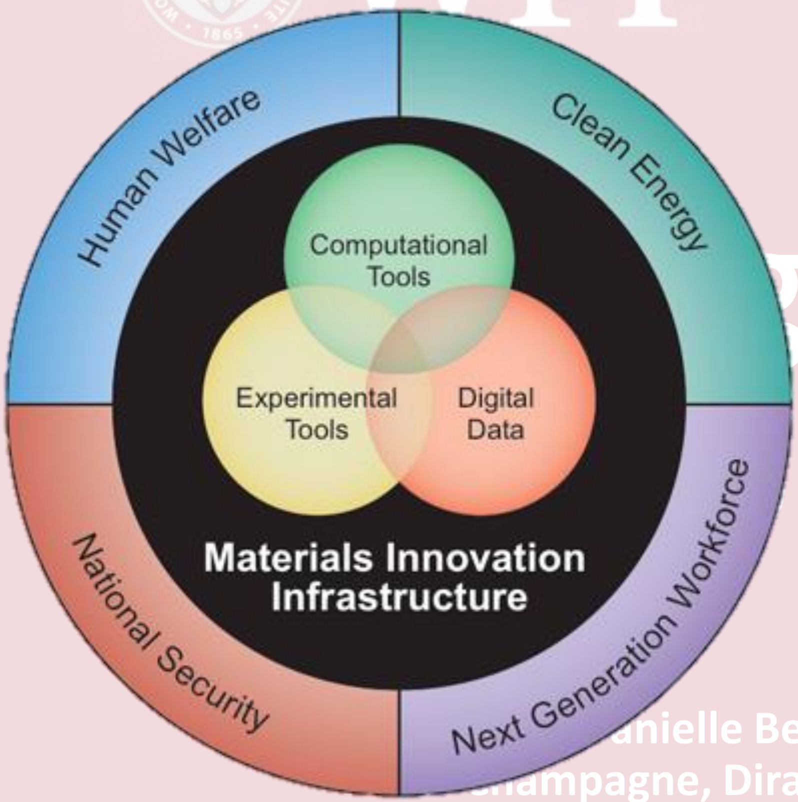
Welcome to WPI

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

- President Obama, 2011



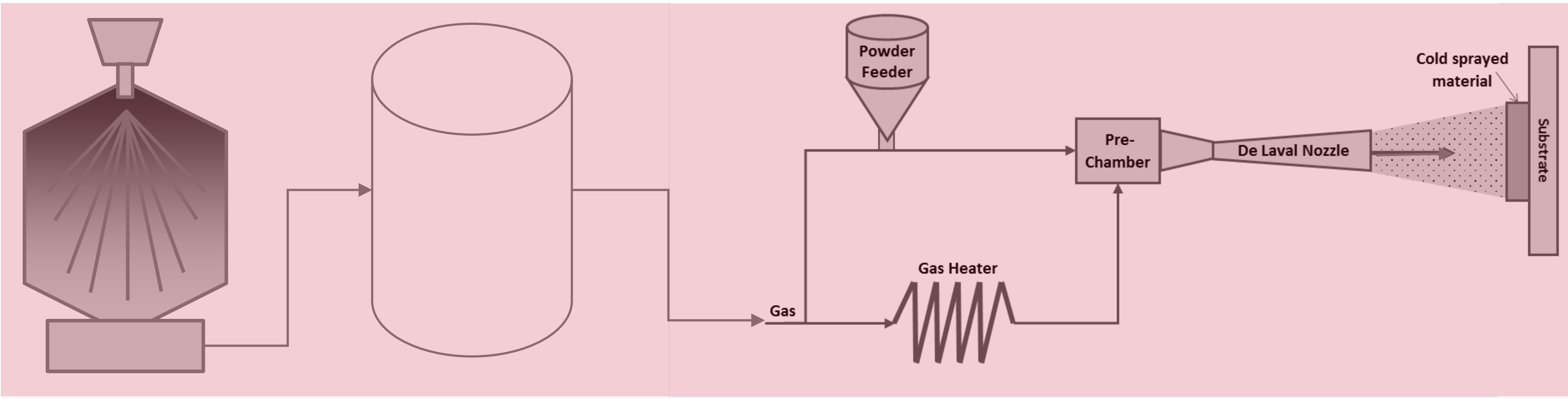
Meeting Societal Needs

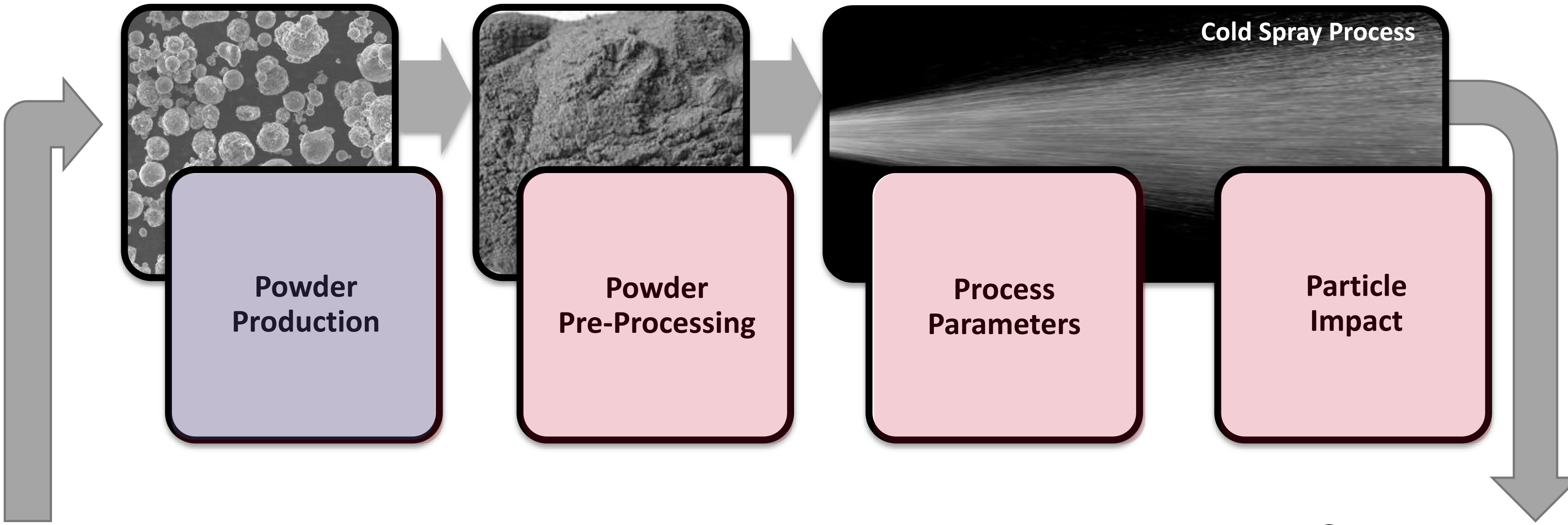
"The **lengthy time frame for materials to move from discovery to market** is due in part to the continued reliance of materials research and development programs