Development of a Microstructural Rapid Solidification Model for Additive Manufacturing Process

A.R.S.M.

03. 18. 2019

What is the Additive Manufacturing(AM)?

: a manufacturing process of making three dimensional solid objects by building up additives

Pros

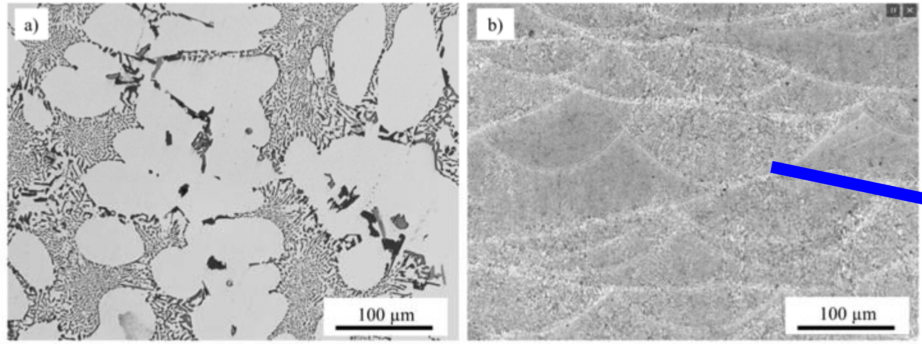
- Lower costs of manufacturing (few additional process, no wastes)
- On-demand manufacturing
- A good option for making extremely complex parts
- Reliability

Cons

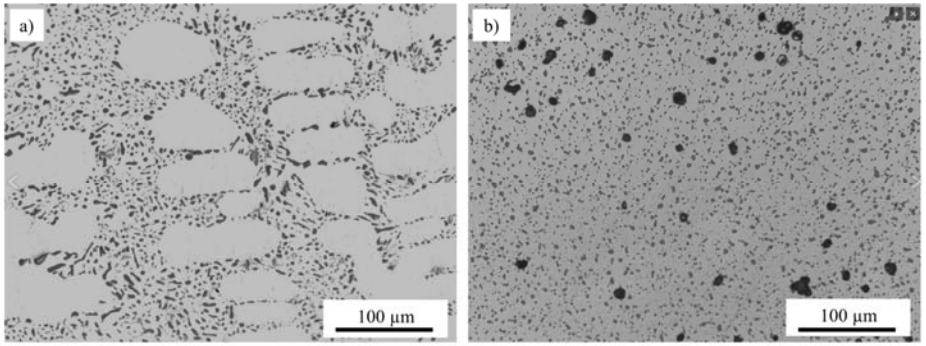
- Low productivity
- Limited materials (e.g. a few steels, Al, Ni, Ti alloys in the case of metal AM)
- Hard to predict mechanical properties (because of dependence of various manufacturing parameters)

→ Solidification model is needed to predict the microstructure which directly decide the mechanical properties of the product

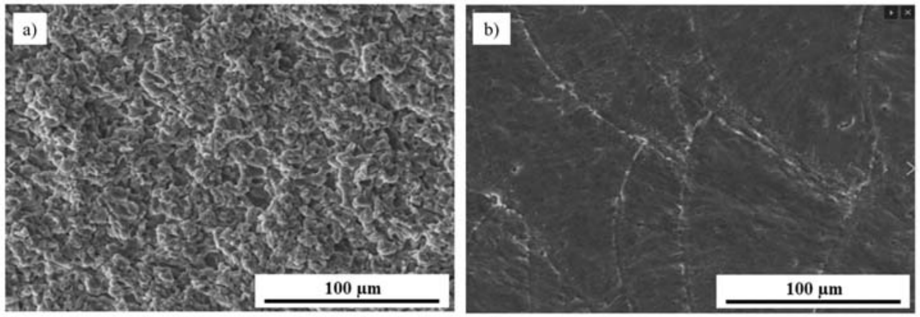
Foundry vs AM



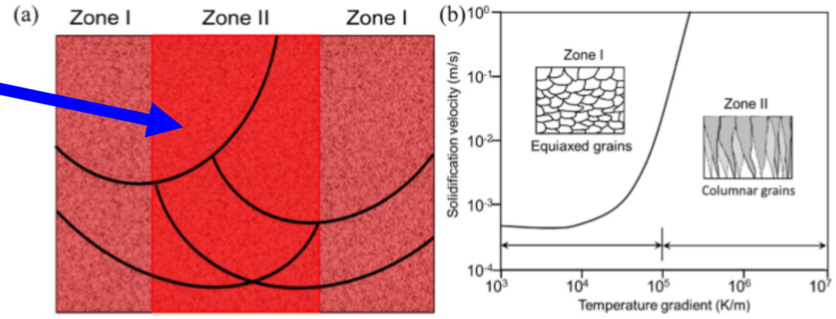
Examples of microstructure under conditions as-produced of AlSi10Mg alloy samples obtained through a) gravity casting and b) AM Item 1 of 4

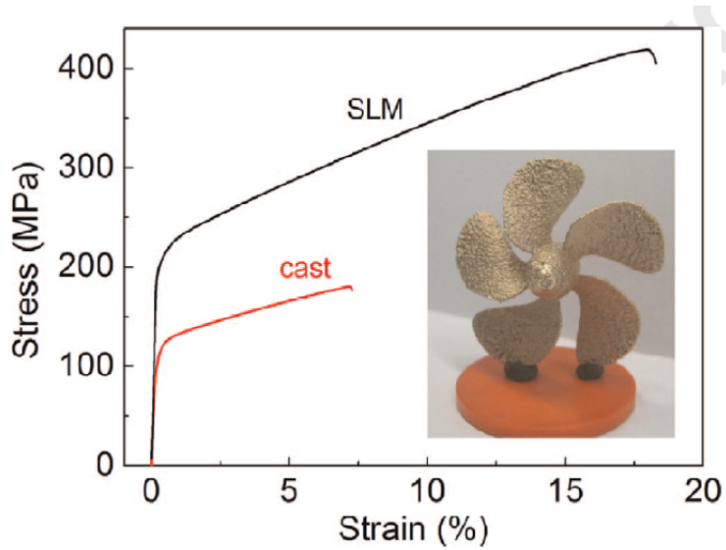


Examples of microstructure under T6 conditions of AlSi10Mg alloy samples obtained through a) gravity casting and b) AM Item 2 of 4



Different morphology of the surface eroded during cavitation tests for AlSi10Mg alloy samples obtained through a) gravity casting and b) AM Item 3 of 4





Introduction

Characteristics of Solidification for AM

- Cooling rate : Conventional casting (~10^3 K/s) vs. Rapid solidification (10^3~10^6 K/s)
- Dimension : layer thickness = 0.03 ~ 0.1 mm , particle size = 0.01 mm (avg)
- Manufacturing parameters : power, scanning rate, printing path > related to thermal history
- Key input variables for model : Alloy composition(C_0), Thermal gradient(G), Growth rate(V)
- Thermodynamic data, Diffusivity and interfacial energy are needed

Research tracks

Follow-up basic theories of conventional solidification → Follow-up solidification modeling method / Analysis for microstructure of 3D-printed product → Presumption and mathematical modeling → Verifying and modifying in certain system

