Worcester Polytechnic Institute

U.S. Army Research Laboratory
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Through-Process Modeling of Cold Spray

Danielle Belsito Cote, Baillie McNally,

Alison Garrett, Matthew Gleason, Robert DelSignore, Derek Tsaknopoulos, Caitlin Walde Victor Champagne, Jr., Richard D. Sisson, Jr.

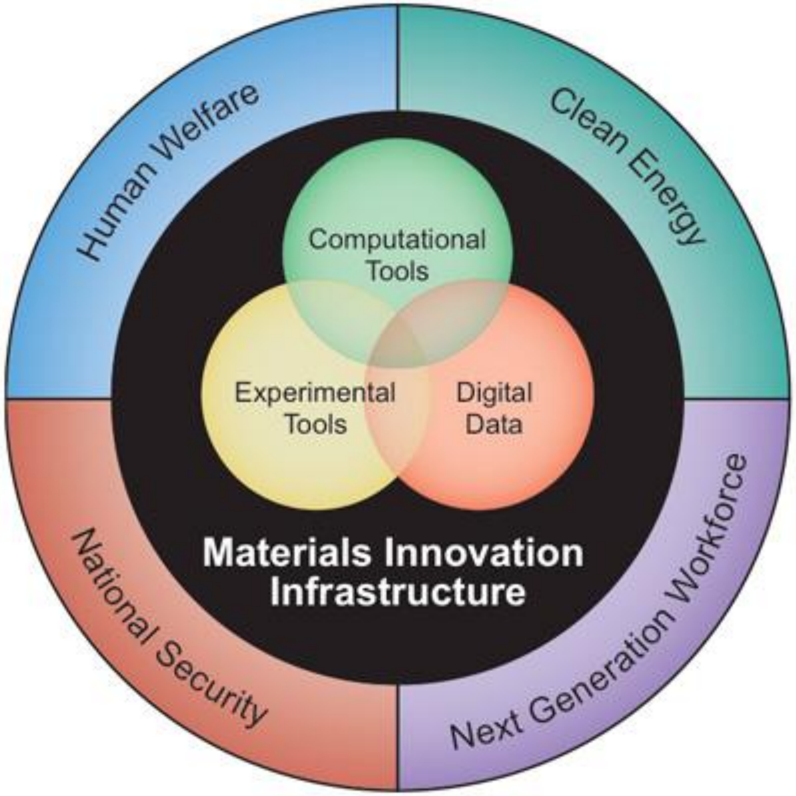
Outline

- Project Motivation
- Project Approach
  - Models
  - Characterization
- Summary

Materials Genome Initiative

“To discover, develop, and deploy new materials twice as fast…”

- President Obama, 2011



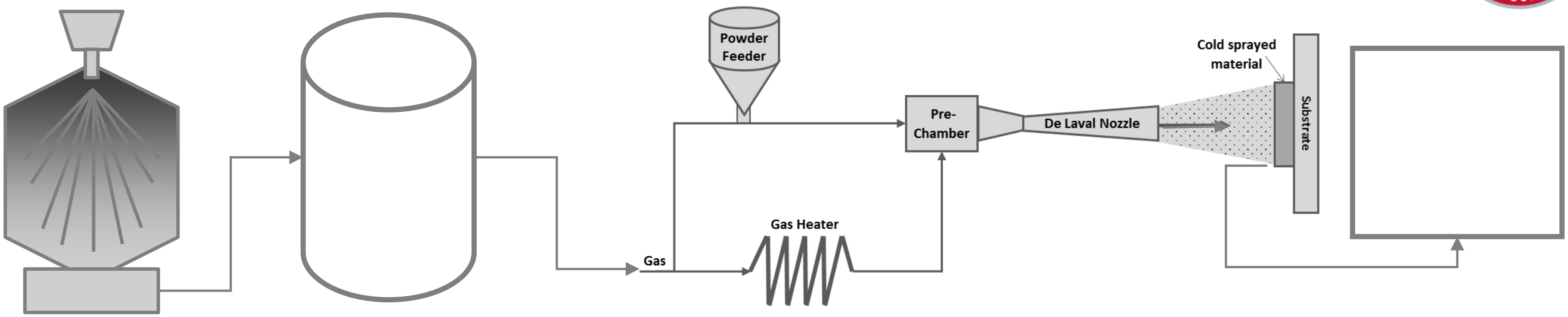
Meeting Societal Needs

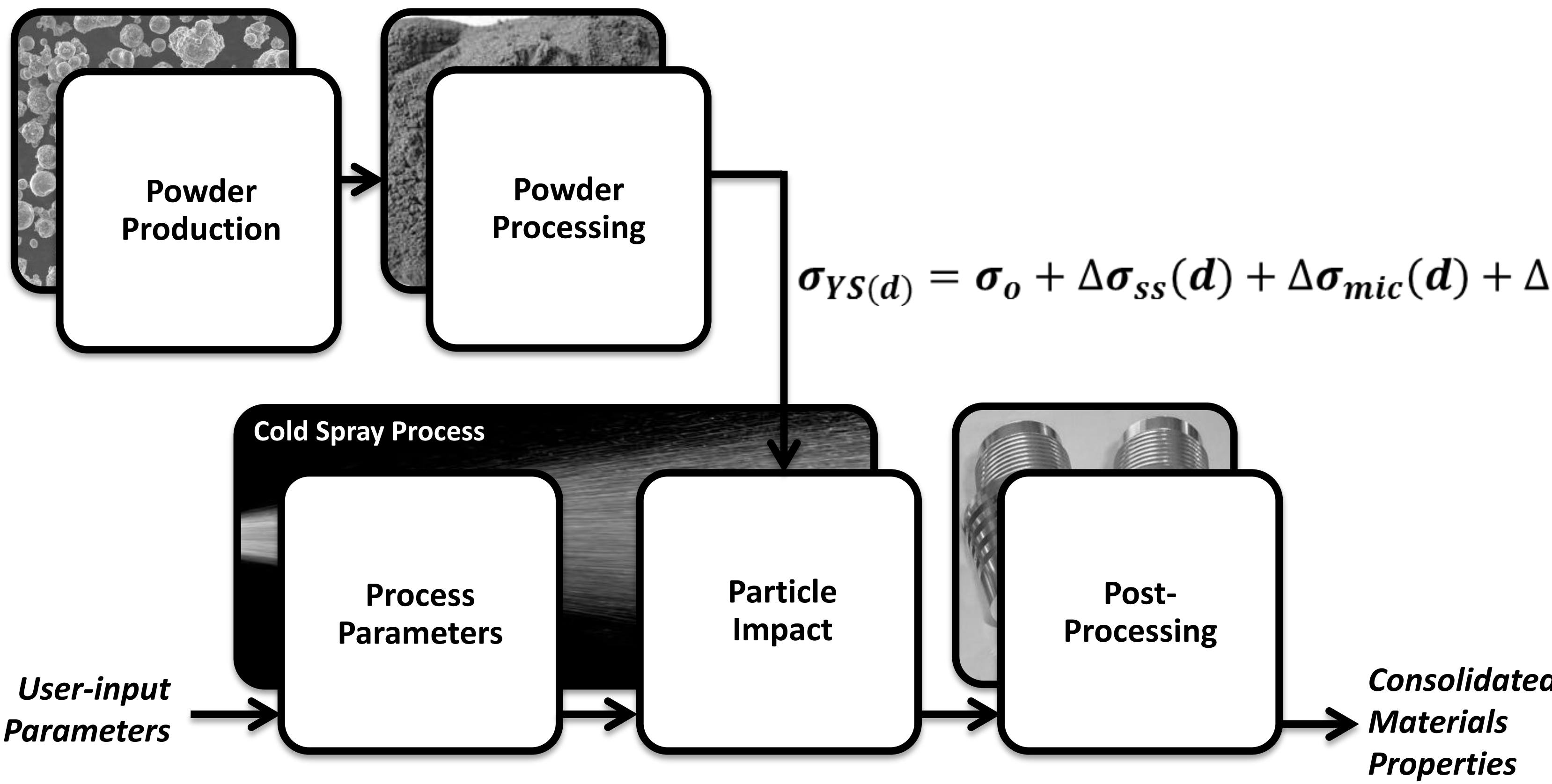
“The **lengthy time frame for materials to move from discovery to market** is due in part to the continued reliance of materials research and development programs on **scientific intuition** and **trial and error experimentation**. Much of the design and testing of materials is currently performed through time-consuming and repetitive experiment and characterization loops. Some of these experiments could potentially **be performed virtually with powerful and accurate computational tools**, but that level of accuracy in such simulations does not yet exist.”

Materials Genome Initiative (2011)

WhiteHouse.gov/MGI (2011)