on **scientific intuition** and **trial and error experimentation**. Much of the design and testing of materials is currently performed through 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)

Cold Spray Through Process Model

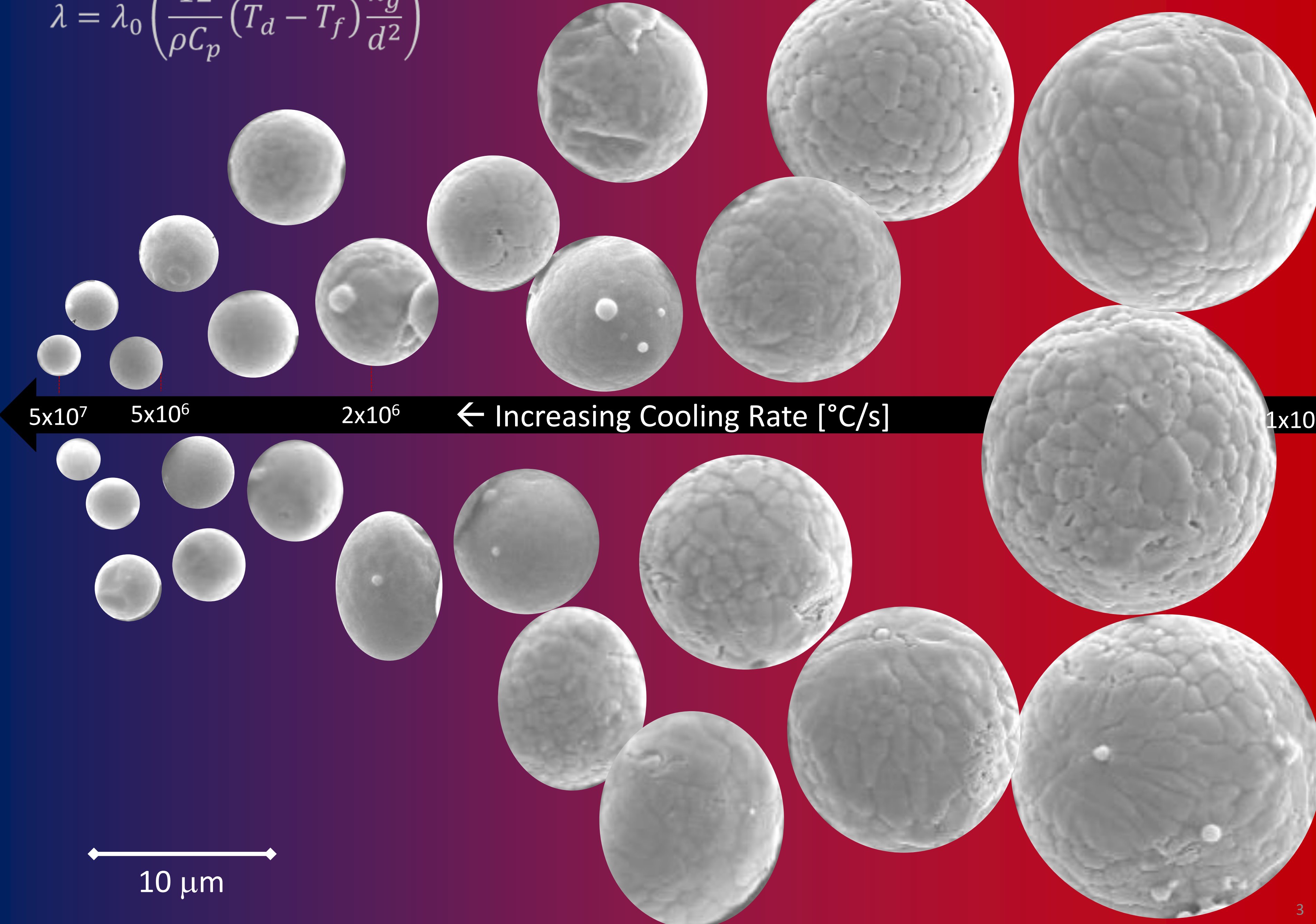




Inputs
- Raw material
- Requirements

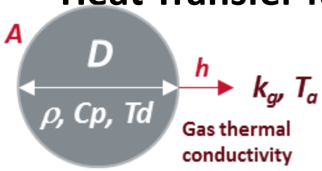
Outputs
- Microstructure
- Mechanical properties

