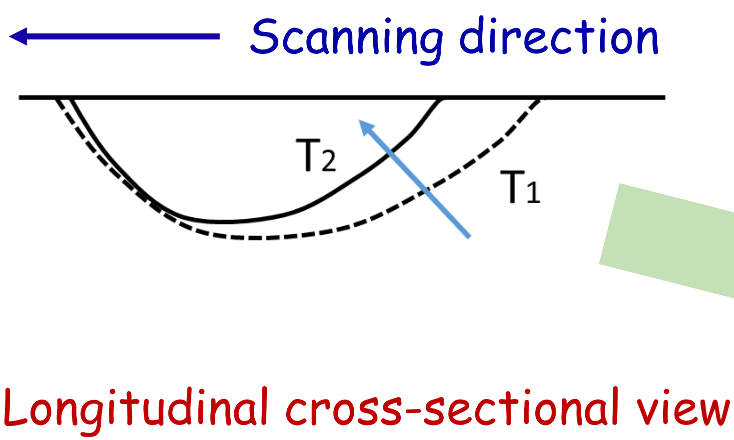


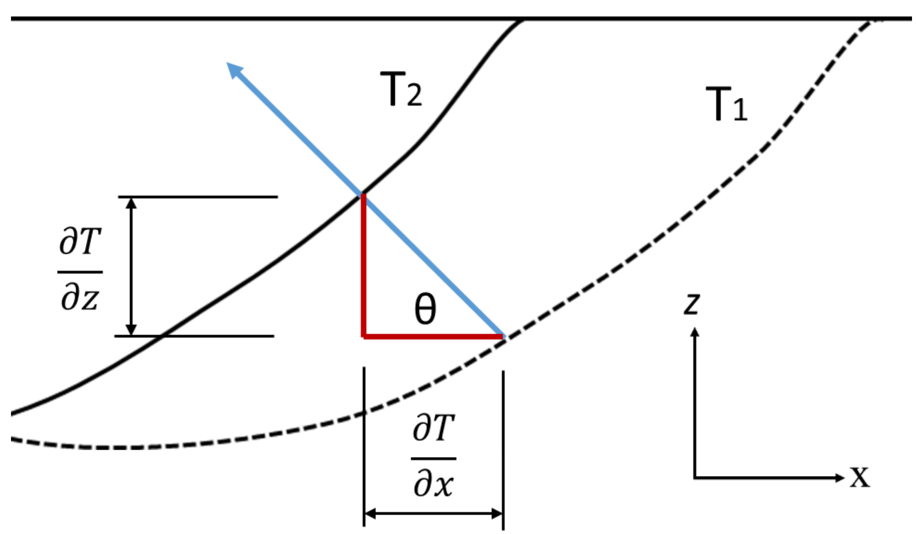
Material	Laser power (W)	Beam radius (mm)	Scanning speed (mm/s)	Layer thickness (mm)	Substrate thickness (mm)
IN 718	250	0.5	20	0.4	4