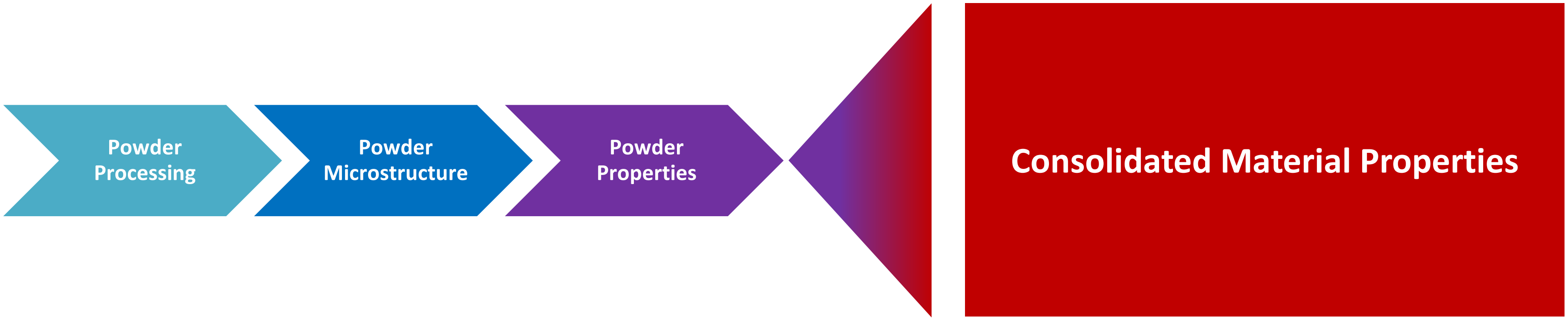
Through-Process Model

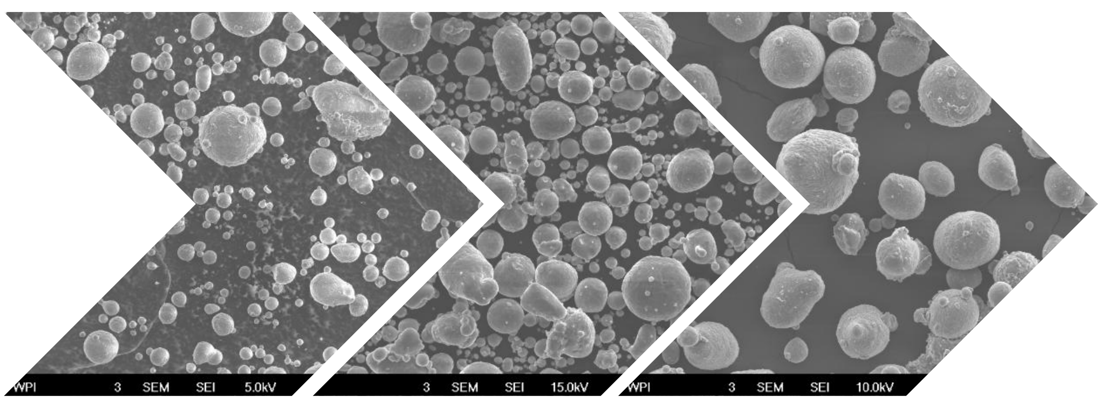




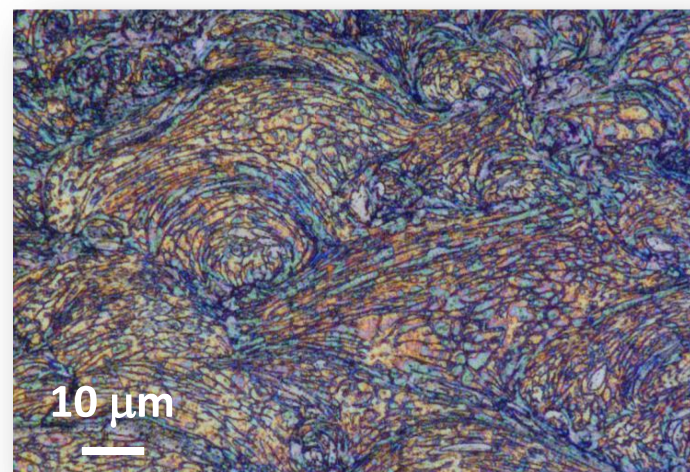
$$\sigma_{YS(d)} = \sigma_o + \Delta\sigma_{ss}(d) + \Delta\sigma_{mic}(d) + \Delta\sigma_{ppt}(d)$$

Powder Significance





Al 5056 Al 6061 Al 7075



Additive Yield Strength Model

Function of:
- **Alloy composition,**
- **Powder particle size,**
- **T, t of heat treatment**

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Solid Solution Strengthening

$$\Delta\sigma_{ss} = \sum_i (G\varepsilon_s{}^{3/2} c^{1/2})/700$$

Substitutional Solid-Solution

Grain Size/Microstructural Influence

$$\Delta\sigma_{mic}(d) = k_{gs}\lambda^{-0.5}$$

Hall-Petch Behavior

Precipitation Strengthening

$$\Delta\sigma_{ppt} = \sum_i [\sigma_{Coherency,\, i} + \sigma_{Modulus,\, i} + \sigma_{Chemical,\, i} + \sigma_{Order,\, i}]$$

$$\Delta\sigma_{Coherency,i} = 7\varepsilon_{coh,i}^{3/2} G \left(\frac{rf}{b}\right)^{1/2}$$

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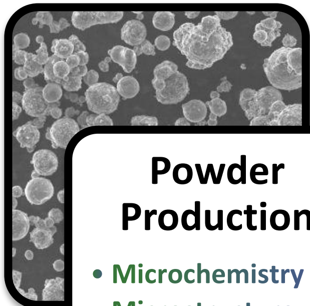
$$\Delta\sigma_{Order,i} = 0.7G \left[\varepsilon_{Ord,i}^{3/2} \left(\frac{rf}{b}\right)^{1/2} - 0.7\right] \varepsilon_{Ord} f$$

Modeling Approach



Powder Production

- Microchemistry
- Microstructure
- Process parameters
- Particle & grain size

$$\sigma_{ys}(d) = \sigma_o + \Delta\sigma_{ss} + \Delta\sigma_{mic} + \Delta\sigma_{ppt}$$

- Predict properties of powders

Powder Pre-Processing

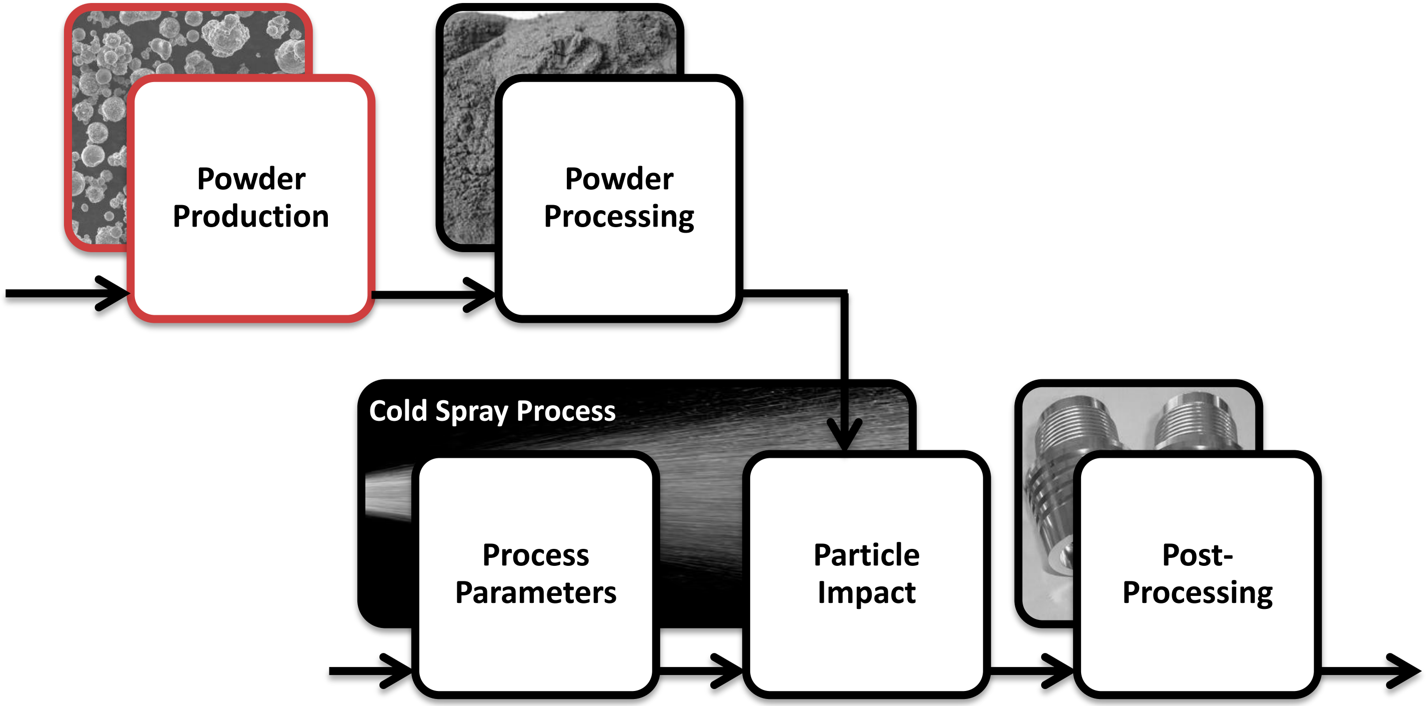
- Degassing
- Heat treating
- Milling
- Blending