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



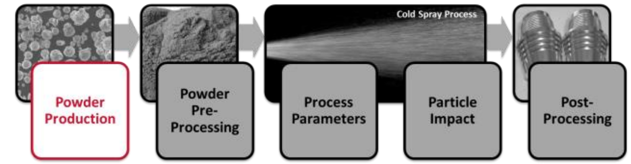
Powder Production Modeling: Solidification

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,

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

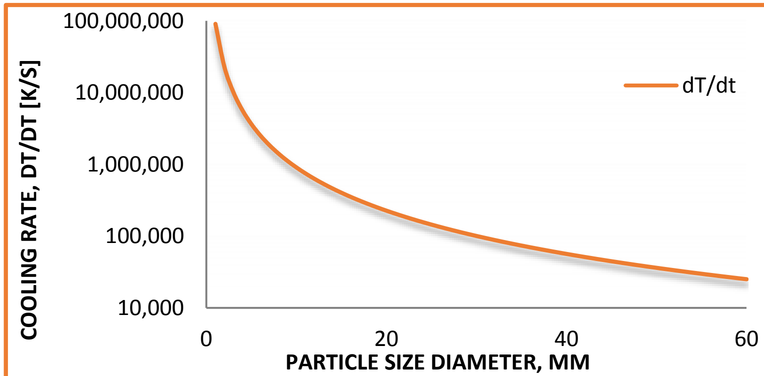
$$h=\frac{k_g}{d}(2.0+0.6\sqrt{R_e}\cdot\sqrt[3]{P_r})^2$$

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

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

$$\left|\frac{dT_d}{dt}\right|=\frac{6}{\rho\cdot C_p}\cdot(T_d-T_f)\cdot\left(\frac{2.0k_g}{d^2}+0.6\frac{k_g}{d}\sqrt{\frac{\rho_g U_0}{\mu_g d}}\cdot\sqrt[3]{P_r}\right)$$

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



Relationships between:

- Cooling Rate & Particle Size
- Cooling Rate & Grain Size

↓

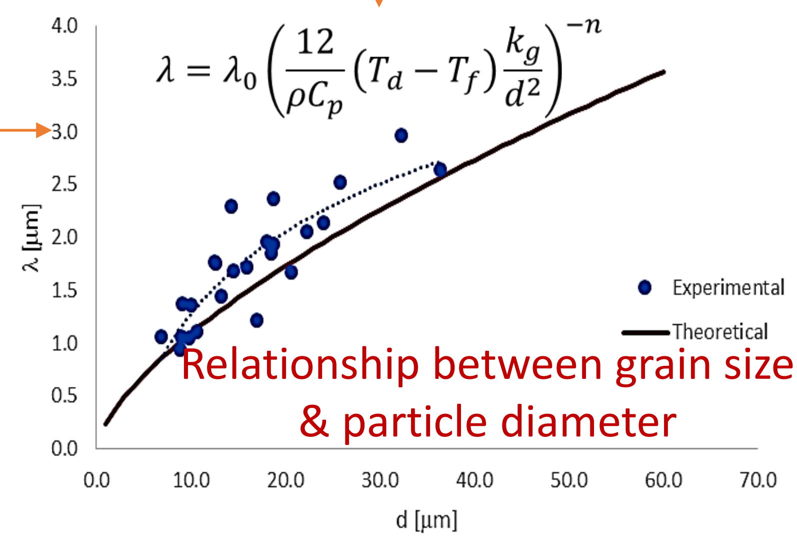
- Particle Size & Grain Size

Relationship Grain Size and Cooling Rate:

$$\lambda_2=\lambda_0\left(\frac{dT_d}{dt}\right)^{-n}$$

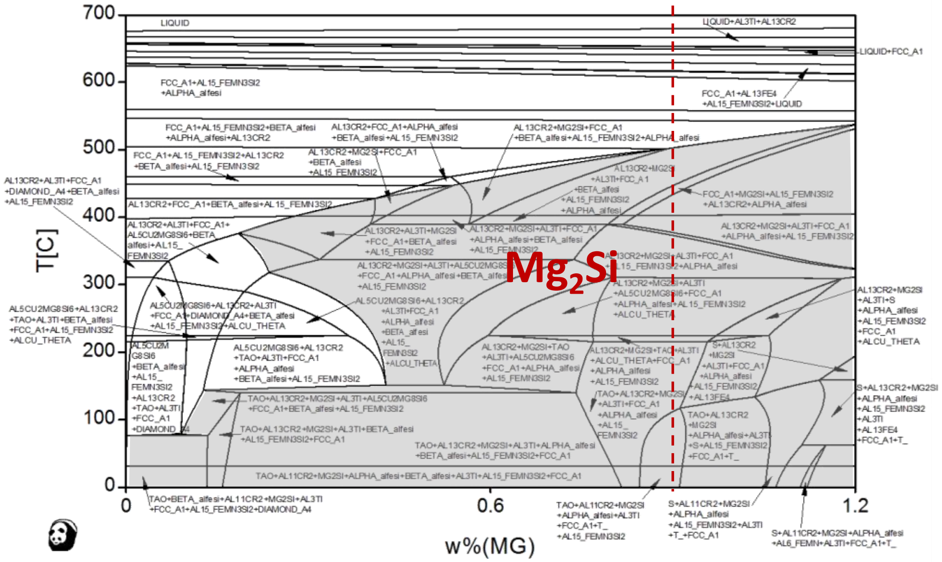
↓

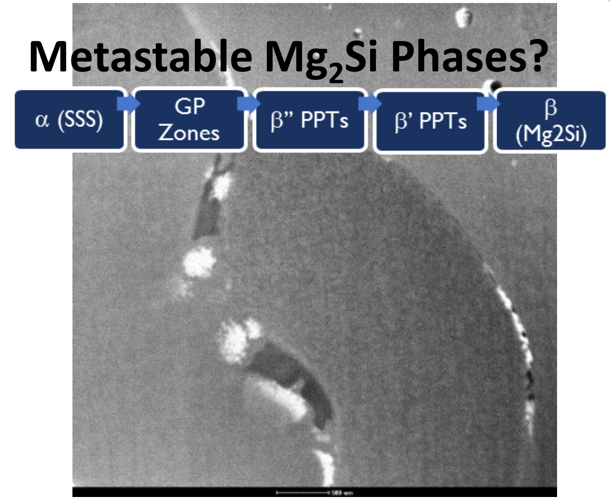
$$\lambda=\lambda_0\left(\frac{12}{\rho C_p}(T_d-T_f)\frac{k_g}{d^2}\right)^{-n}$$