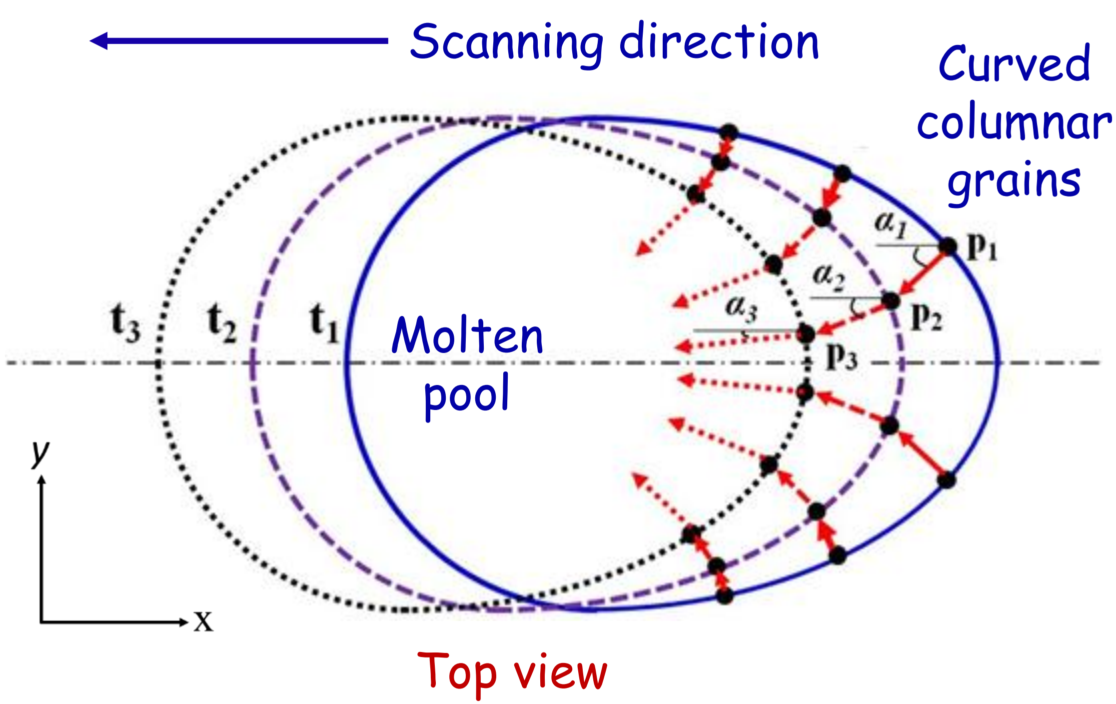
3D grain growth model: algorithm



Maximum heat flow direction







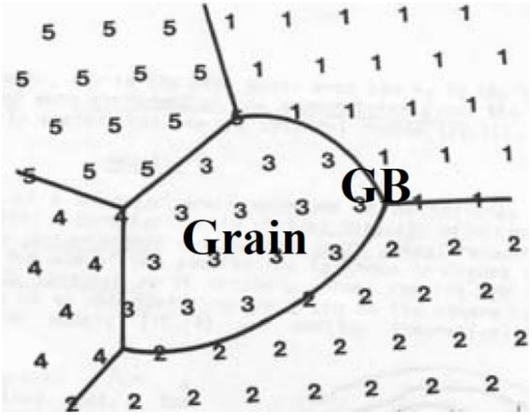
Wei et al. Acta Mater. 2016.

Wei et al. Sci. Rep. 2015.

Monte Carlo grain growth model

Step 1

Each grid point is assigned a random orientation number between 1 and Q > 32



Step 2

Calculate the local interaction energy $E_1 = -J \sum_{j=1}^{n} \left(\delta_{S_i S_j} - 1\right)$

J => positive constant to set the scale of grain-boundary energy

δ => Kronecker's delta function

Si => orientation at a randomly selected site i

S_j => orientation of its nearest neighbors

n => total number of the nearest-neighbor sites

Monte Carlo grain growth model

Step 3

Grain boundary migration:

1. Select a random site
2. Select the neighbors along maximum heat flow direction
3. Change its orientation to one of the nearest-neighbor orientations

Step 4

Calculate the local interaction energy $E_2 = -J \sum_{j=1}^{n} \left(\delta_{S_i S_j} - 1\right)$