Chemical Composition

Solidification Properties

Thermal Treatment

Thermodynamic, Kinetic, and Solidification Models



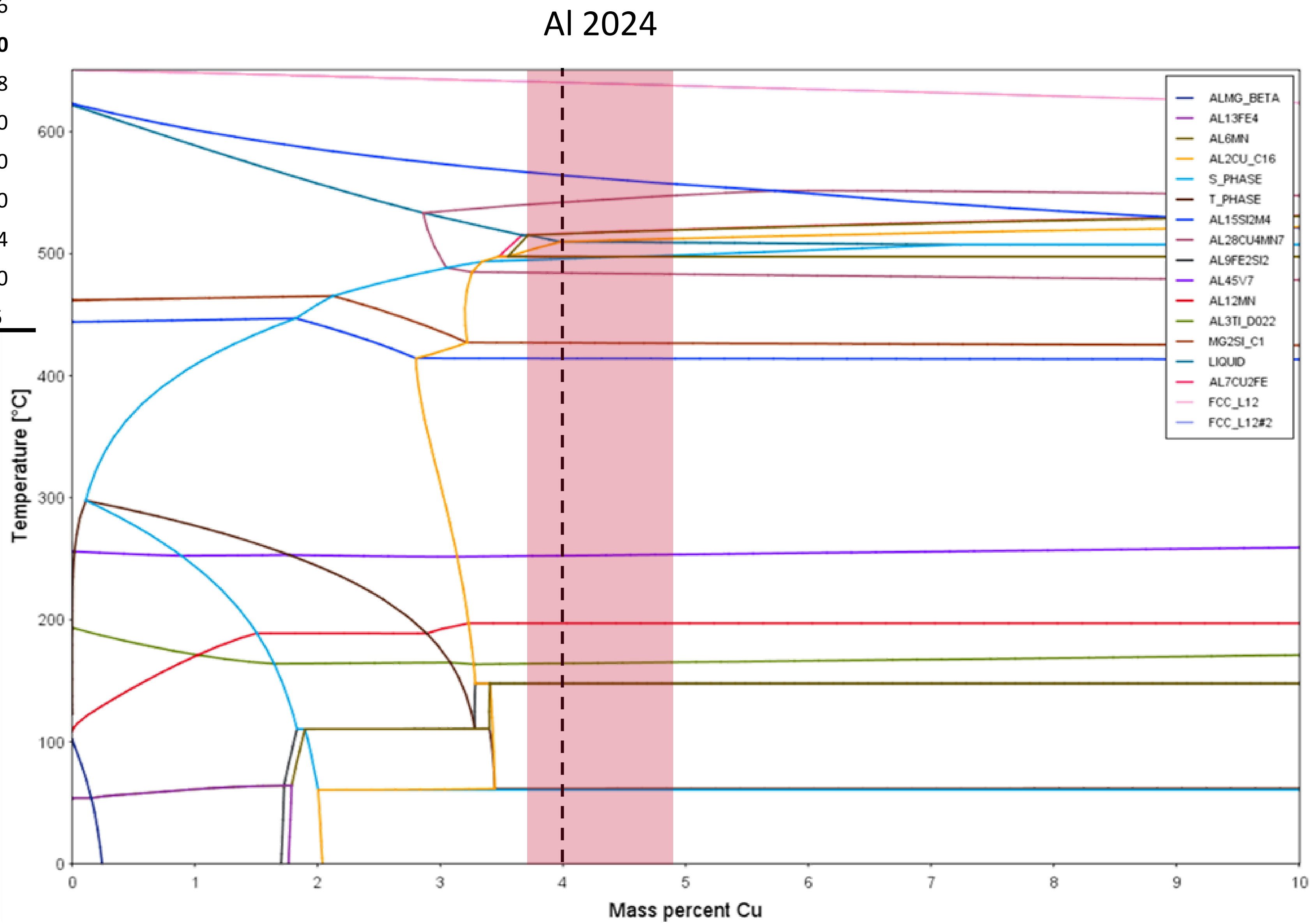
Powder Production

Thermodynamic & Solidification Models

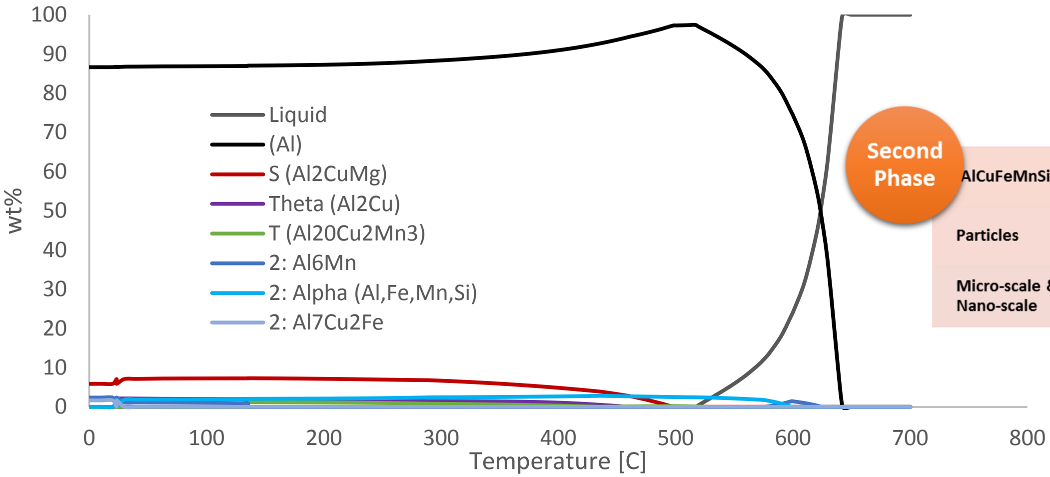
Characterization: SEM & EDS

Thermodynamic Modeling

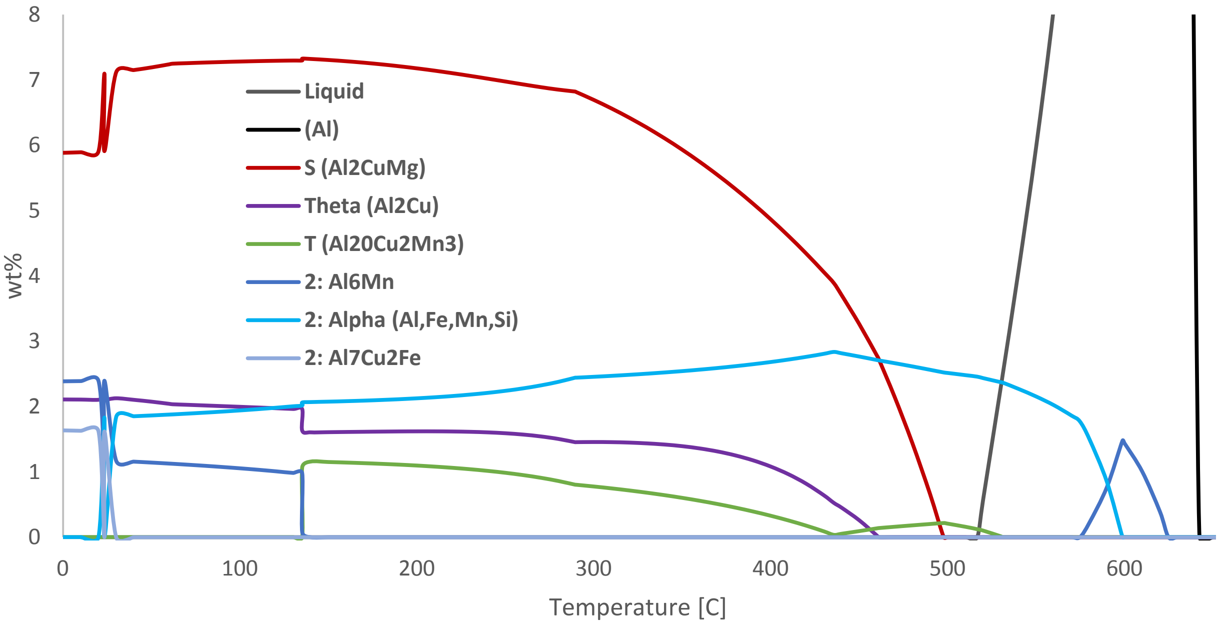
wt%	Al 2024
Cr	0.006
Cu	**4.000**
Fe	0.078
Mg	1.500
Mn	0.610
Ti	0.100
Zn	0.014
Si	0.130
Al	93.6



Thermodynamic Modeling



Second Phase	S-Phase	θ-Phase	T-Phase
AlCuFeMnSi	Al2CuMg	Al2Cu	Al20Cu2Mn3
Particles	Precipitates	Precipitates	Dispersoids
Micro-scale & Nano-scale	Micro-scale	Micro-scale	Nano-scale

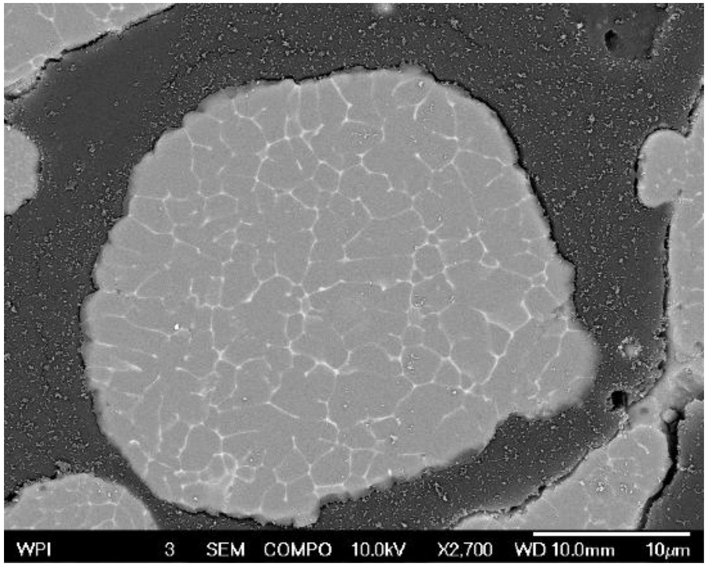


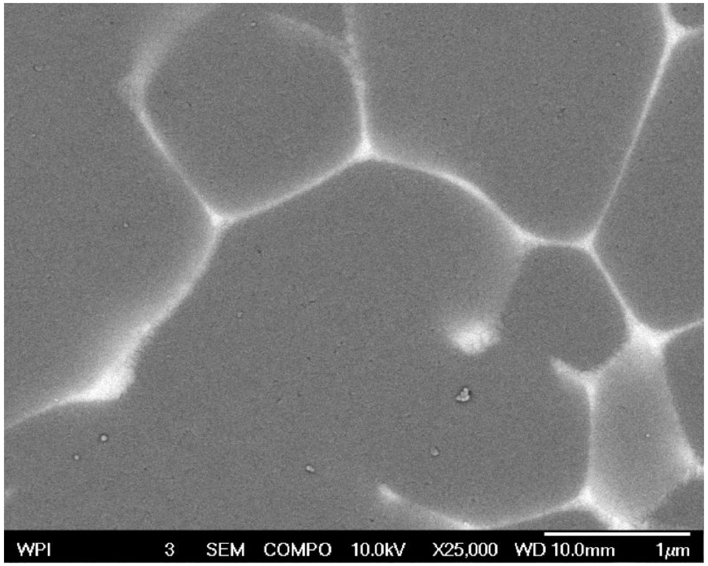
$$\Delta\tau_{Coherency,i} = 7\varepsilon_{coh,i}^{3/2} G \left(\frac{rf}{b}\right)^{1/2}$$

$$\sigma_{YS(d)} = \sigma_o + \Delta\sigma_{ss}(d) + \Delta\sigma_{mic}(d) + \Delta\sigma_{ppt}(d)$$

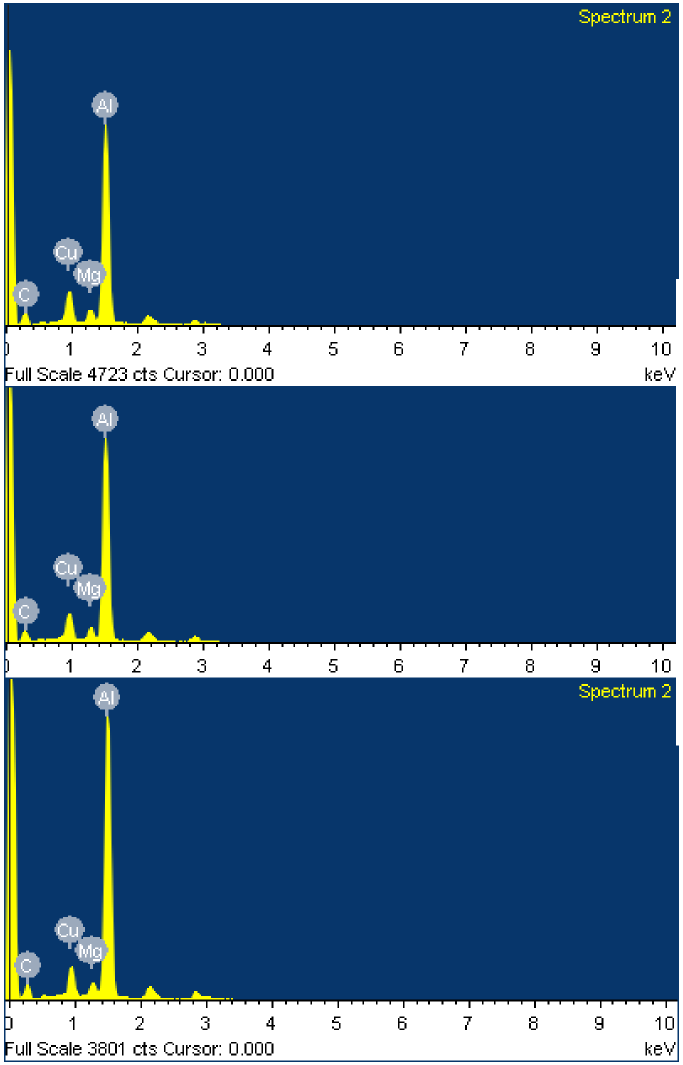
Al 2024

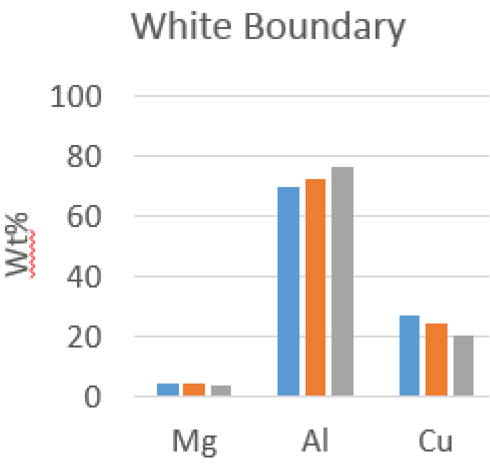
Thermodynamic Characterization – SEM/EDS