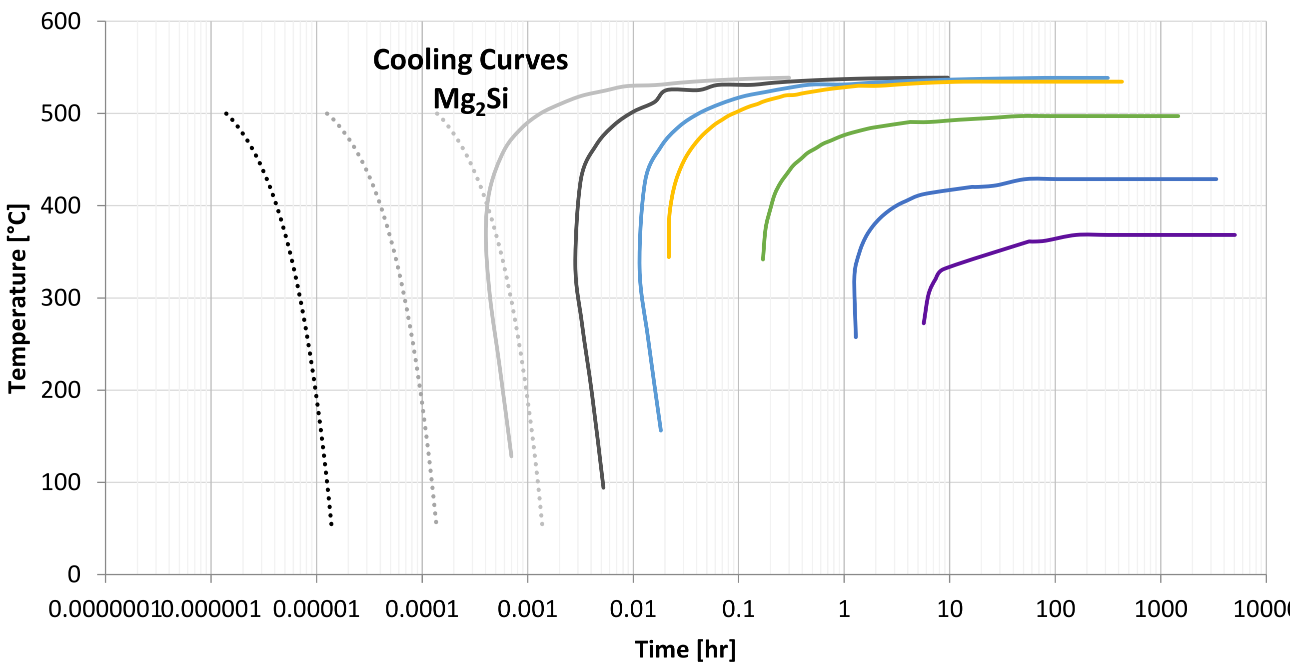


Relationship between grain size & particle diameter

Predictive Phase Modeling



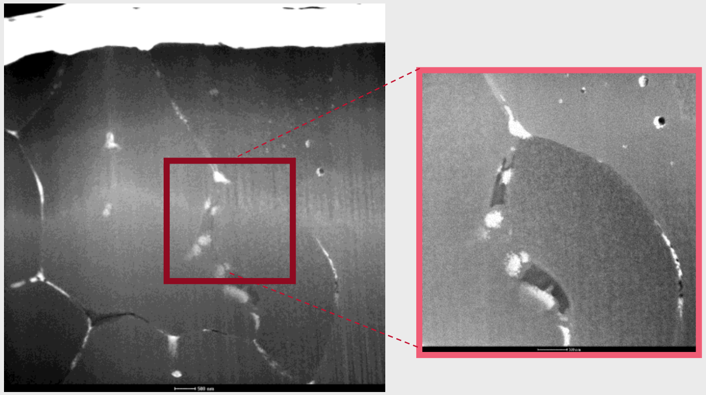




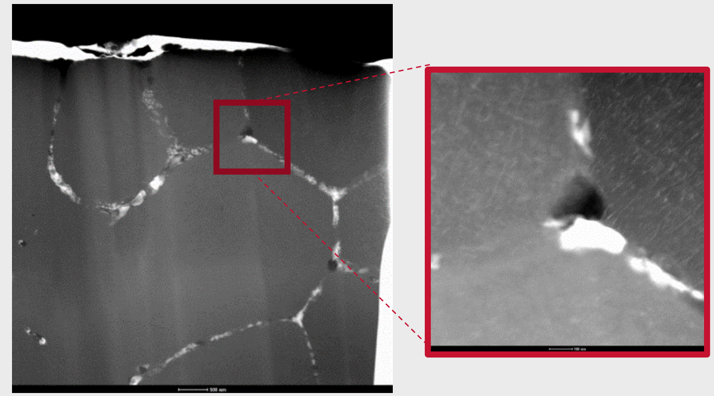
Gas atomization cooling rates: ~10^4-10^5 °C/s