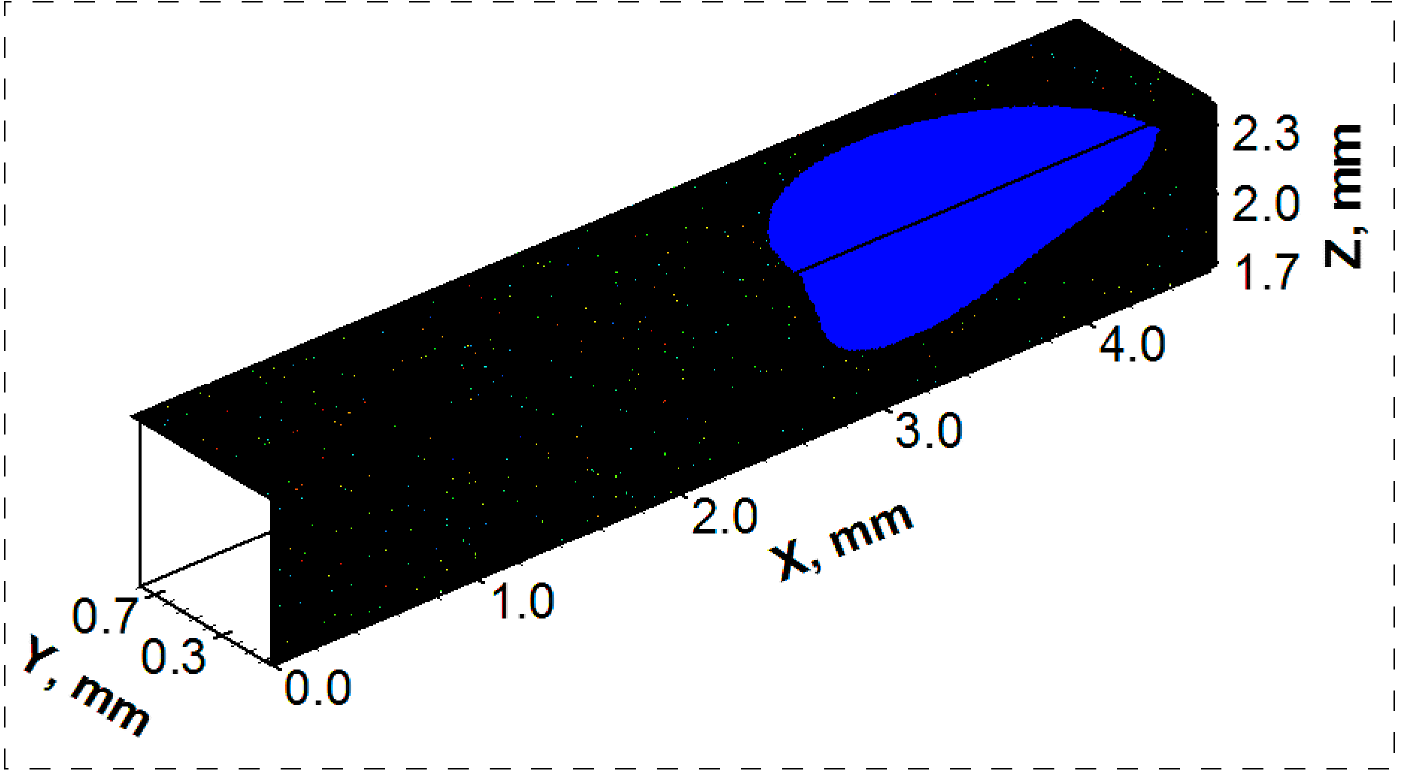
The probability of orientation change corresponds to boundary migration

If, $E_2 - E_1 \leq 0$ Probability = 1

If, $E_2 - E_1 > 0$ Probability = $e^{-(E_2 - E_1)/k_B T}$

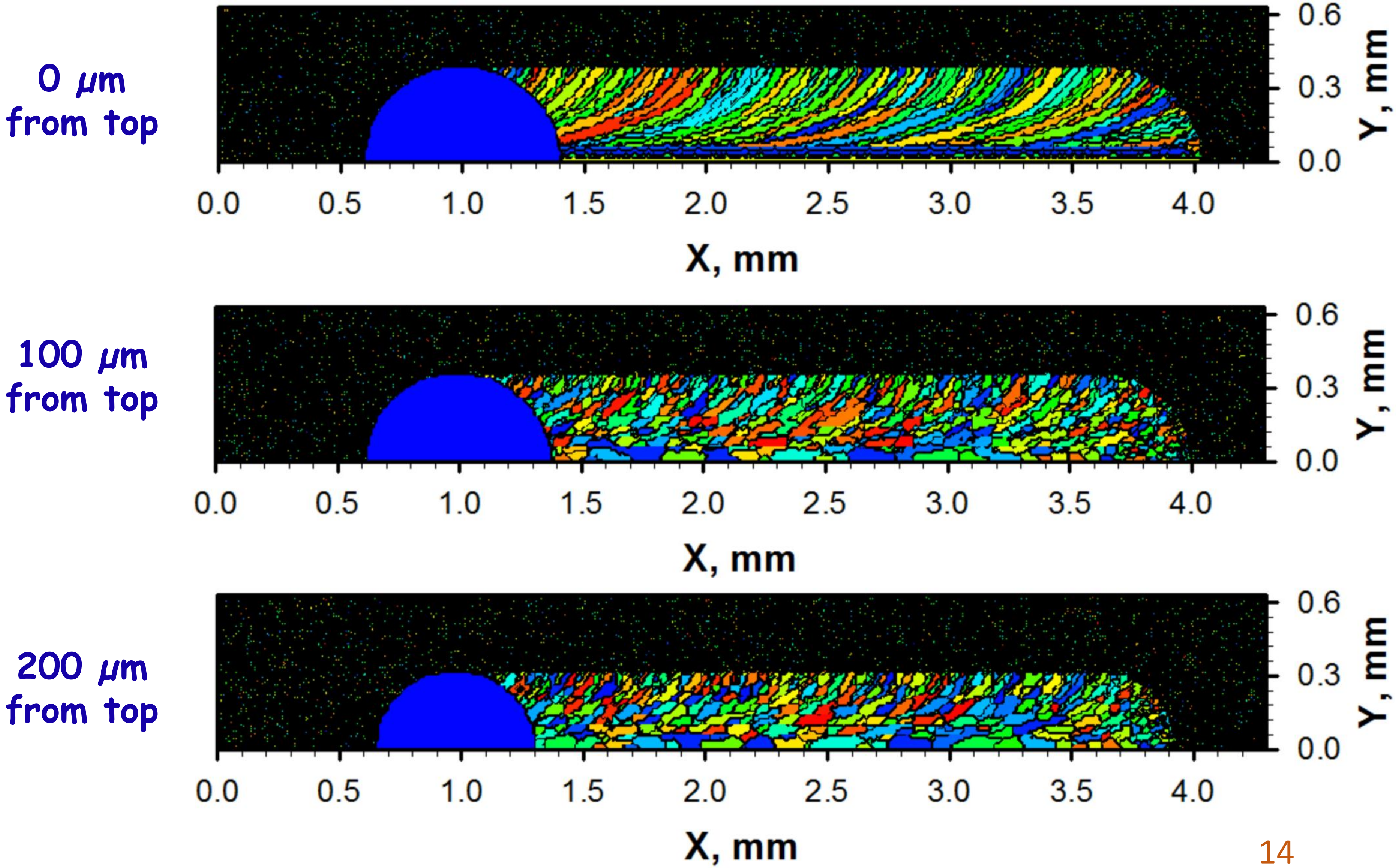
k_B is Boltzman constant and T is temperature