S-Phase & θ

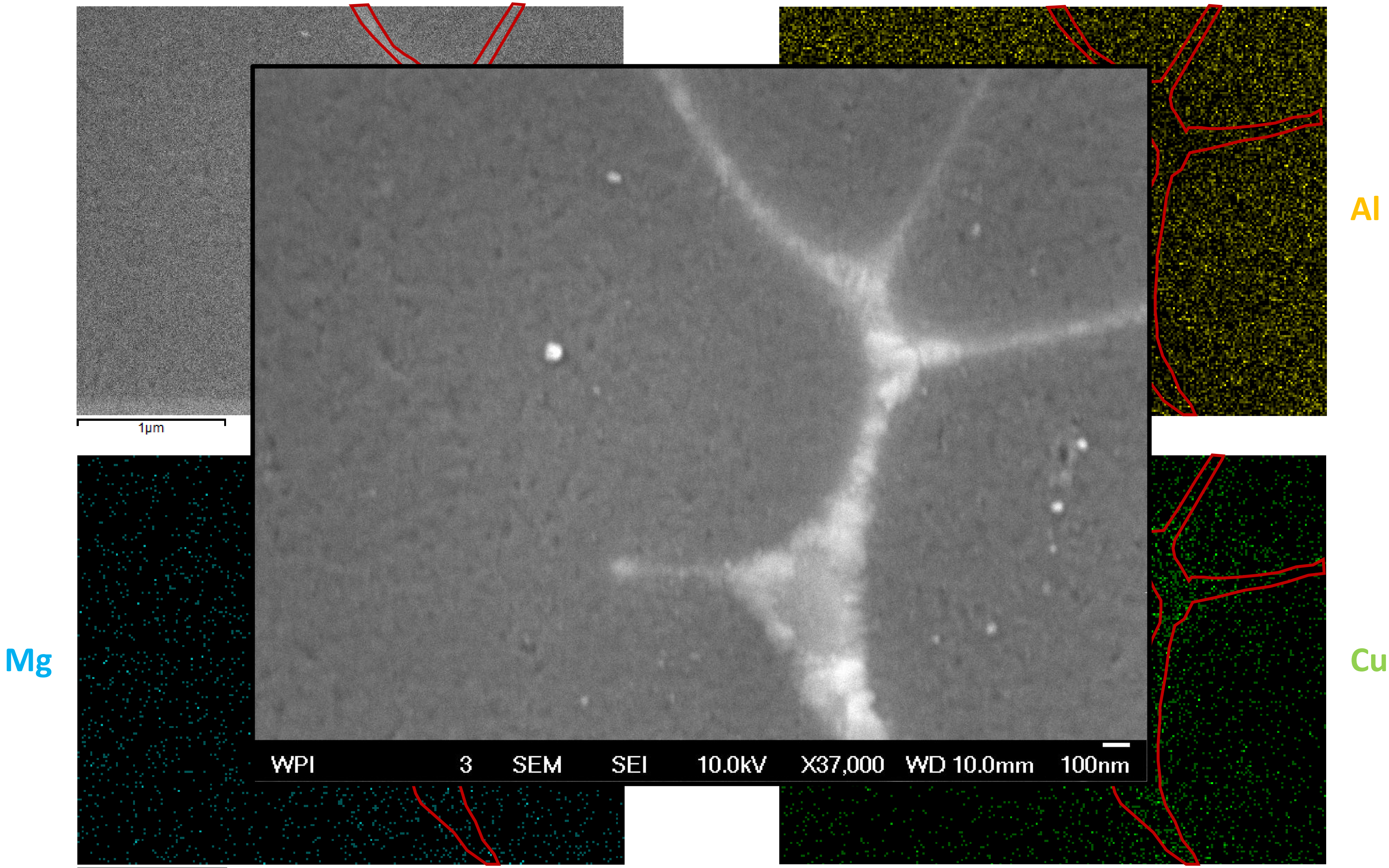




$$\sigma_{YS(d)} = \sigma_o + \Delta\sigma_{ss}(d) + \Delta\sigma_{mic}(d) + \Delta\sigma_{ppt}(d)$$

Al 2024

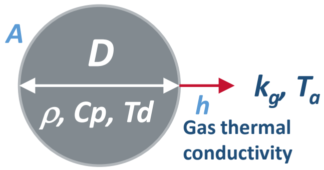
Thermodynamic Characterization – EDS Map



Al 2024

Solidification Model

Heat Transfer Model Gas Atomization Process



Gas Atomization: Newtonian Heat Flow

- Heat transfer from droplet: forced convection
- Radiational cooling: neglected
- Heat conduction (w/in droplet): neglected (small size – Biot number < 0.1)

Heat balance,

$$-V\cdot\rho\cdot C_p\cdot\frac{dT_d}{dt}=h\cdot A\cdot(T_d-T_f)+\sigma\varepsilon\left(T_d^4-T_f^4\right)$$

$$h=\frac{k_g}{d}\left(2.0+0.6\sqrt{R_e}\cdot\sqrt[3]{P_r}\right)$$ [2]

$$R_e=\frac{U\cdot\rho_g\cdot d}{\mu_g}$$

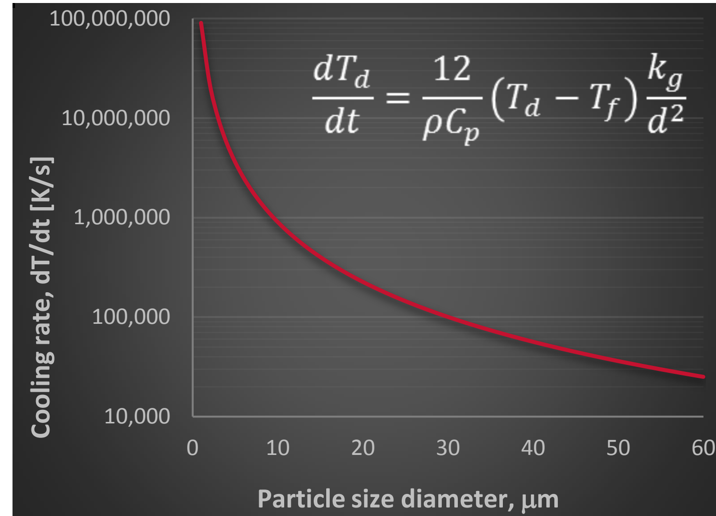
$$Pr=(C_g\mu_g/k_g)$$

$$\left|\frac{dT_d}{dt}\right|=\frac{6}{\rho\cdot C_p}\cdot(T_d-T_f)\cdot\left(\frac{2.0k_g}{d^2}+0.6\frac{k_g}{d}\sqrt{\frac{\rho_g U}{\mu_g d}}\cdot\sqrt[3]{P_r}\right)$$

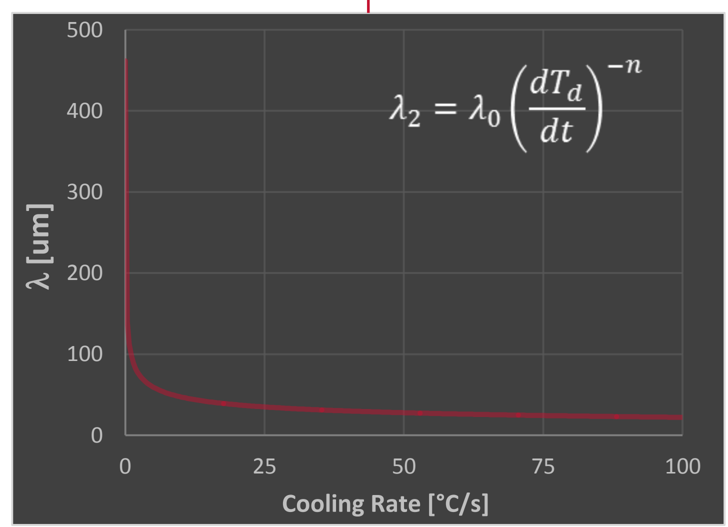
0

$$\left|\frac{dT_d}{dt}\right|=\frac{12}{\rho\cdot C_p}\cdot(T_d-T_f)\cdot\frac{k_g}{d^2}$$ [3]

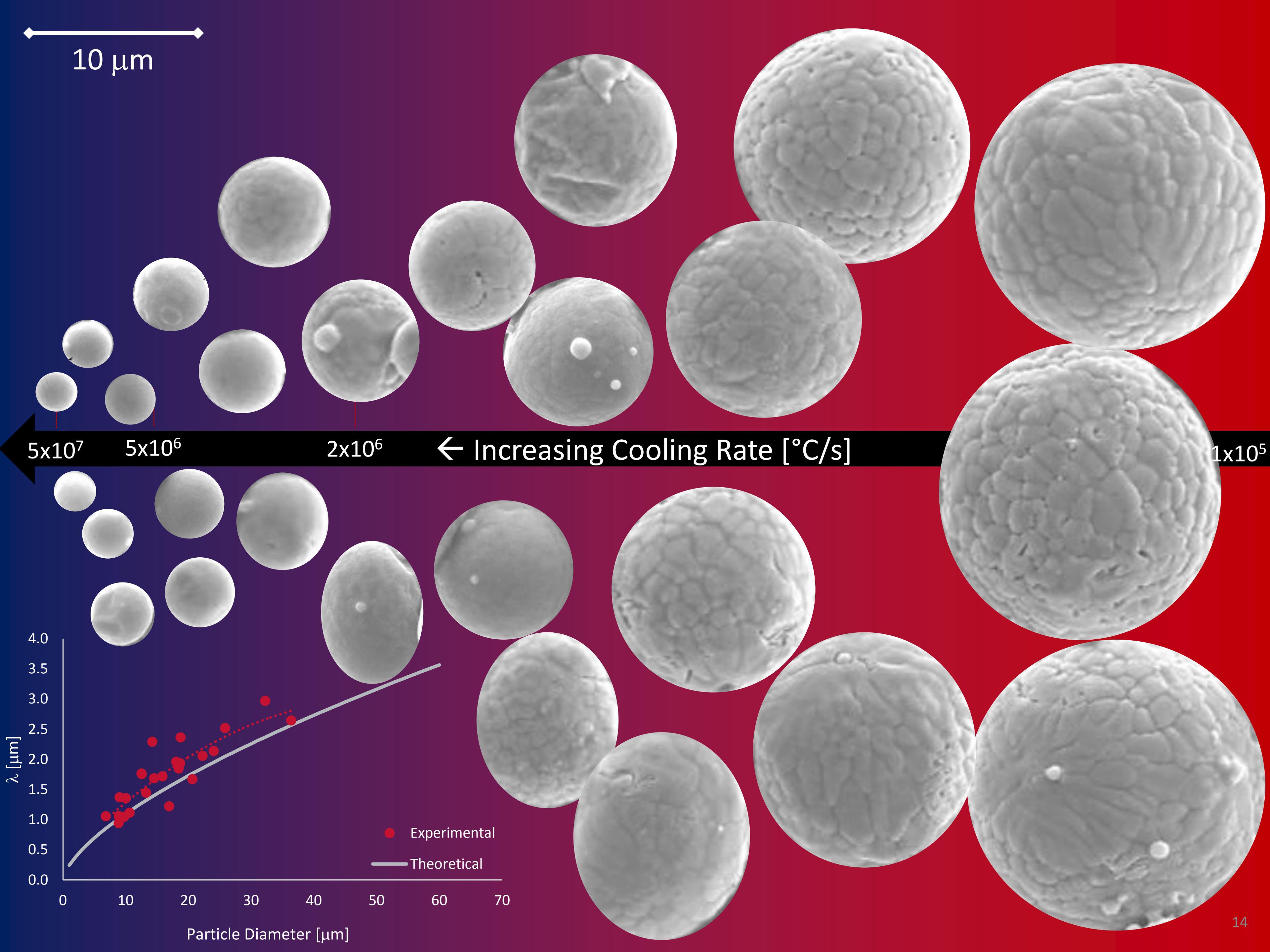
Thermophysical Properties of Al 6061[1]				
Ar Atomizing Gas		Molten Droplet		
T_f	K_g	ρ	C_p	T_d
[K]	[W/(mK)]	[kg/m³]	[J/(kgK)]	[K]
300	1.79E-02	2380	1170	1473