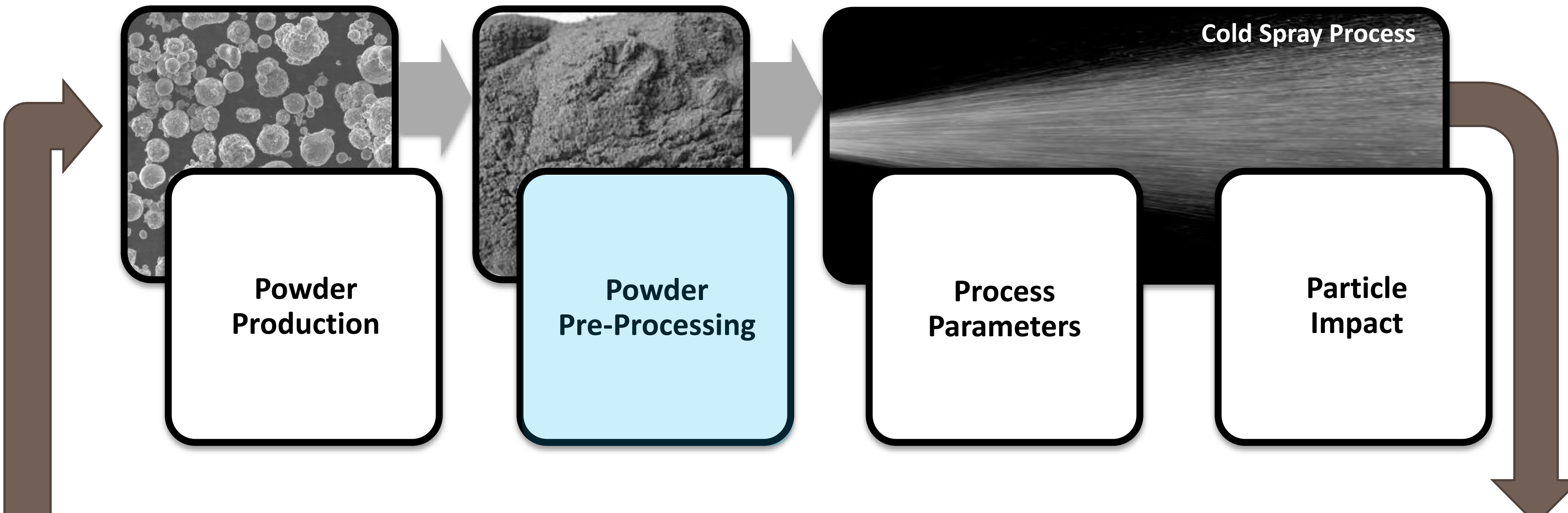
Powder Pre-Processing

Before Heat Treat



After Heat Treat



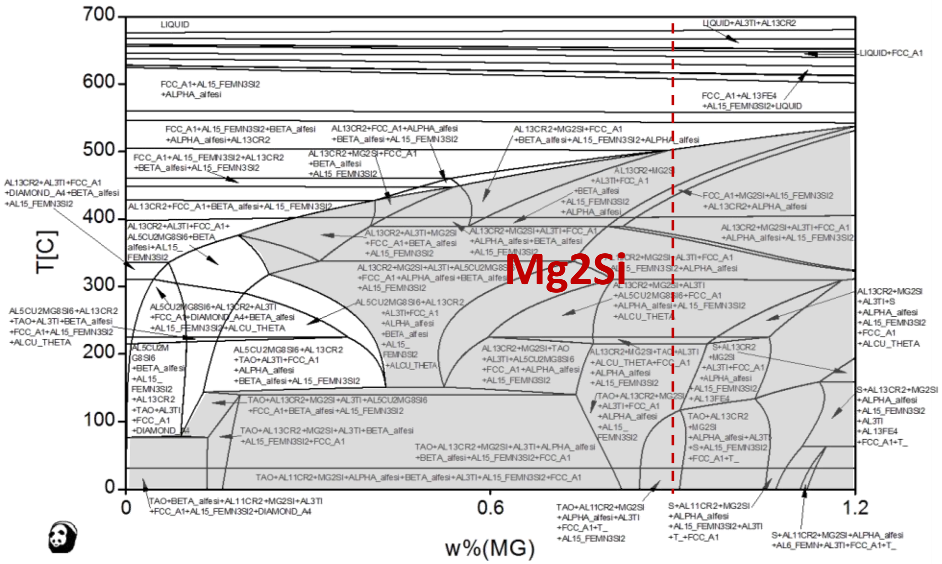


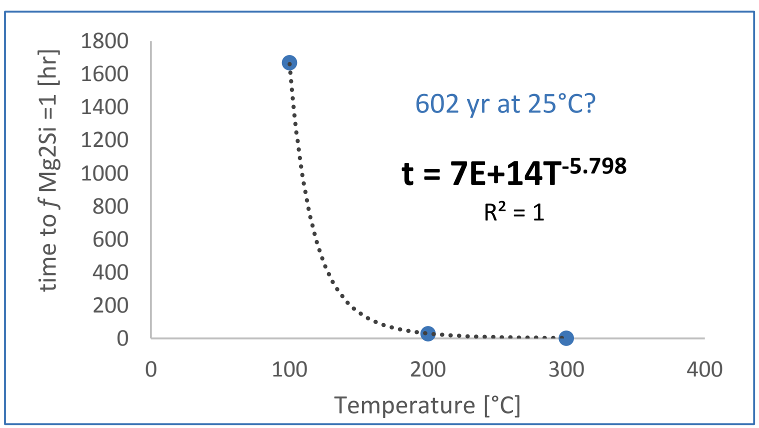
Inputs
- Raw material
- Requirements

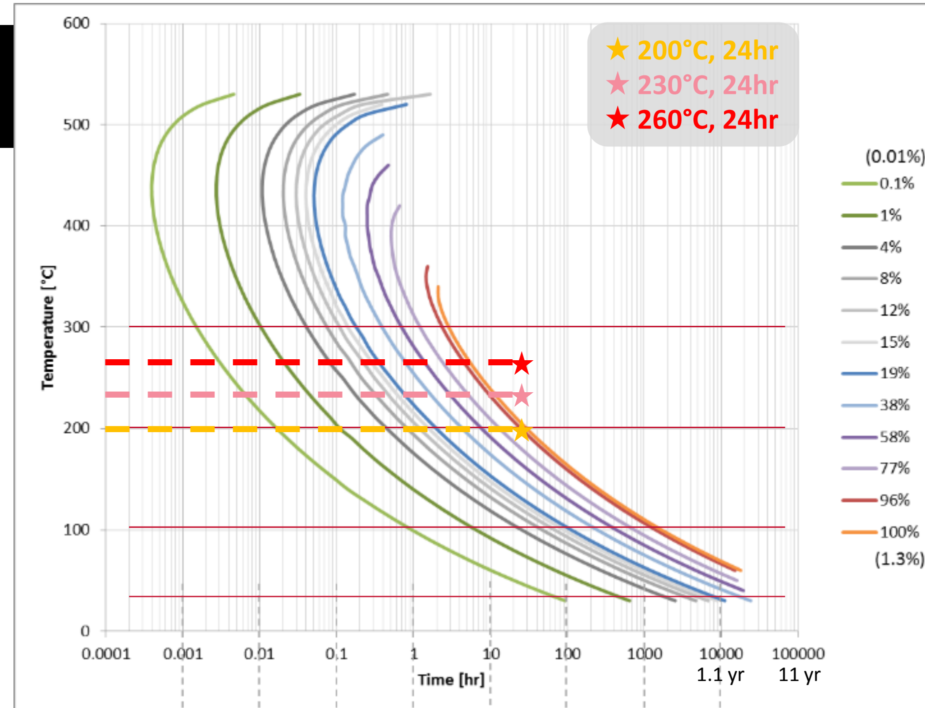
Outputs
- Microstructure
- Mechanical properties