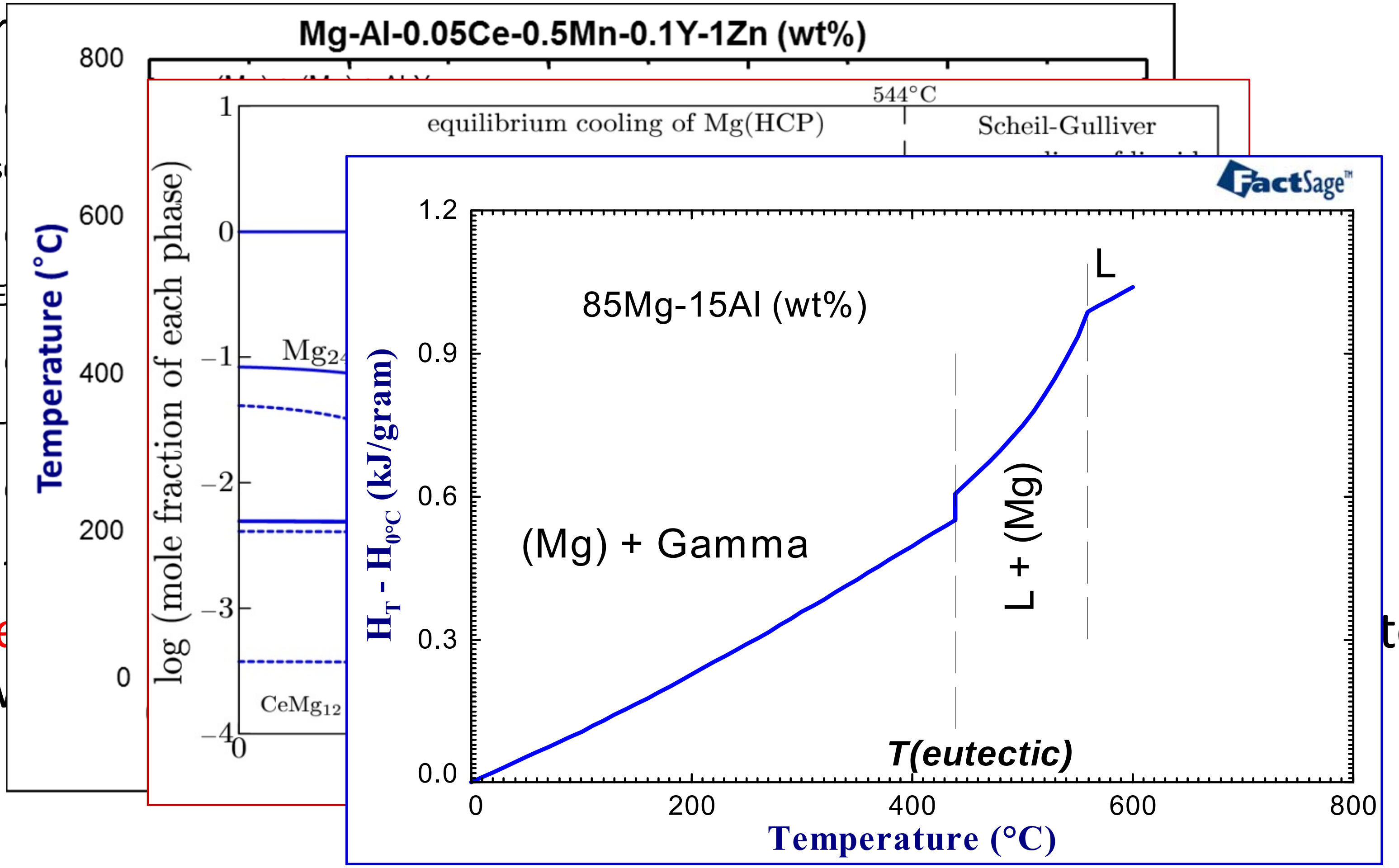
2018 2nd semester | 2019 1st semester (now) | 2019 2nd semester ~

What can we do using Thermodynamic Data?

The thermodynamic database can be used along with the Gibbs
ener

- is
- (E
- (-
-

The
force to
softw



Background

<Commercial Software and databases>

FactSage™

MTDATA

Thermo-Calc Software

SGTE

MatCalc The Materials Calculator

JMatPro Practical Software for Materials Properties

1970' 1980' 1990'

Background

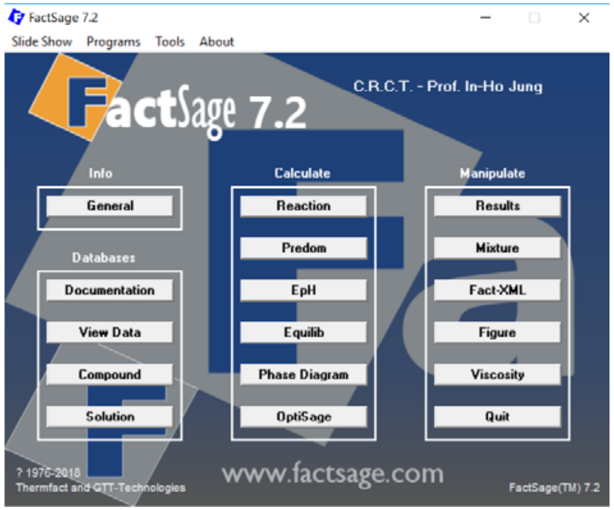
Thermodynamic database

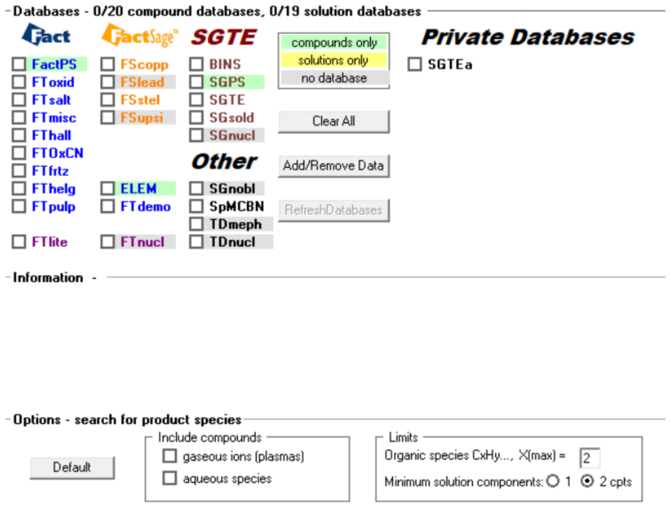
ÉCOLE POLYTECHNIQUE MONTRÉAL

McGill

UNIVERSITÉ Concordia UNIVERSITY

서 울 대 학 교 SEOUL NATIONAL UNIVERSITY





Microstructural simulation (2009 ~)

McGill

서 울 대 학 교 SEOUL NATIONAL UNIVERSITY

Predictions of microstructure evolution : from solidification to annealing

1) Matrix composition distribution

2) Amount and chemistry of Secondary phases and precipitates

Key experiment & simulation code development

Various solidification models

Complexity in calculations

Scheil Cooling Model

> Energy scale (gibbs E)

- Short calculation time (~seconds)
- No morphology
- No cooling rate
- No diffusion

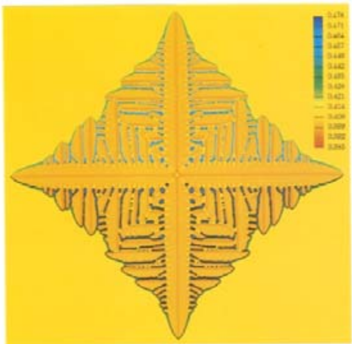
Solidification Model (1D)

> Energy scale + Time scale

- Short calculation time (~ minutes)
- Cooling rate (G·V)
- Concentration profile in dendrite
- Morphology Calc. (+SDAS/PDAS, fraction)
- Multicomponent system
- Based on FVM, FEM code

Phase Field Model

> Energy scale + Time scale + Length(Dimension) scale



- Calculation of morphology
- Concentration profile (diffusion)
- Long calculation time (~ hours, days)
- Difficulty in Multicomponent system

An Integrated tool for microstructure prediction

Solidification

= *f* (*G*, *V*, C_0)

- Solute profile/microsegregation
- Second phase fraction
- SDAS/PDAS
- Morphology

Homogenization

= *f* (*T*, *t*)

- Solute distribution
- Second phase fraction

Precipitation

= *f* (*T*, *t*)

- Solute distribution
- Ppts: Size, Number, Volume

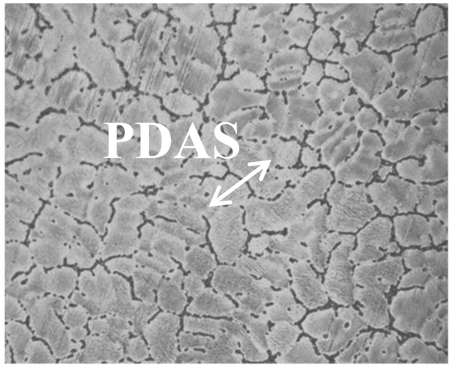
1 Dimension numerical model with

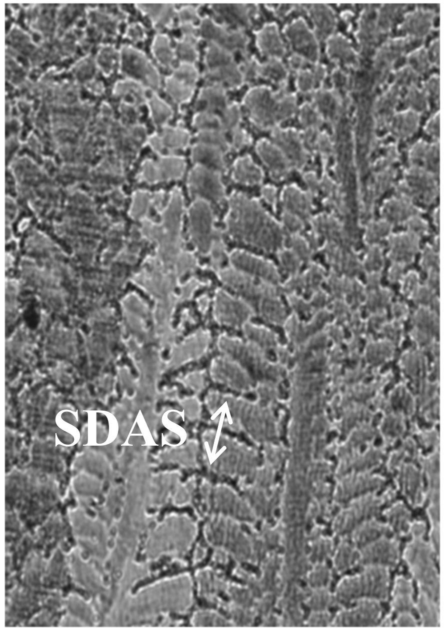
- Multicomponent (2 to 5 components)
- Max. 3 different secondary (or ppts) phases
- Dynamically linked to FactSage thermodynamic database
- Diffusivity (mobility) and interfacial energy: user inputs