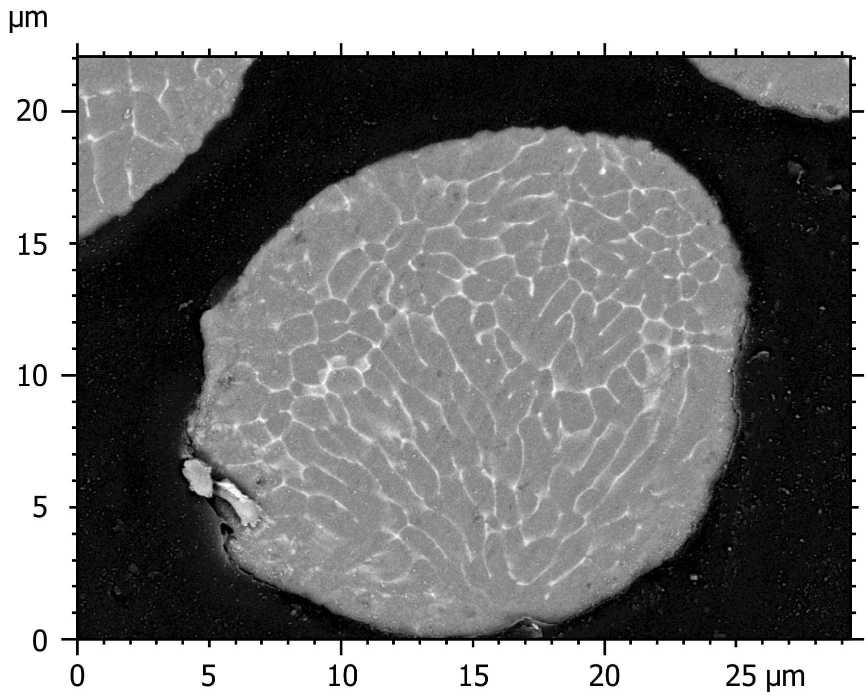
$$\lambda=\lambda_0\left(\frac{12}{\rho C_p}(T_d-T_f)\frac{k_g}{d^2}\right)^{-n}$$

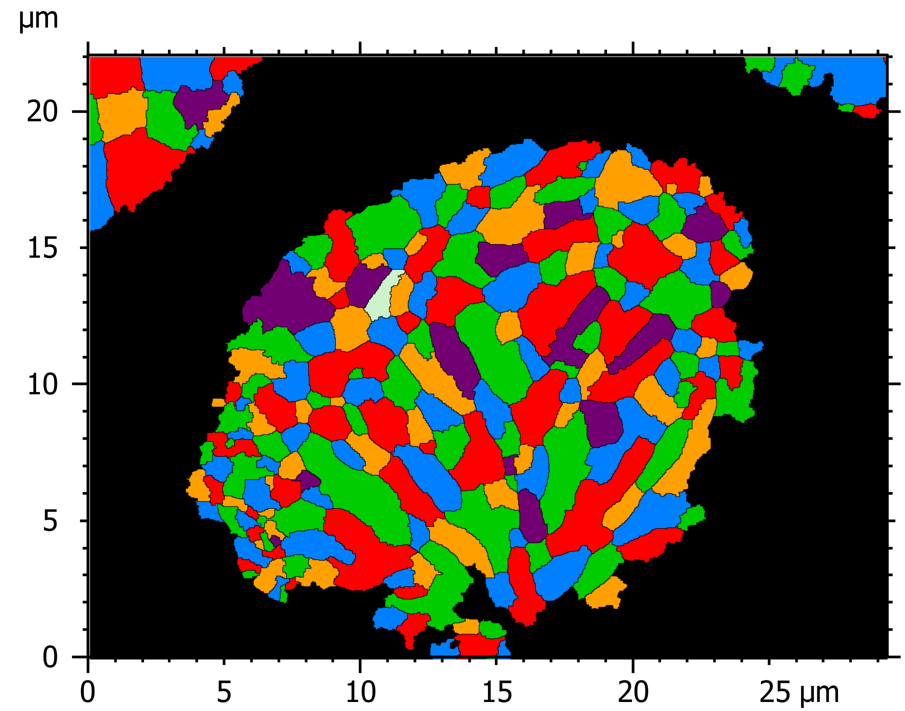


$$\sigma_{YS(d)}=\sigma_o+\Delta\sigma_{ss}(d)+\Delta\sigma_{mic}(d)+\Delta\sigma_{ppt}(d)$$


10 μm
5x10⁷
5x10⁶
2x10⁶
← Increasing Cooling Rate [°C/s]
1x10⁵
λ [μm]
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
10
20
30
40
50
60
70
Particle Diameter [μm]
Experimental
Theoretical

Grain Size Characterization





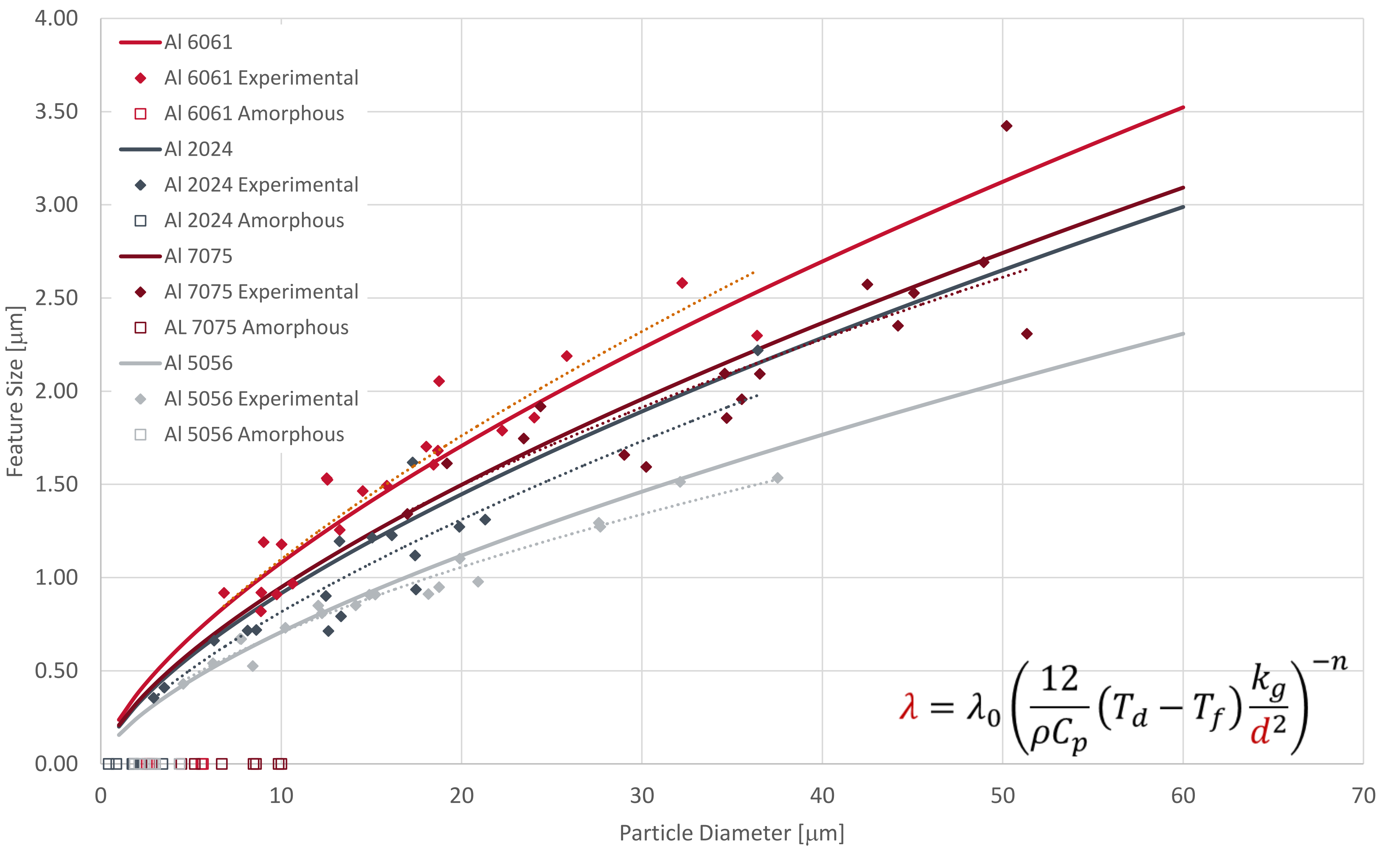
Statistics over all grains - Separated / merged

Global information	Value		
Number of grains	227		
Total area occupied by the grains	281 µm² (43.4%)		
Density of grains	0.351 Grains/µm²		
Grain parameters	Unit	Mean	Std dev
Area	µm²	1.24	1.21
Perimeter	nm	5277	3007

Mountains® by Digital Surf

$$\sigma_{YS(d)} = \sigma_o + \Delta\sigma_{ss}(d) + \Delta\sigma_{mic}(d) + \Delta\sigma_{ppt}(d)$$