3D grain growth during AM of IN 718



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

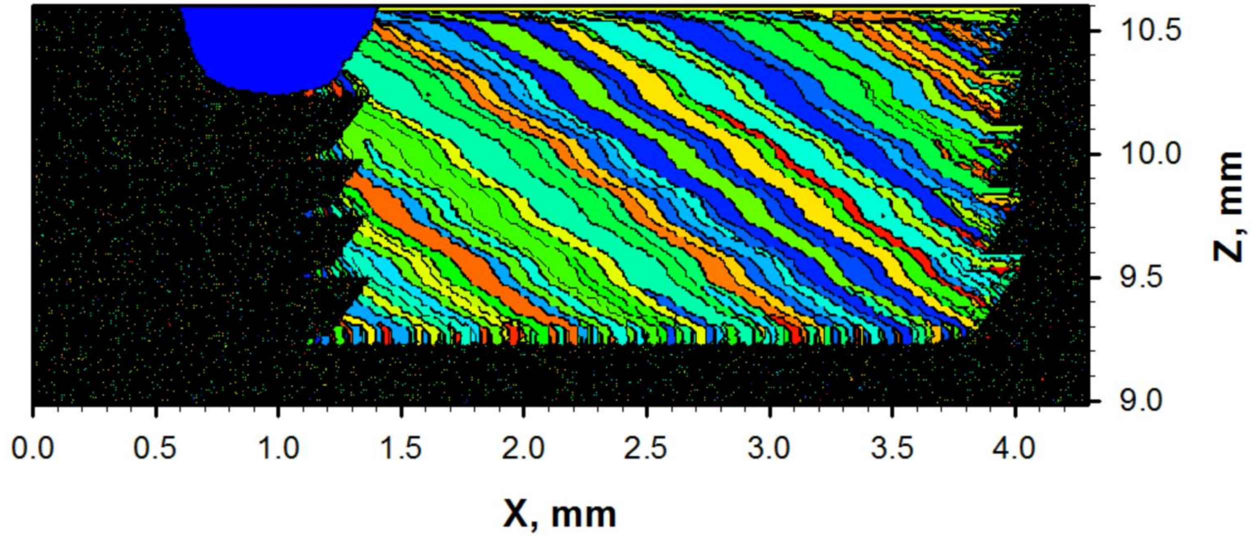
Spatial distribution of grain shape and size at various horizontal planes of the deposit