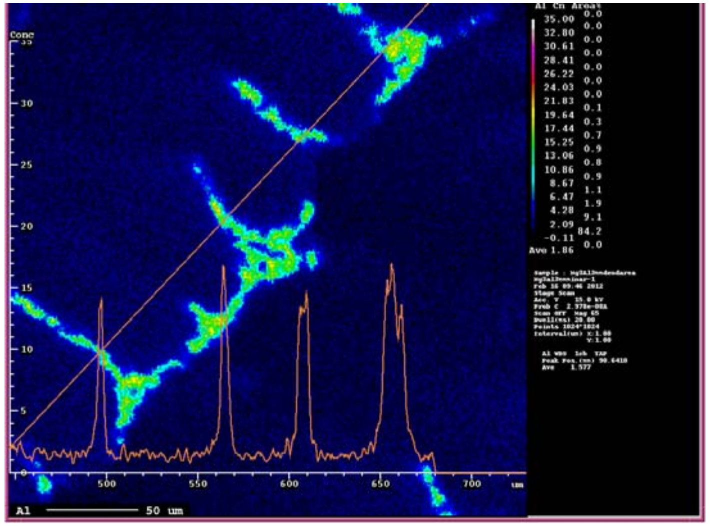
Thermodynamics

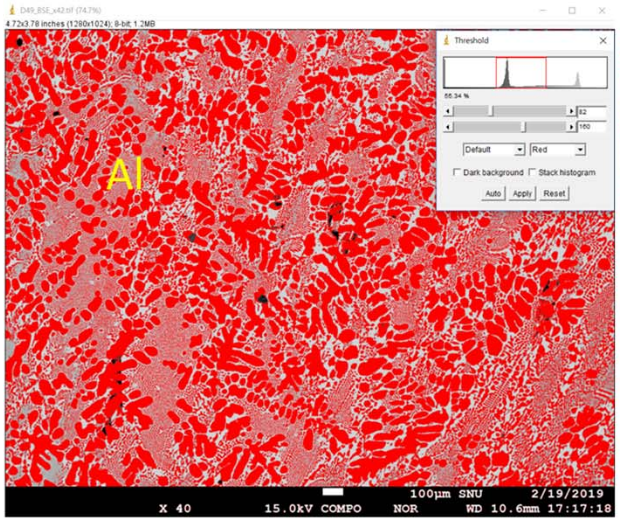
Diffusivity & interfacial energy

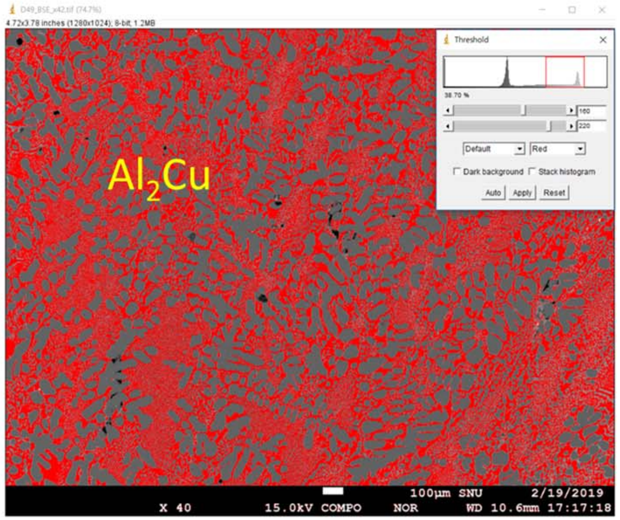
As-cast microstructure



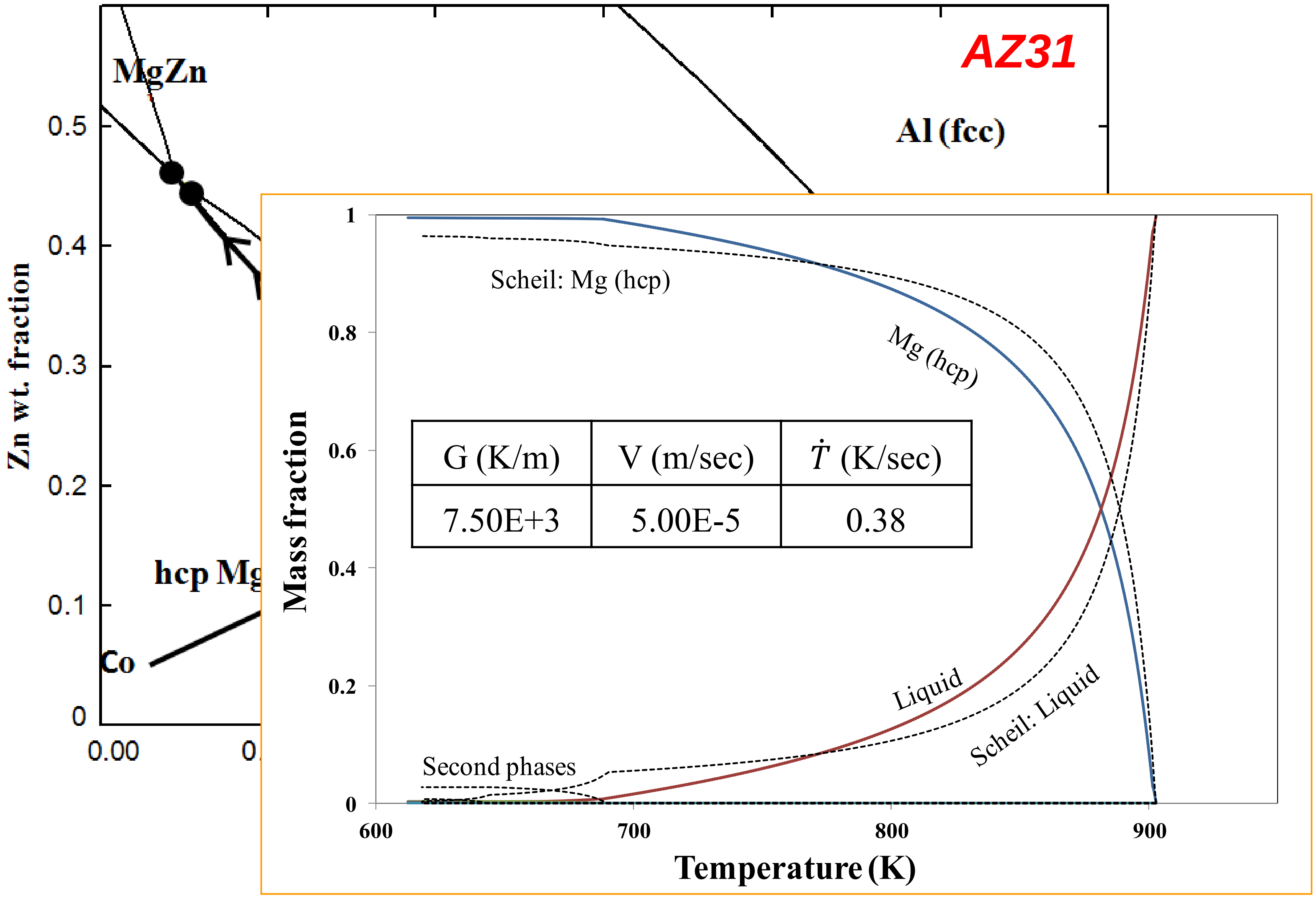