Grain Size Variation with Alloy



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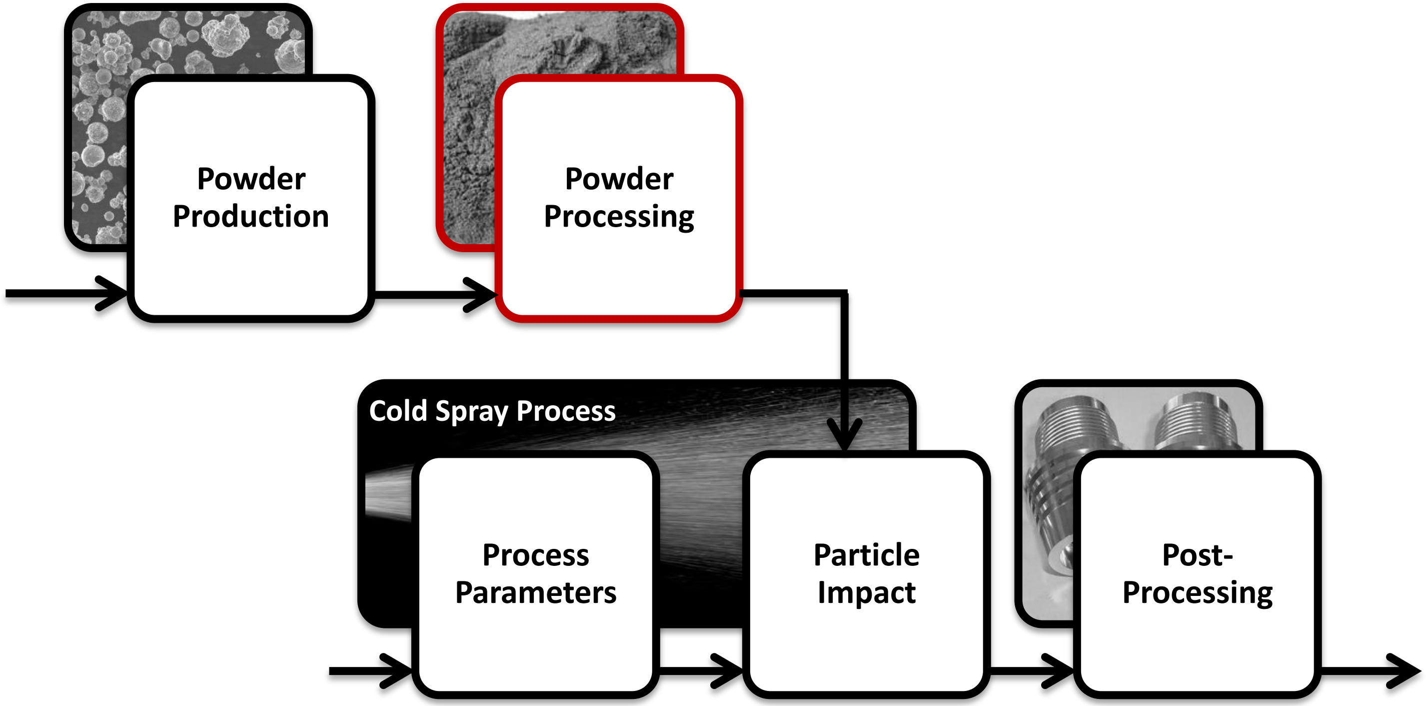


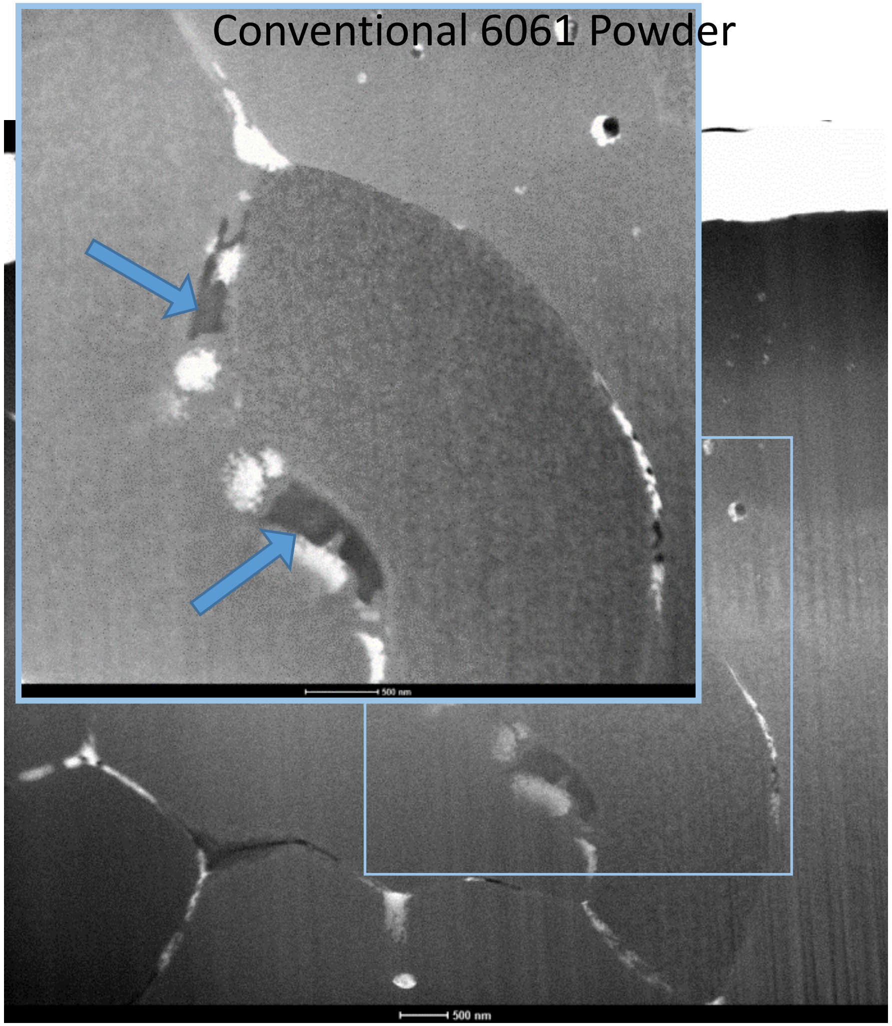
Powder Processing

Kinetic Modeling: TTT, CCT

Characterization: STEM

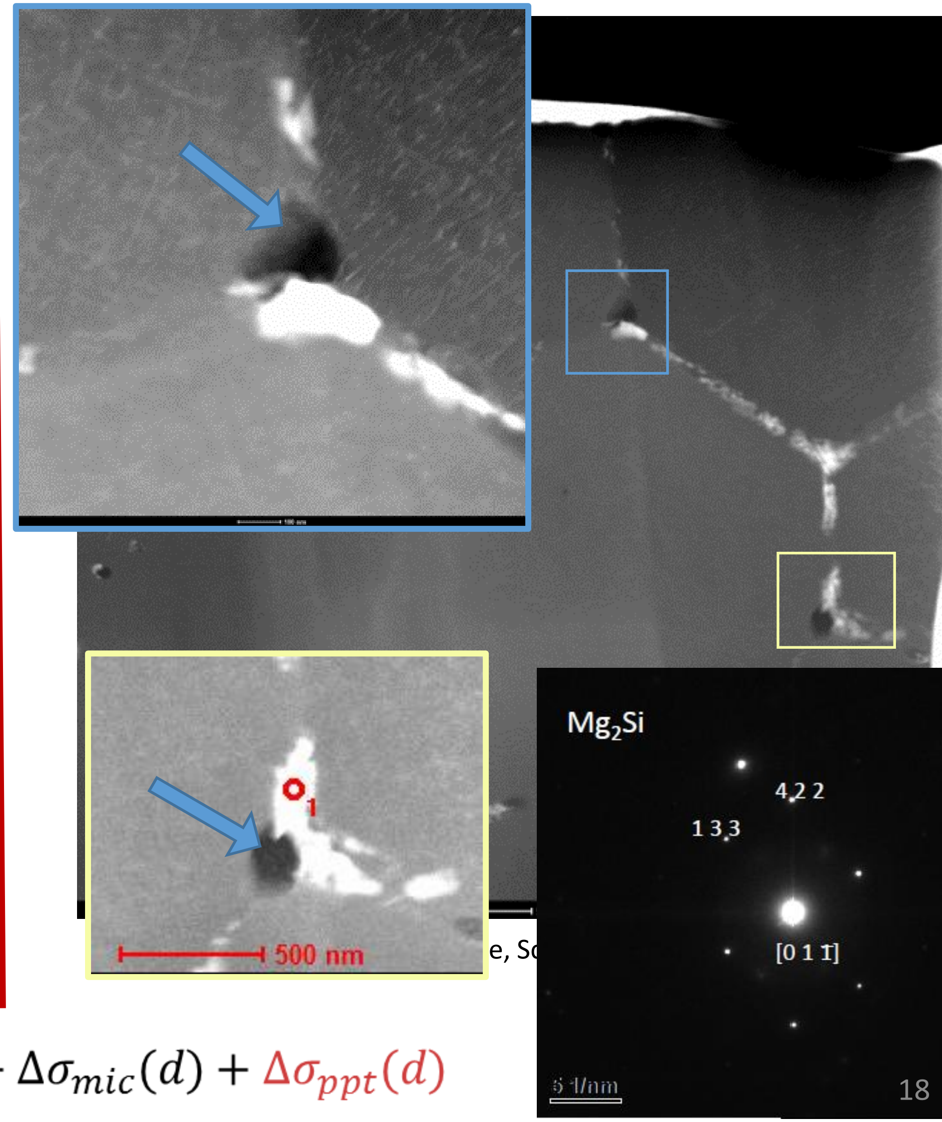
Kinetic Modeling Characterization: STEM

Conventional 6061 Powder



STEM DF Image, Scale Bar 500μm

Degassed 6061 Powder



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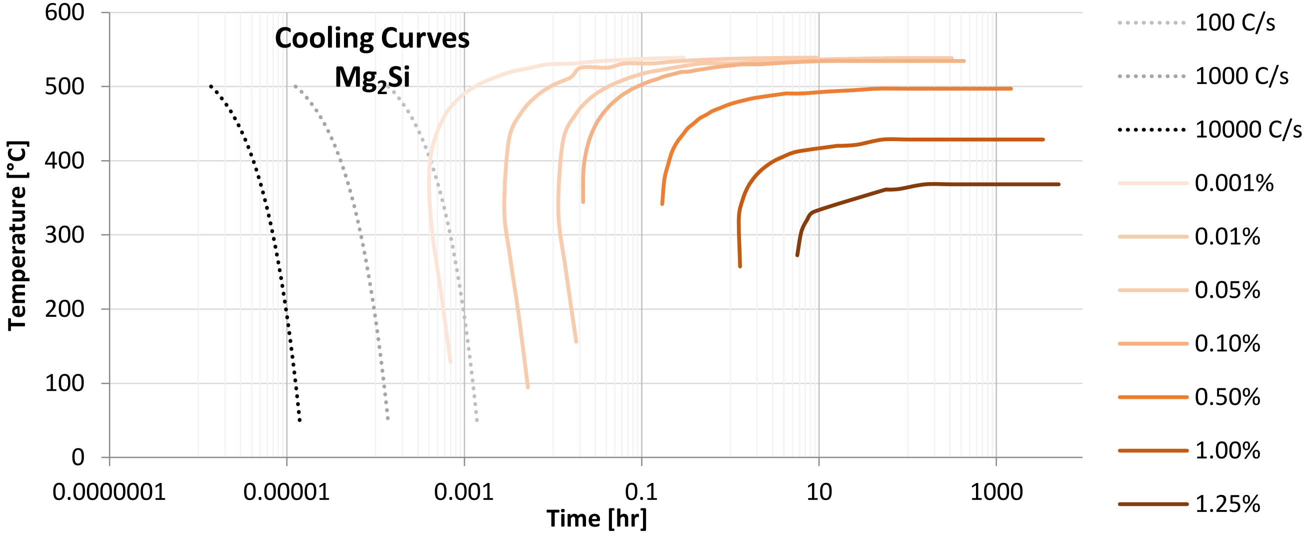
Al 6061