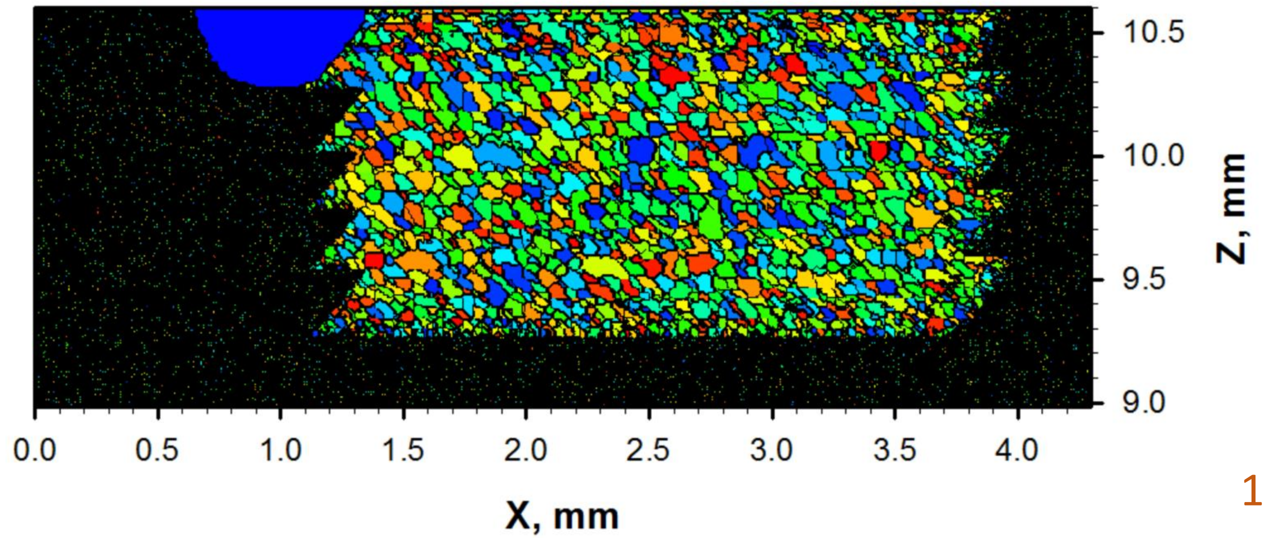
Spatial distribution of grain shape and size at various longitudinal planes of the deposit