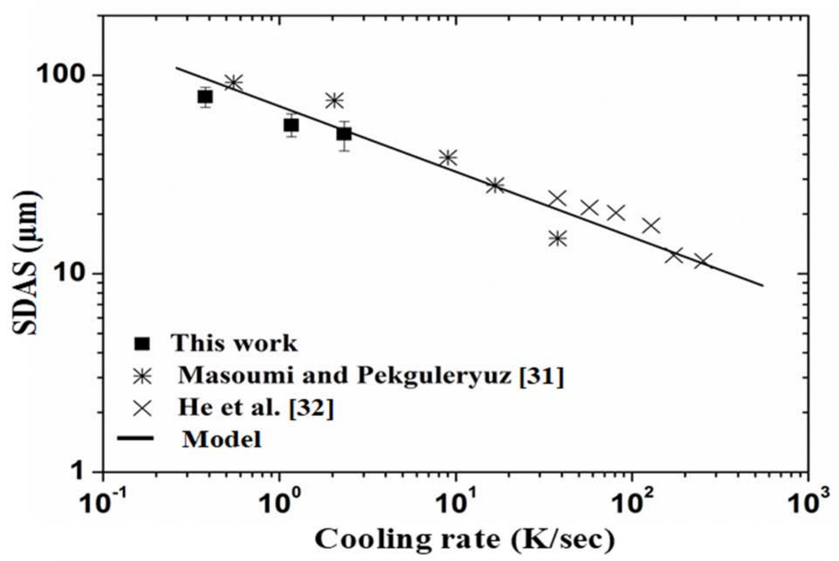


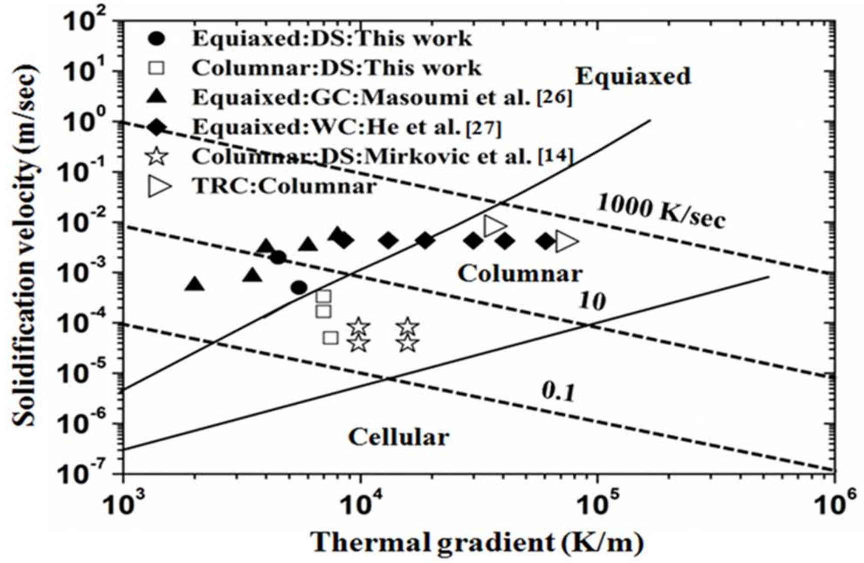
Some previous results

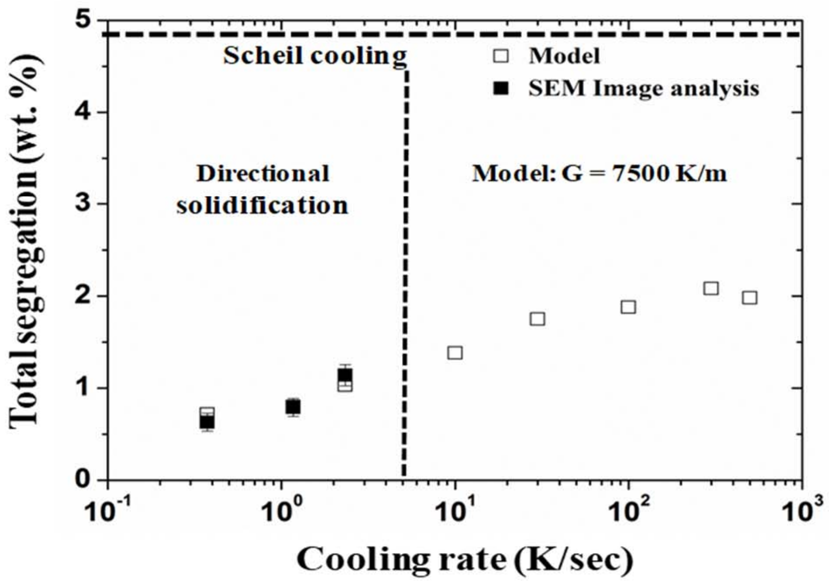


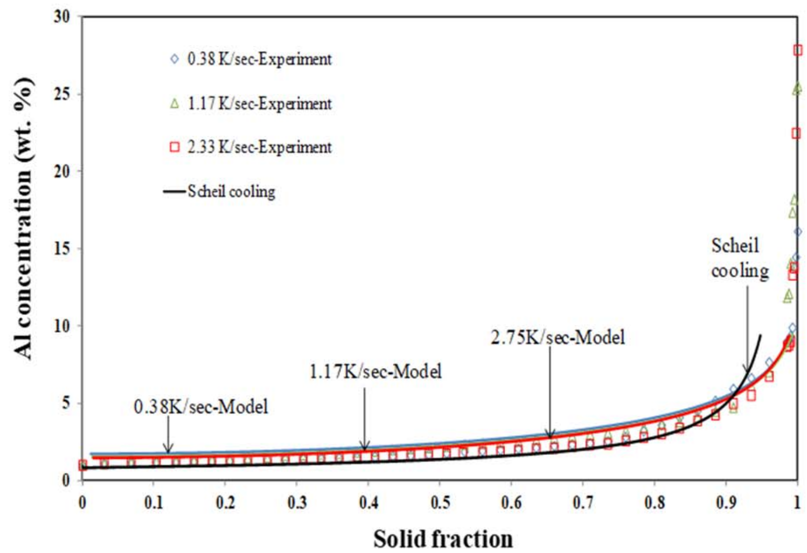
G (K/m)	V (m/sec)	$\dot{T}$ (K/sec)
7.50E+3	5.00E-5	0.38