Kinetic Modeling: CCT Diagram



Gas atomization cooling rates: ~10^4-10^5 °C/s

Metastable Mg_2Si Phases

$$\Delta\tau_{Coherency,i} = 7\varepsilon_{coh,i}^{3/2} G \left(\frac{rf}{b}\right)^{1/2}$$

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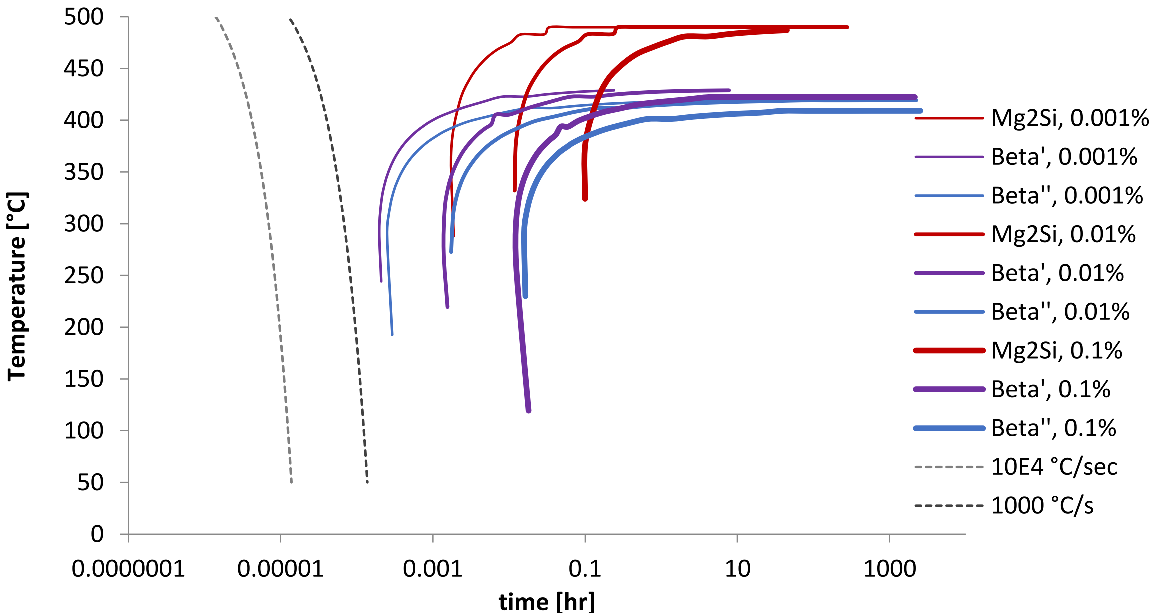
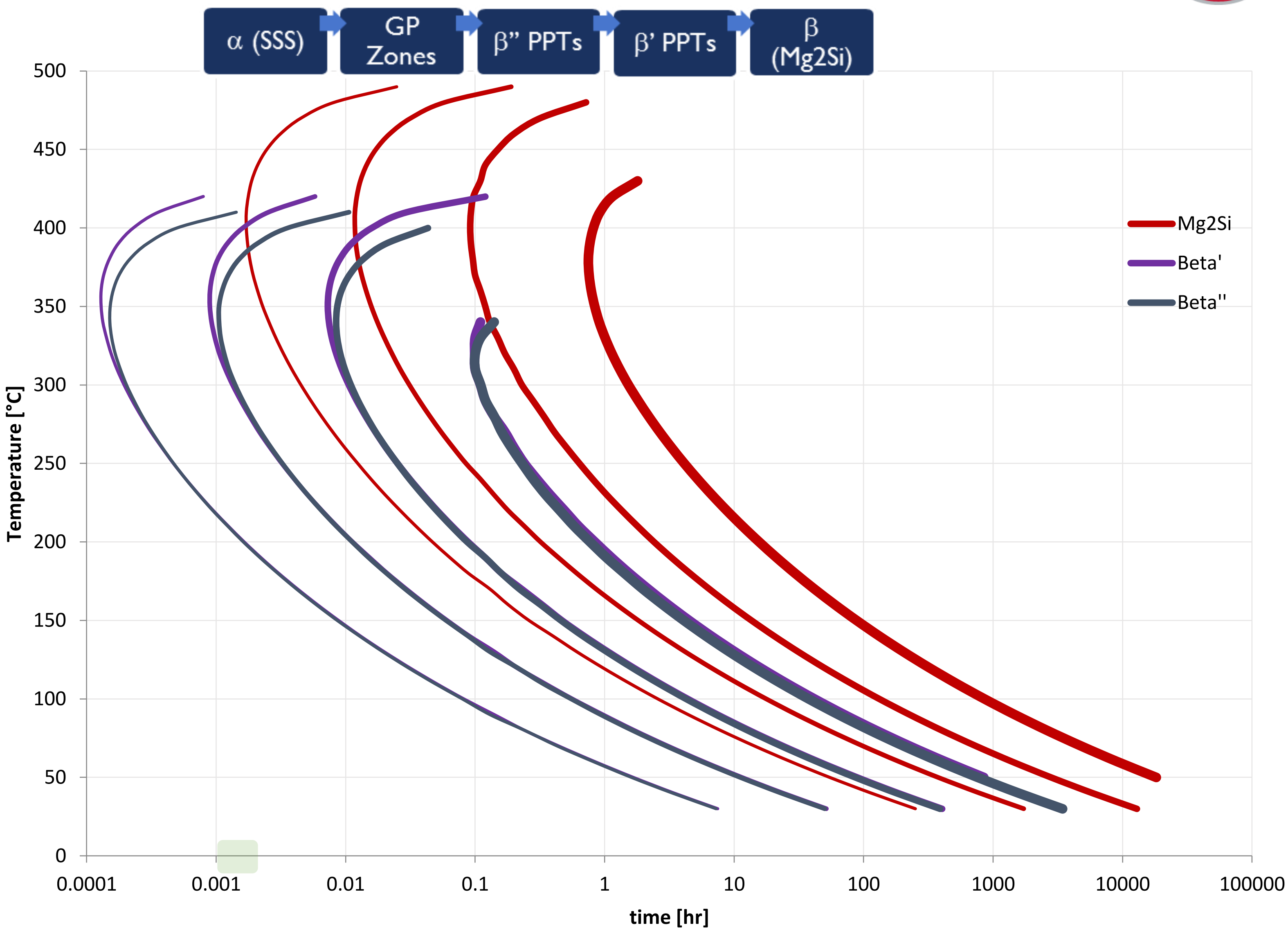
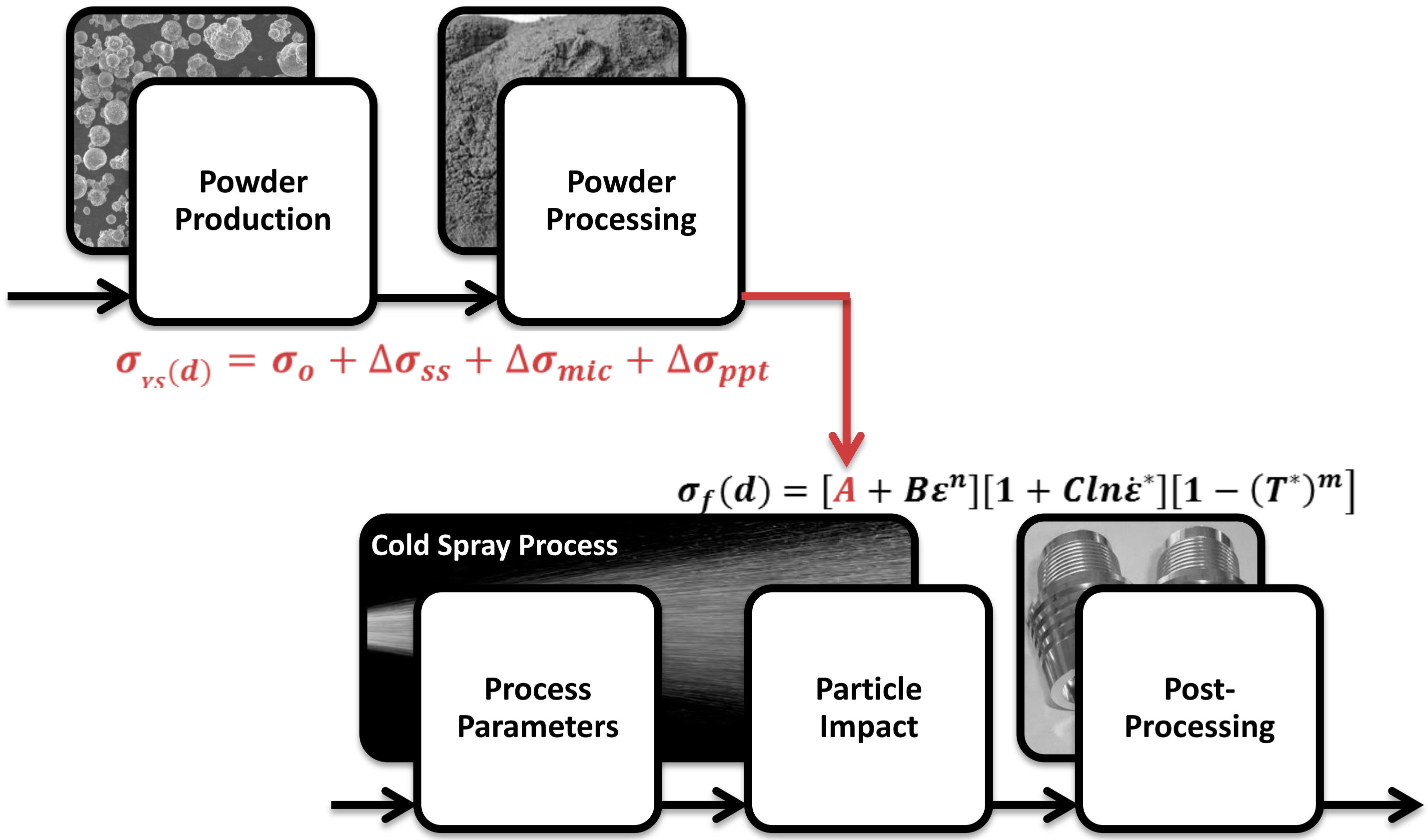