Scanning direction

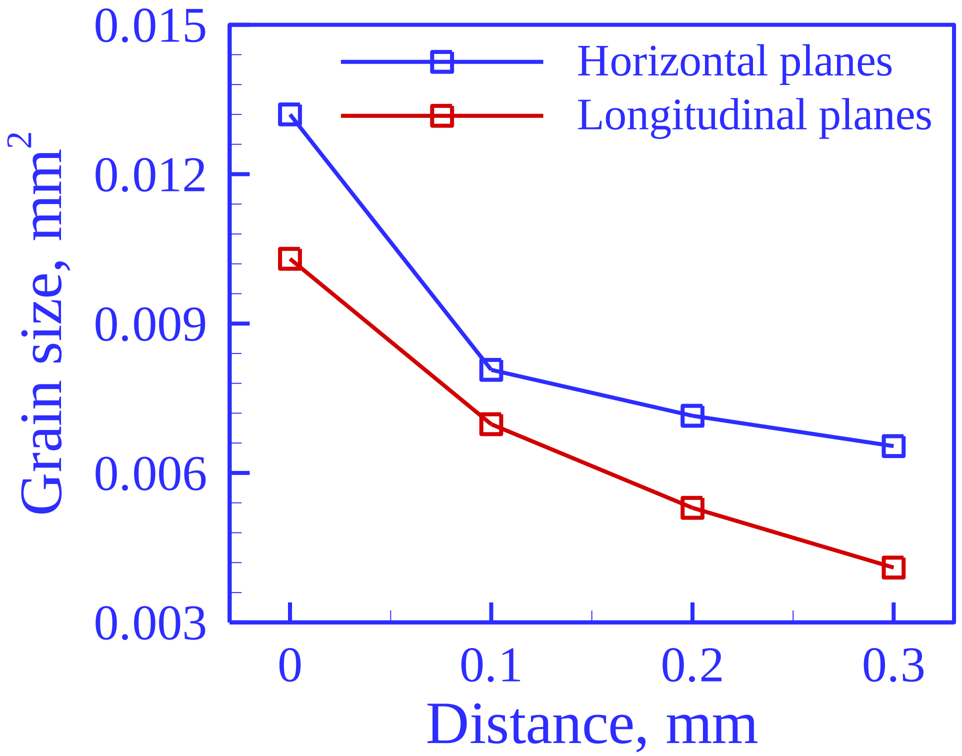
At the center of the pool



200 μm from the center of the pool

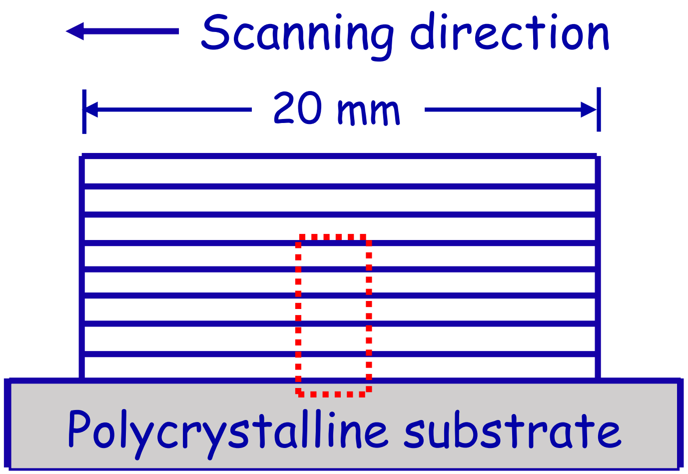


Spatial distribution of grain size

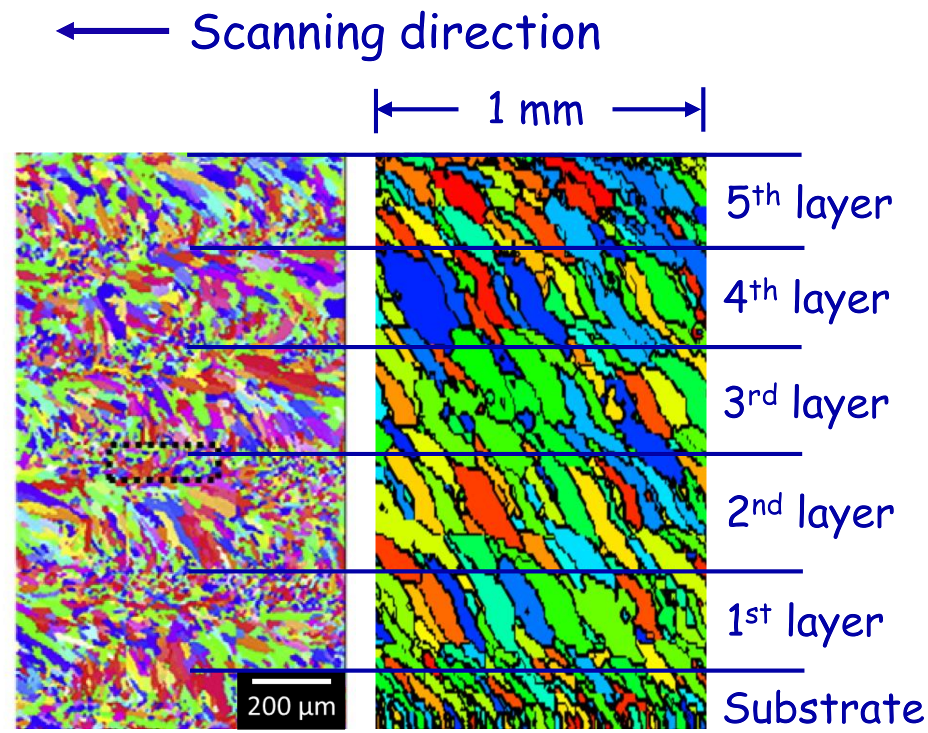


- Distances for horizontal planes are measured from top surface
- Distances for longitudinal planes are measured from pool center
- Grain sizes are smaller at the locations away from the center of the molten pool because of the lower growth rate of grains.