Solidification model: AZ31

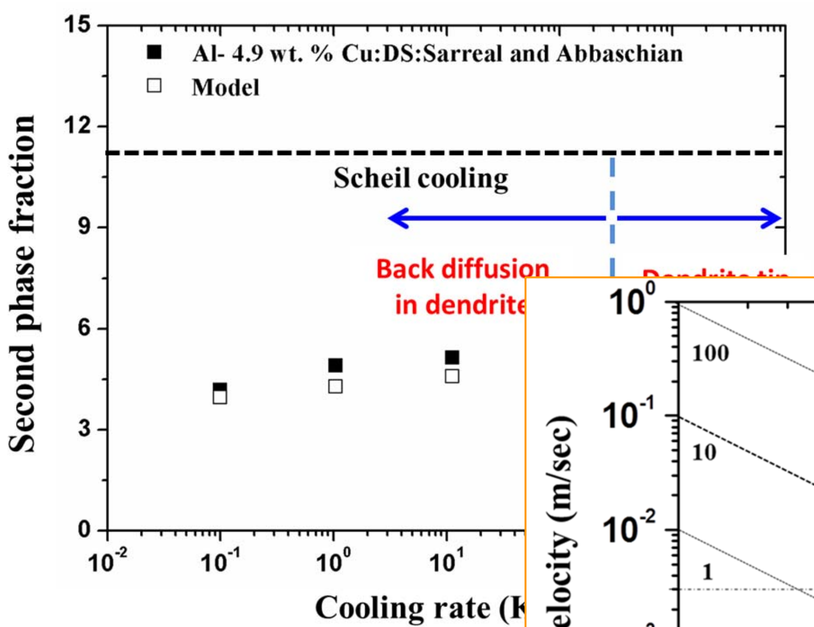


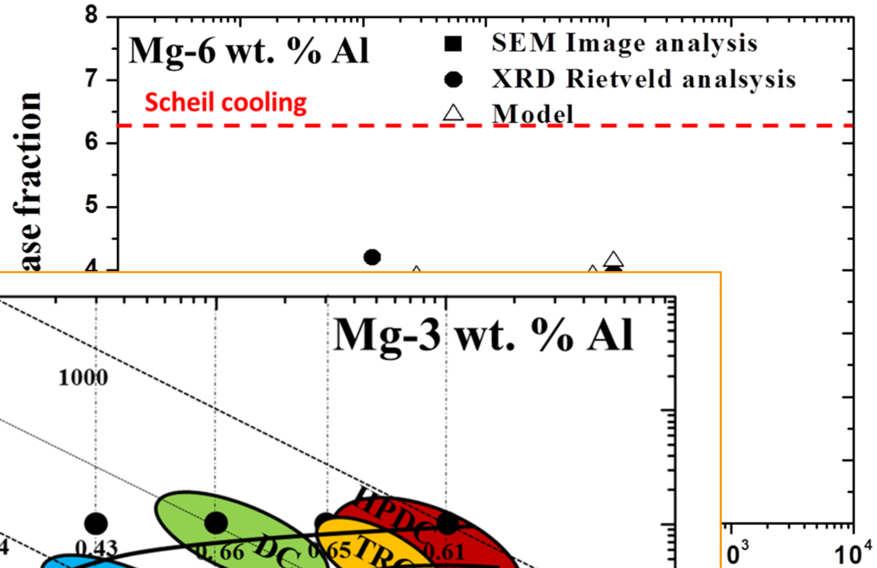




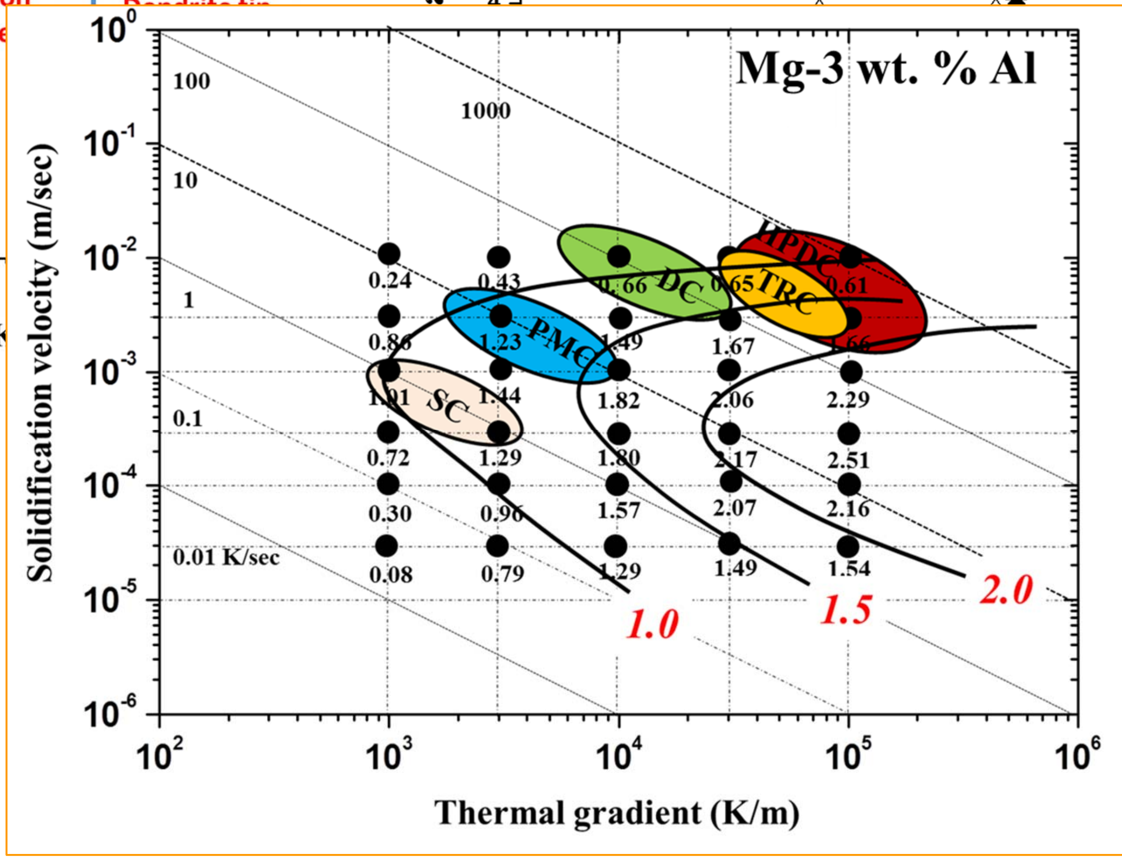


Solidification model: Second phase fractions





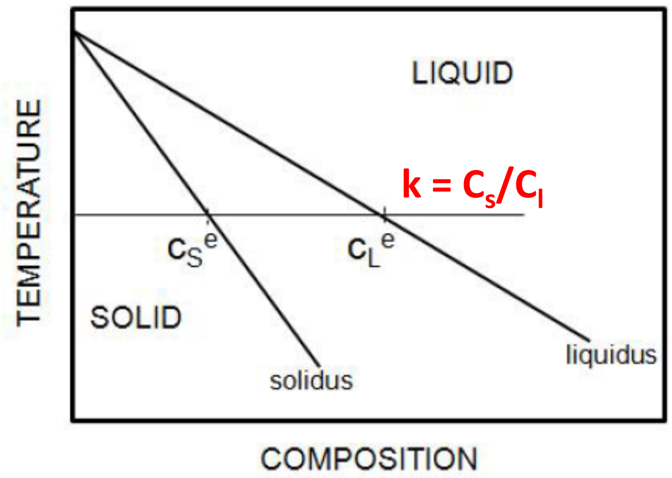
Secondary phase fraction mapping



Rapid Solidification: Departure from Equilibrium

Slow vs Rapid or Equil'm vs Non-equil'm

Thermodynamics of solidification



Local thermodynamic equilibrium at S/L interface

VS

Experimental evidences of non-equil'm

TABLE II. Comparison of distribution coefficients under equilibrium (k_0) and laser-annealed (k') regrowth conditions.

Dopant	(a) Tetrahedral covalent radius (Å)	(b) k_0	k'	$\frac{k'}{k_0}$
As	1.18	0.3	1.0	3.3
Sb	1.36	0.023	0.7	30
Bi	1.46	0.0007	0.4	571
Ga	1.26	0.008	0.2	25
In	1.44	0.0004	0.15	375

White et al. Ion implantation followed by laser annealing of solutes in Si

Theories: Aziz's model for solute trapping

Michael J. Aziz 1981

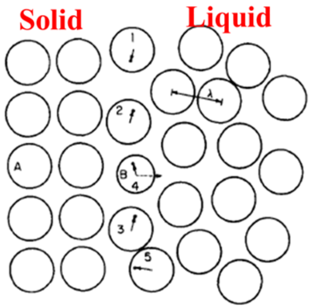


FIG. 1. Choreography of solute trapping.

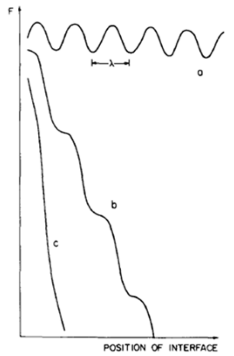


FIG. 2. Free energy of system as a function of interface position. (a) Small driving force, (b) critical driving force, and (c) large driving force.

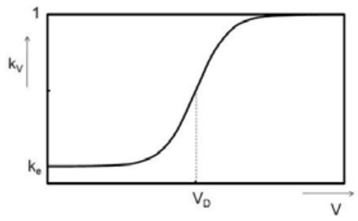
$$\tau = \frac{\lambda}{v}$$

Stepwise growth model

Continuous growth model

- Chemical rate theory
- Flux balance at interface

$$k^{non-eqb} = \frac{k + v / v_d}{v / v_d + 1}$$



$v =$ solidification velocity

$v_d = \frac{D}{\lambda} =$ diffusive velocity of a solute atom

k = equilibrium partition coefficient

No dependence on composition

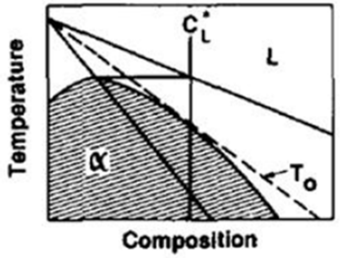
Laser melting experiments

Materials	V_D (m/s)
Si-As	0.46
Si-Ge	2.03
Si-Bi	32
Si-Sn	17
Si-Ge	22
Si-In	57
Si-Sb	0.64
Al-Sn	36
Al-In	38
Al-Ge	6.1
Al-Cu	6.7
Ni-Zr	26

v_d :Obtained by fitting solute profile with Aziz's model

Boettinger-Coriell-Sekerka 1984

- Turnbull's collision limited growth model
- The rate at which atoms attach on the solid phase is limited by the rate of collision with the solid phase