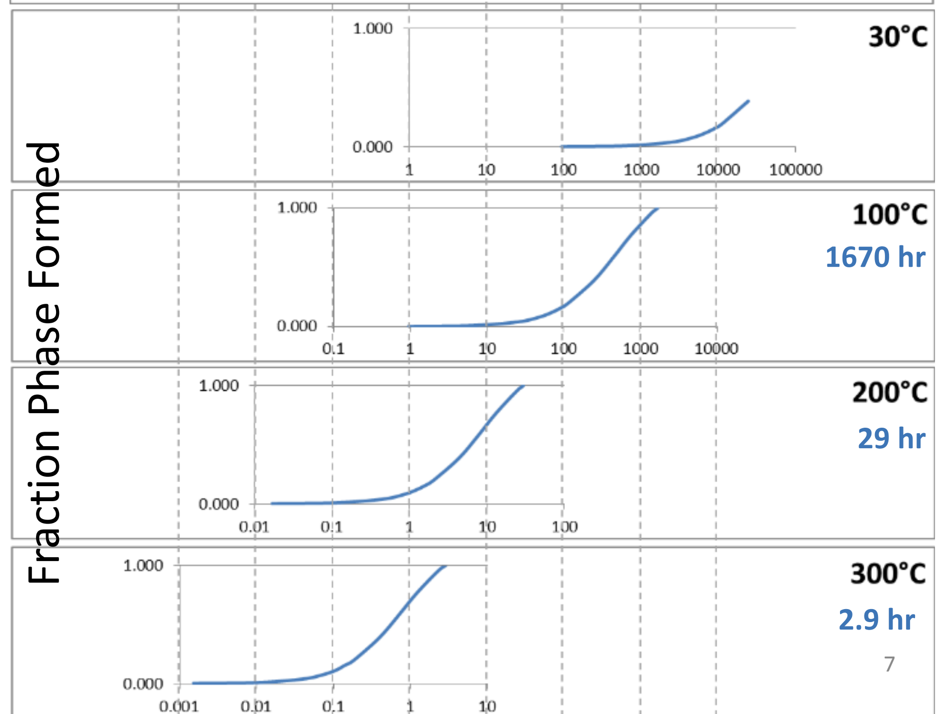
Mg_2Si TTT Diagram

At Equilibrium,



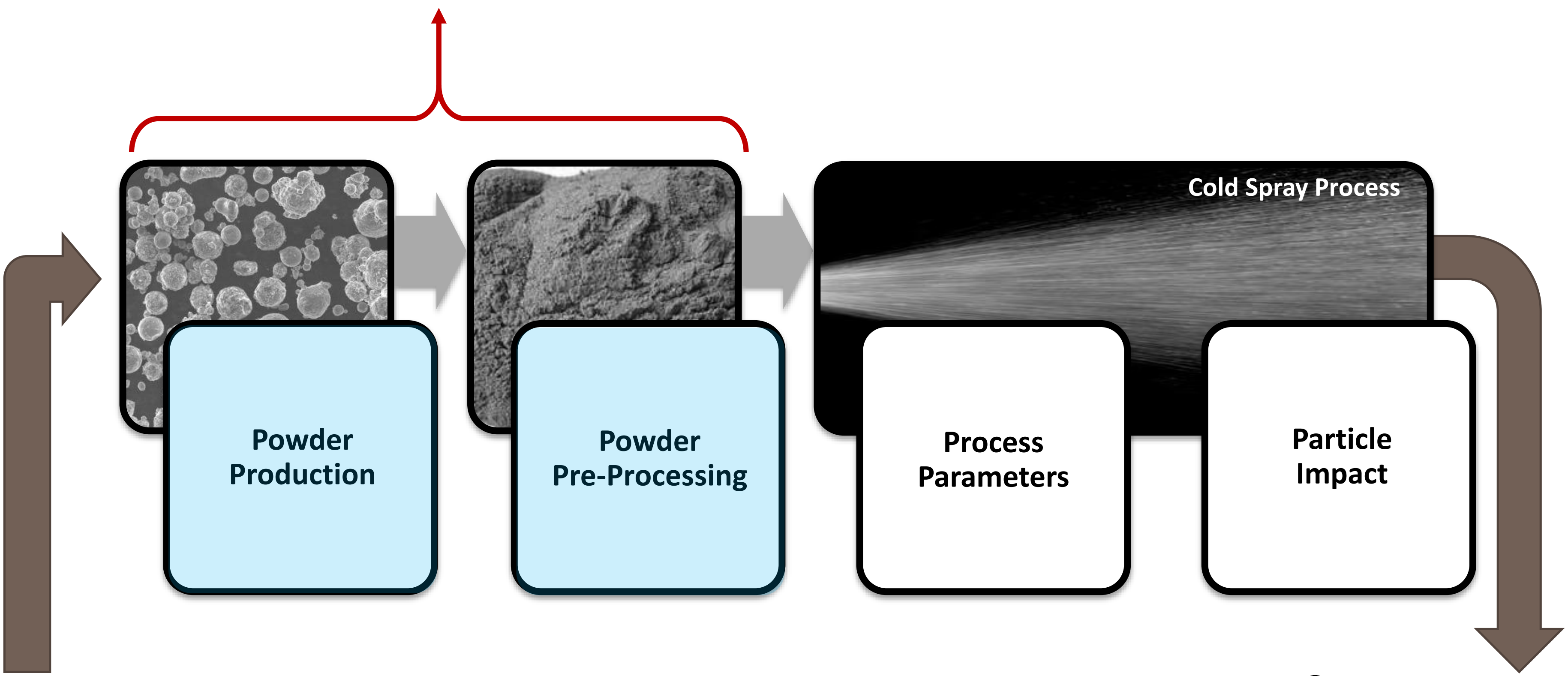






Model Development

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



Inputs
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Additive Hardness Model

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

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

Solid Solution Strengthening

Heat-treat dependent (↓ ss due to diffusion)

$$\Delta\sigma_{ss} = \sum_i x_i \Omega_i$$

Composition dependent

Linear approximation

Grain Size/Microstructural Influence

Heat-treat dependent

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

Particle size, composition dependent

Hall-Petch Behavior

Precipitation Strengthening

Heat-treat dependent

$$\Delta\sigma_{ppt,i} = \sum_i 0.84M\left[\frac{1.2Gb}{2\pi L_i}\right] ln\left(\frac{r_i}{b}\right)$$