Experimental validation: EBSD map of grain growth



Longitudinal cross section

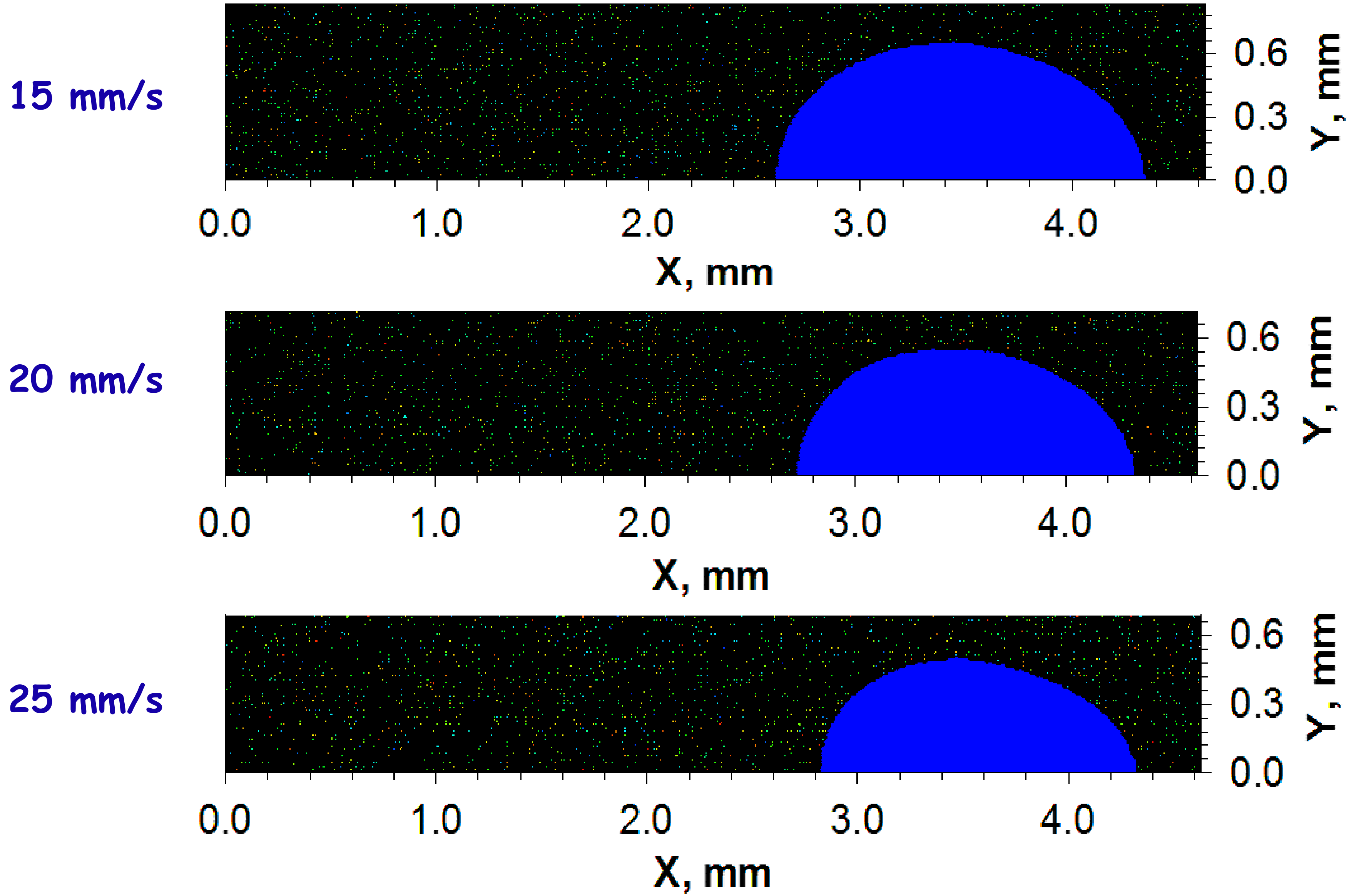


Parimi et al. Mater. Character. 2014.

Columnar grains curve towards the scanning direction and grow along the maximum heat flow direction