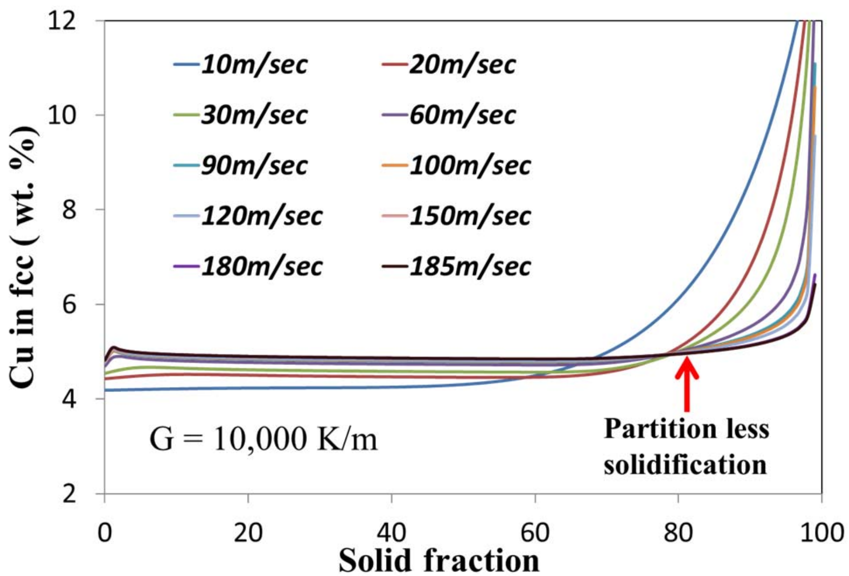


$$m^{non-eqb} = m_e\left(1 + \frac{k - k^{non-eqbm}\left(1 - \ln \frac{k^{non-eqbm}}{k}\right)}{1-k}\right)$$

Theories: Aziz's model for solute trapping

* Some experimental evidences

Solute distribution: Al- 4.9 wt. % Cu



TOF-SIMS analysis AA2199 alloy

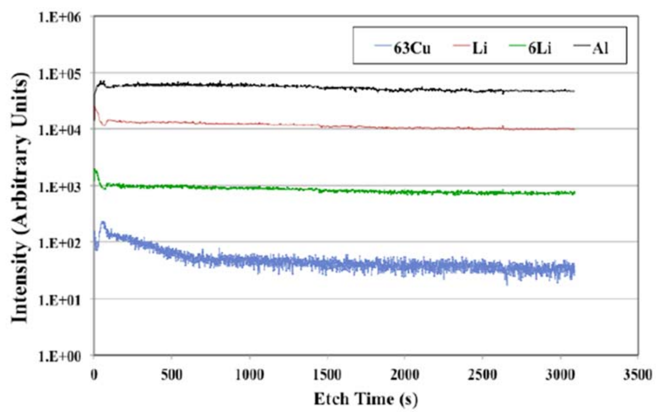


Figure 6-7- TOF-SIMS depth profile revealing homogeneous solute (lithium and copper) distribution.

Phd Thesis Dave Heard, McGill 2013

Summary

Inputs: G, V and C_o

Solidification Model

ChemApp

Thermodynamic Database

Diffusivity (Mobility) & Interfacial Energy Database

Morphology (KGT model):
- Dendrite tip radius
- Total undercooling
- Initial SDAS
- PDAS

Microsegregation:
- Solute profiles (back diffusion)
- Second phase fraction
- Final SDAS

Rapid Solidification:
- Solute trapping model
- Collison limited growth model
- or another new model

Experiments:
Additive Manufacturing
Experimental Data

Thank you for listening!

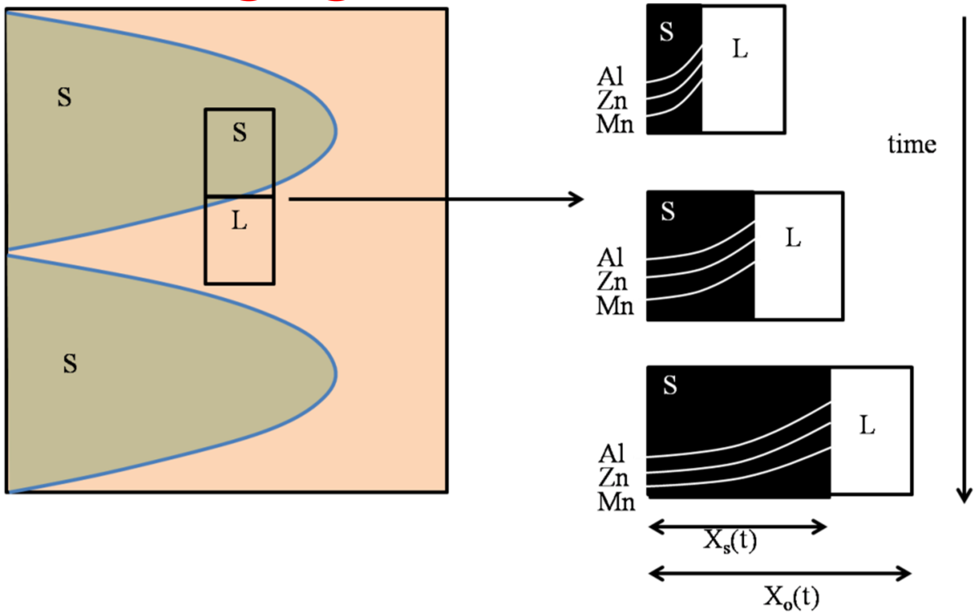
APPENDIX

Solidification modeling

Morphology

Kurz, Giovanola and Trivedi (KGT model)[1]

Microsegregation



Solute balance

$$\int_{0}^{Xsi} C_{si}dx + \int_{Xsi}^{Xo} C_{li}dx = X_o C_{oi}$$

Coarsening[2]

$$X_o(t)^3 - X_o(0)^3 = \int_o^t M_i dt$$

Back diffusion

$$\frac{\partial C_{si}}{\partial t} = D_{si}\frac{\partial^2 C_{si}}{\partial x^2}$$

Local thermodynamic Equilib at solid/liquid interface. (TD database)

$$C_{si} = k_i C_{li}$$

[1]Kurz W, Giovanola B, Trivedi R. Acta Metall. 1986:34:823

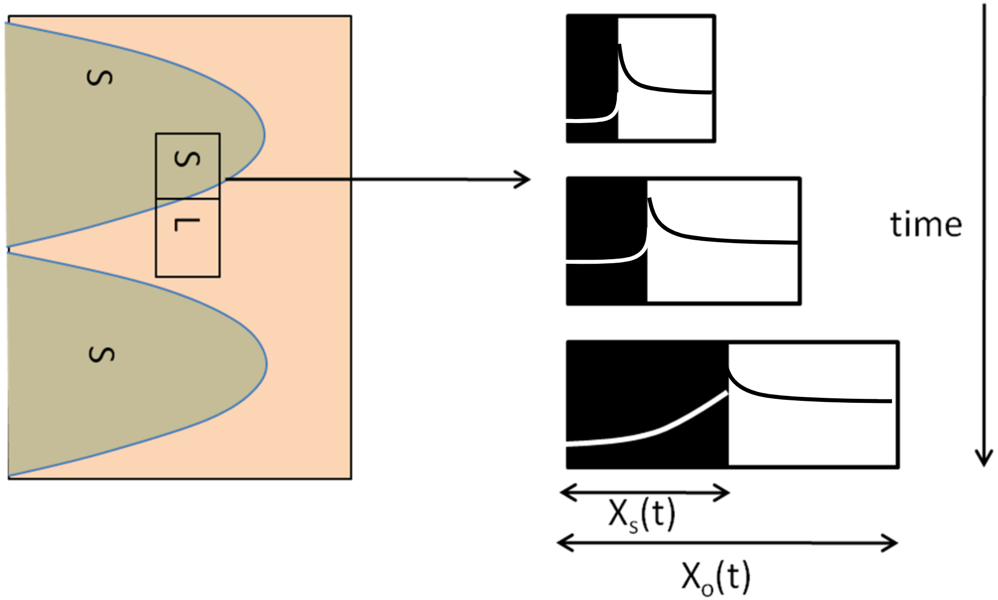
[2] Roosz et al. Mat. Sci. Tech. 1986:2:1149