Al 6061

Al 6061 Kinetic Diagrams



$$\sigma_{YS(d)} = \sigma_o + \Delta\sigma_{ss}(d) + \Delta\sigma_{mic}(d) + \Delta\sigma_{ppt}(d) \longrightarrow \Delta\tau_{Coherency,i} = 7\varepsilon_{coh,i}^{3/2} G \left(\frac{rf}{b}\right)^{1/2}$$



Quantification for Integration

Additive Yield Strength Model

Characterization: Nanohardness

Additive Yield Strength Model

Function of:
- **Alloy composition,**
- **Powder particle size,**
- **T, t of heat treatment**

Solid Solution Strengthening

$$\Delta\sigma_{ss} = \sum_i (G\varepsilon_s^{3/2} c^{1/2})/700$$

Substitutional Solid-Solution

Grain Size/Microstructural Influence

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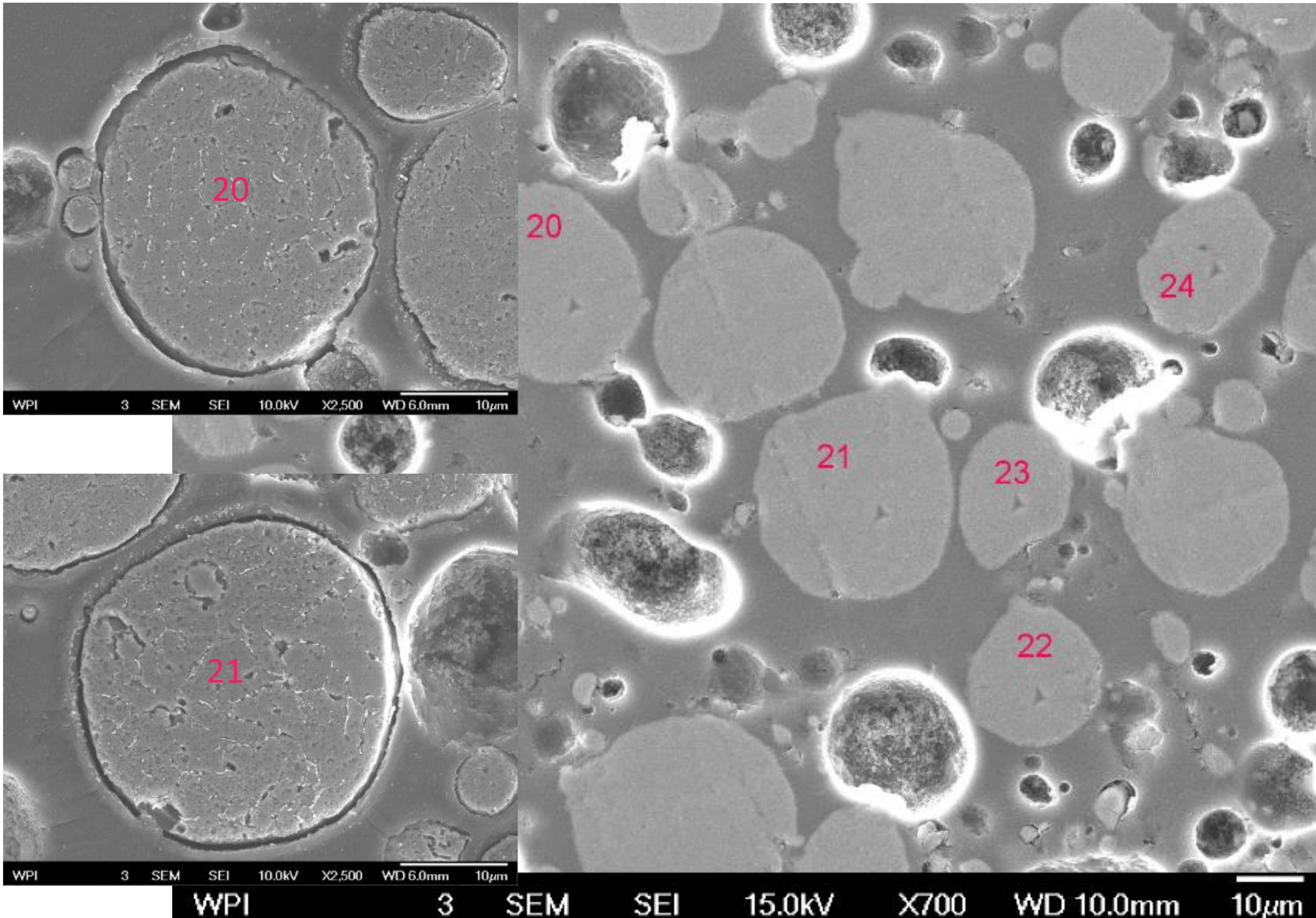
$$\Delta\sigma_{Order,i} = 0.7G \left[\varepsilon_{Ord,i}^{3/2} \left(\frac{rf}{b}\right)^{1/2} - 0.7\right] \varepsilon_{Ord} f$$

Additive Hardness Model

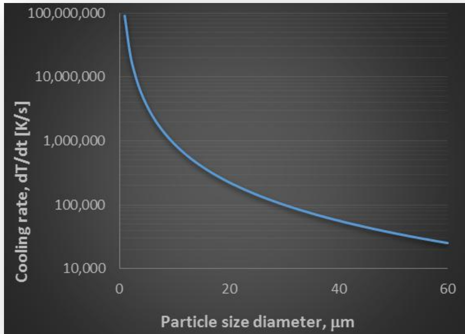


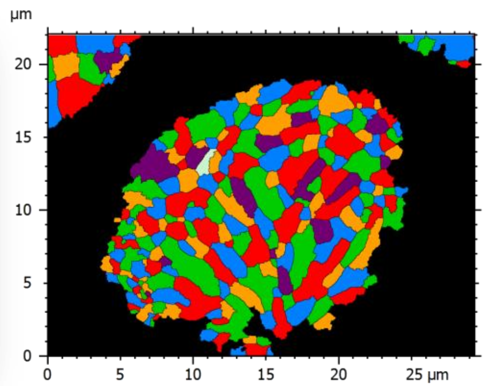
Al 6061

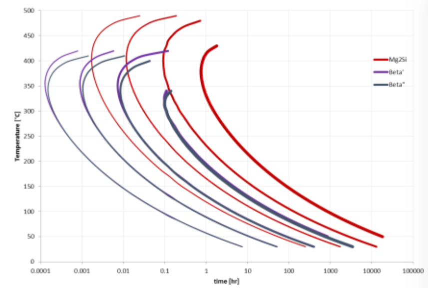
70

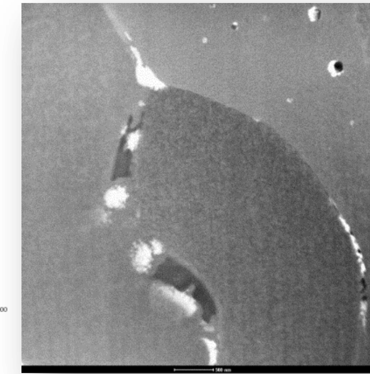
Al 6061

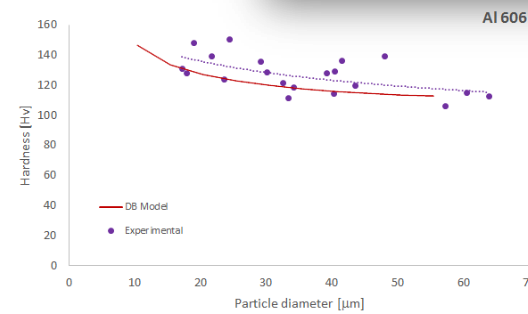
WPI Overview

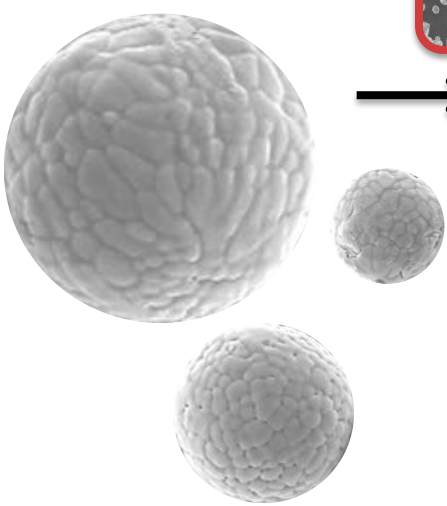


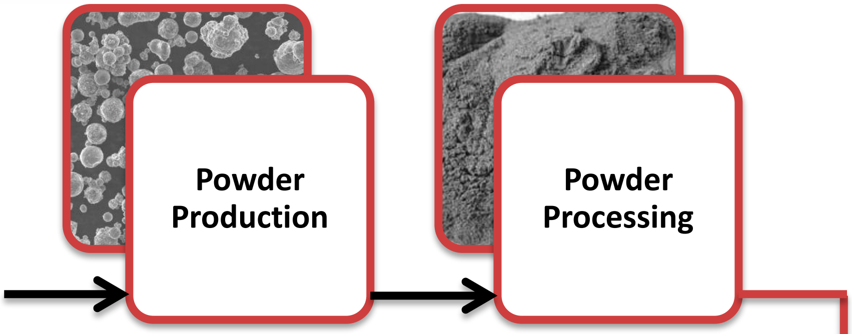


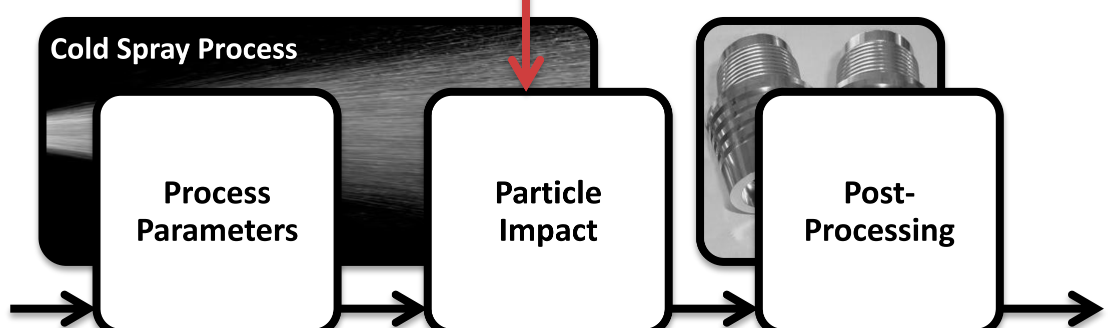












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Contact email:
dbelsito@wpi.edu
bamcnally@wpi.edu

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Le Zhong
Yongho Sohn