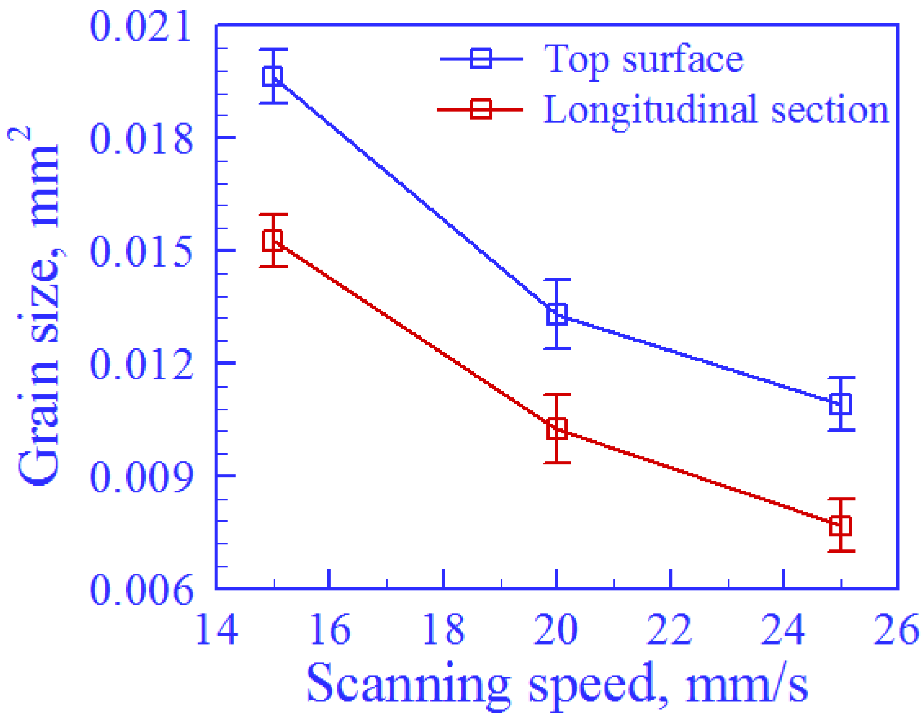
Material	Laser power (W)	Beam radius (mm)	Scanning speed (mm/s)	Layer thickness (mm)	Substrate thickness (mm)
IN 718	390	0.35	3.3	0.3	10

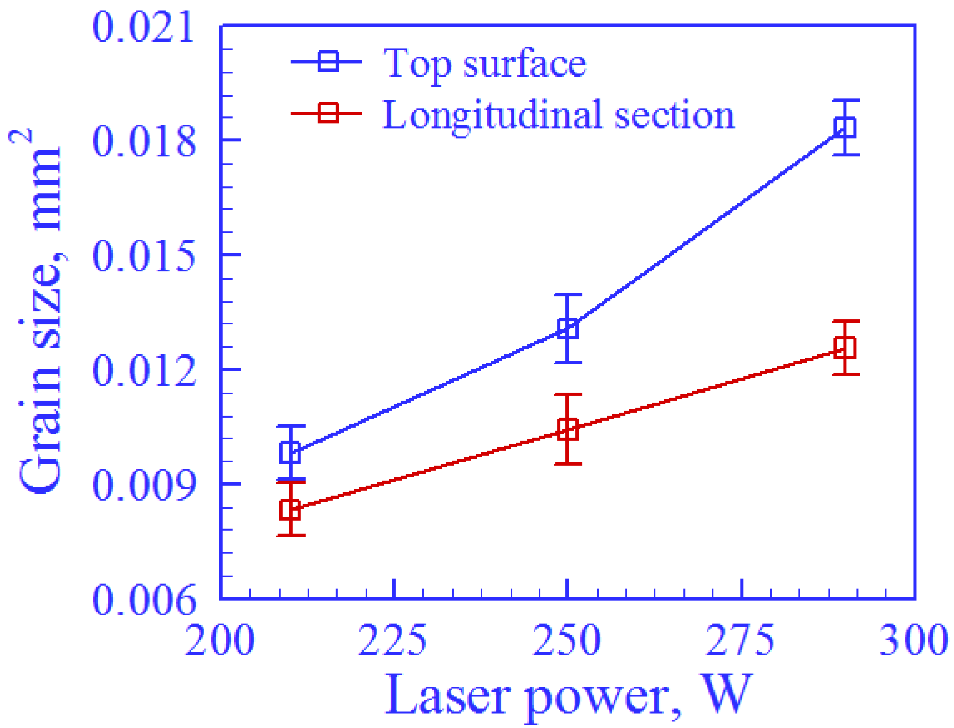
Effect of laser scanning speed on grain growth



Laser power = 250 W Top view of deposit Inconel 718

Effect of laser power and scanning speed on grain size





High scanning speed low laser power => Low linear heat input

Low linear heat input => High cooling rate

High cooling rate => Smaller grain size

Summary and conclusions

- A 3D transient heat transfer and fluid flow model is used to calculate the temperature field during the deposition.
- A Monte Carlo grain growth model is used to simulate the grain growth along the maximum heat flow direction.
- Columnar grains curve along the scanning direction to follow the maximum heat flow direction.
- Grain sizes are smaller at the locations away from the center of the molten pool because of the lower growth rate of grains.
- Higher scanning speed and lower power promotes a rapid cooling rate and therefore smaller grain size .