Solidification modeling-diffusion in liquid phase

$$\frac{dC_l}{dt} = \frac{cr}{m}$$

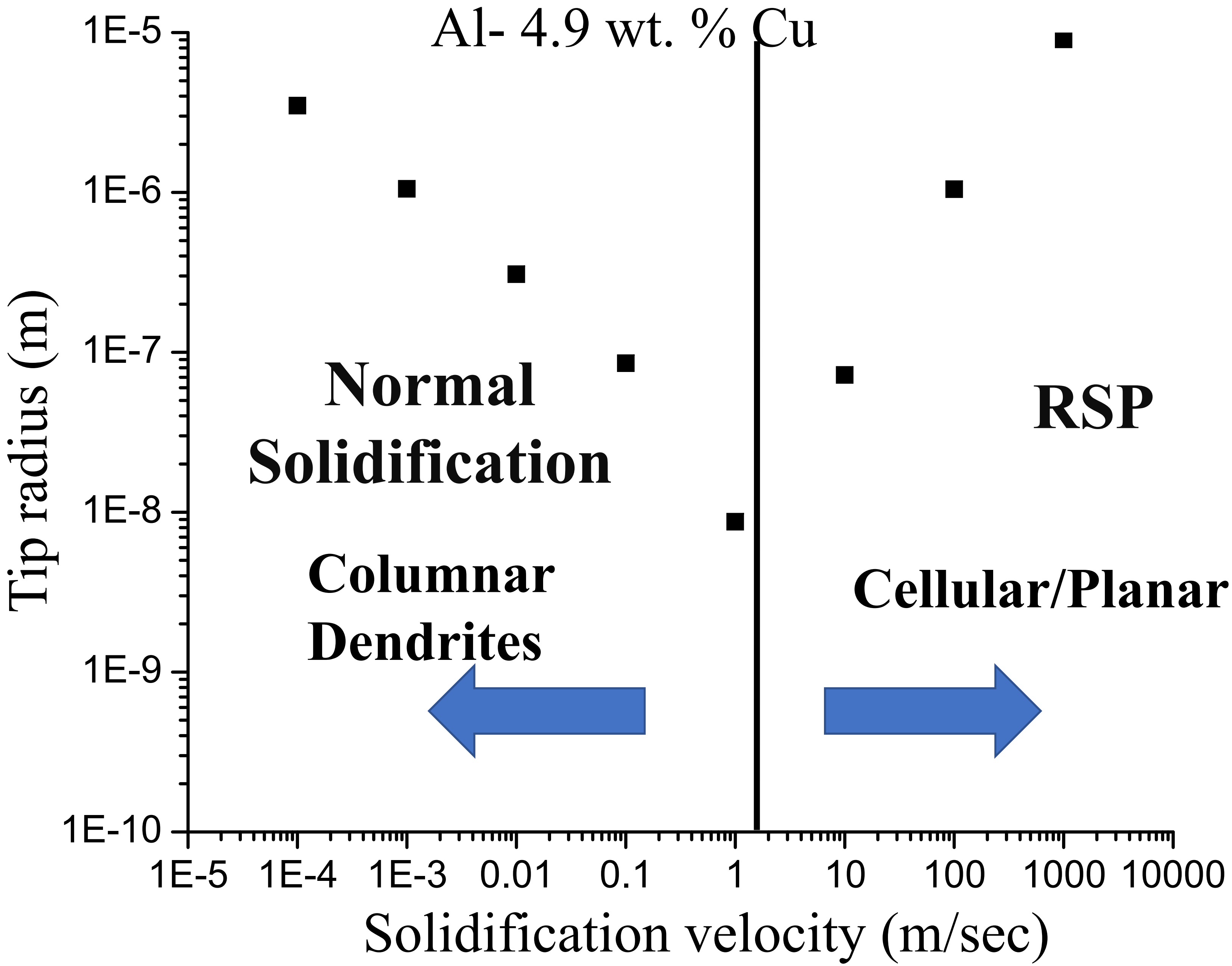
$$\frac{\partial C_s}{\partial t} = D_s \frac{\partial^2 C_s}{\partial x^2}$$

$$\frac{\partial C_l}{\partial t} = D_l \frac{\partial^2 C_l}{\partial x^2}$$

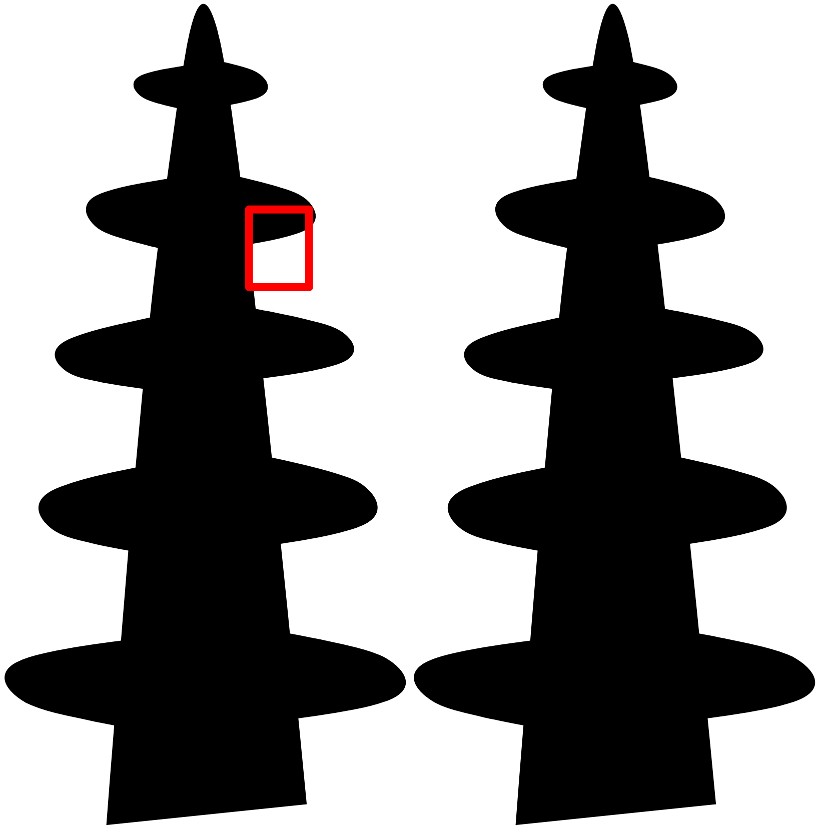


$$x_s^{new} = x_s^{old} + \Delta t \left[\frac{\left| D_s \frac{\partial C_s}{\partial x} \right|_{x=x_s}^{old} - \left| D_l \frac{\partial C_l}{\partial x} \right|_{x=x_s}^{old} (C_l - C_o) \frac{dx_o}{dt}}{(1-k)C_l} \right]$$

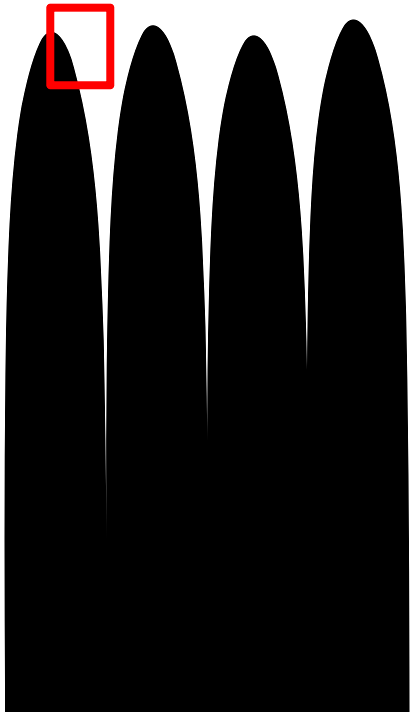
Solidification modeling-Morphology consideration



Solidification modeling-Morphology consideration



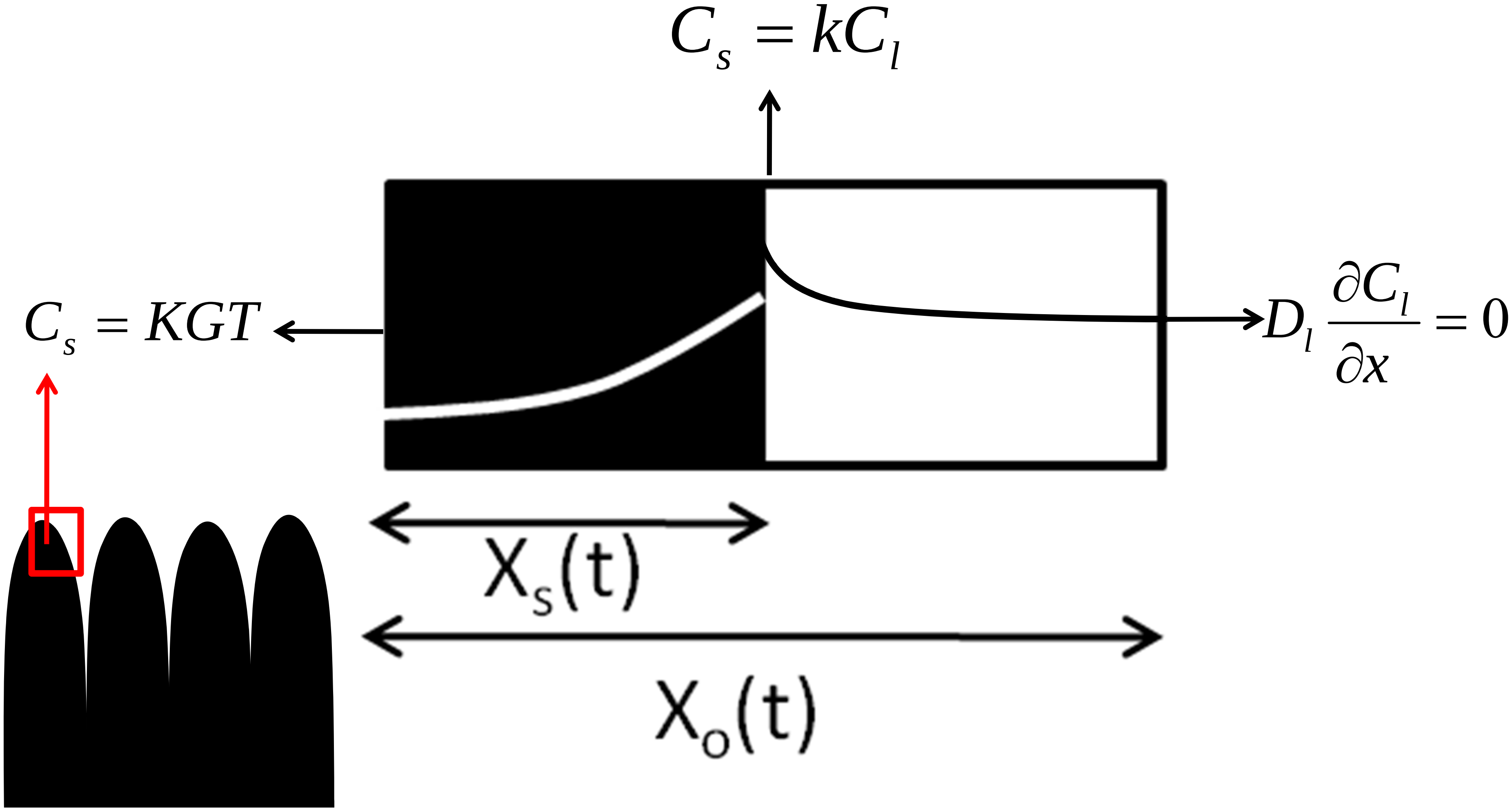
Columnar dendrite



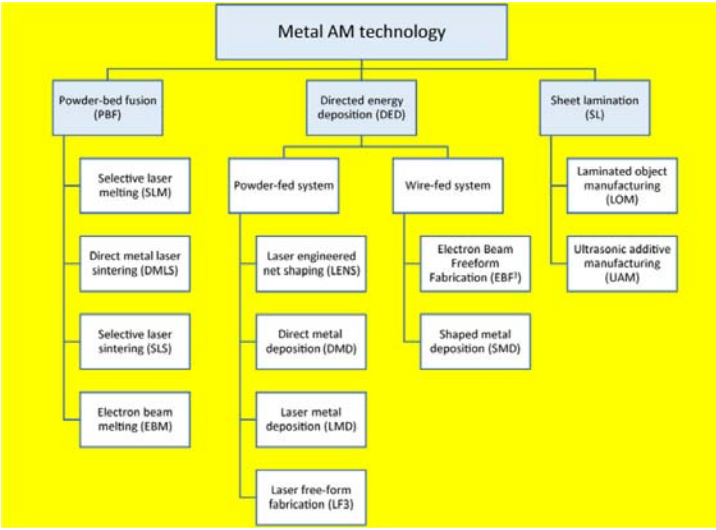
Cellular

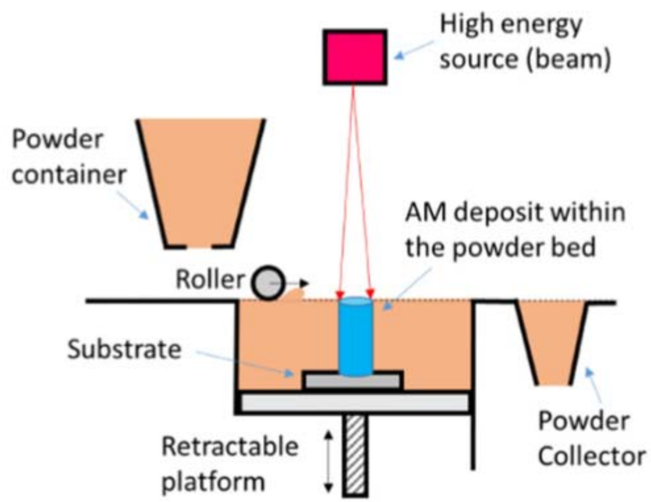
Length scale of the microsegregation calculation changes

Solidification model with diffusion (solid, liquid phases and morphology considerations)



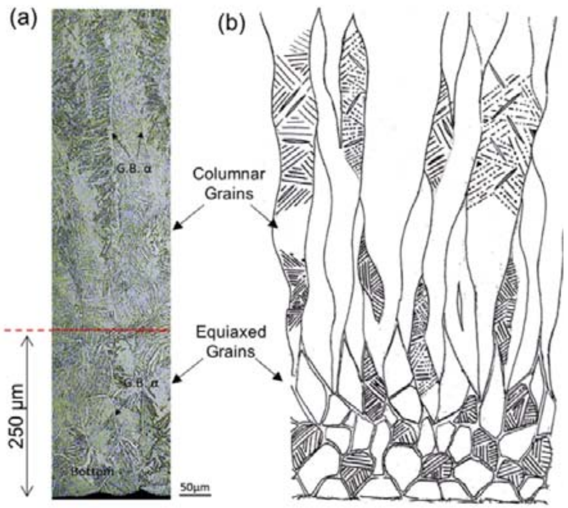
Additive Manufacturing(AM)?

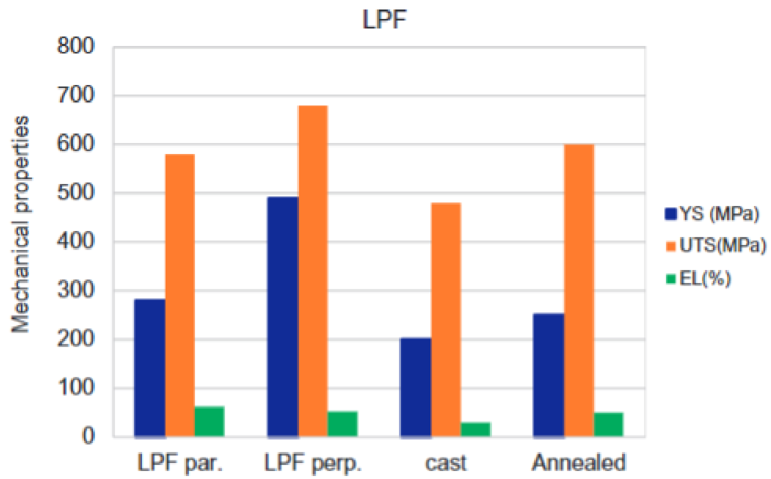




Y. Kok et al. / Materials and Design 139 (2018) 565–586

Equiaxed-to-columnar grain transition





Additive Manufacturing(AM)?