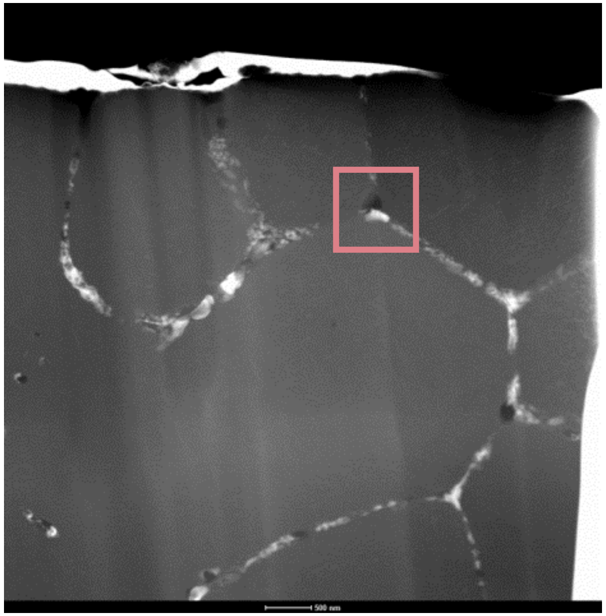
Particle size, composition dependent

$$L = \left[1.23\sqrt{\frac{2\pi}{3f_{ppt,i}}} - 2\sqrt{\frac{2}{3}}\right] r$$

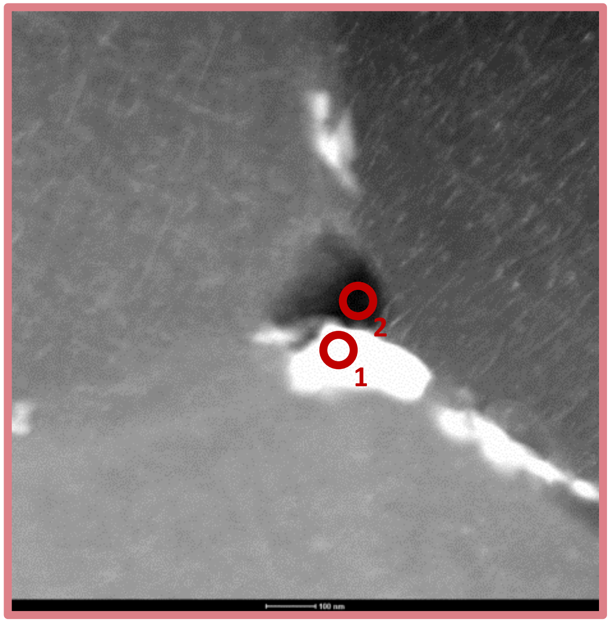
Ashby-Orowan Relationship

Al 6061 Powder Precipitates

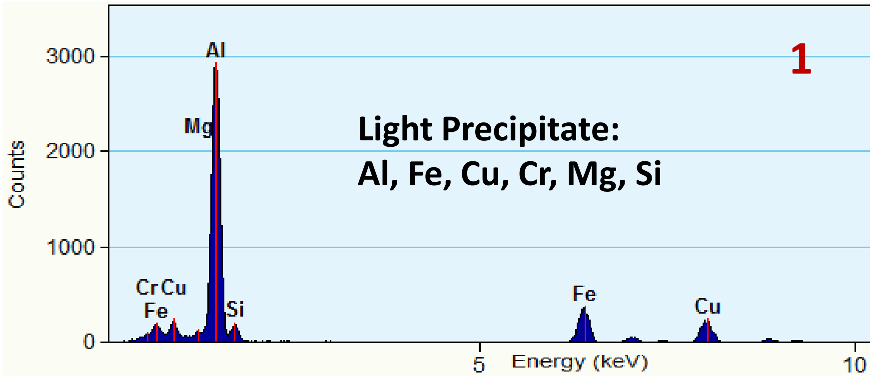
Phase	Wt%	Composition
Al	96.5	Al + trace Zn
Mg2Si	1.41	Mg_2Si ← 2
Al7Cu2M	0.76	Al_7Cu_2Fe } 1
Alpha	0.65	$Al_{47}(Fe,Mn,Cr)_{11}Si_5$ } 1
E	0.23	$Al_{18}Cr_2Mg_3$
Al3Fe	0.18	$Al_3(Fe,Cr)$ ← 1
Al13Cr4Si4	0.17	$Al_{13}Cr_4Si_4$
Al3M	0.06	Al_3Ti

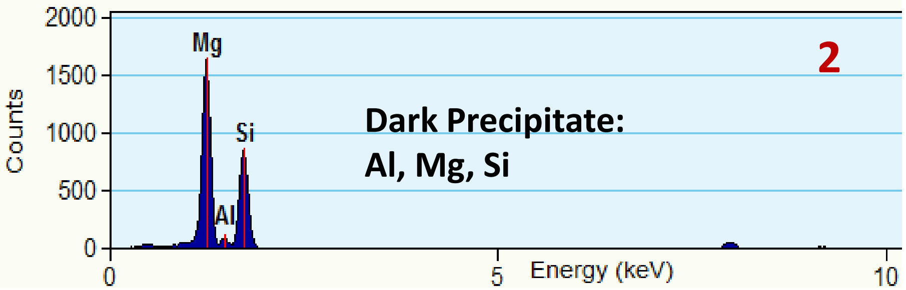


STEM DF Image, scale bar 500 nm



STEM DF Image, scale bar 100 nm

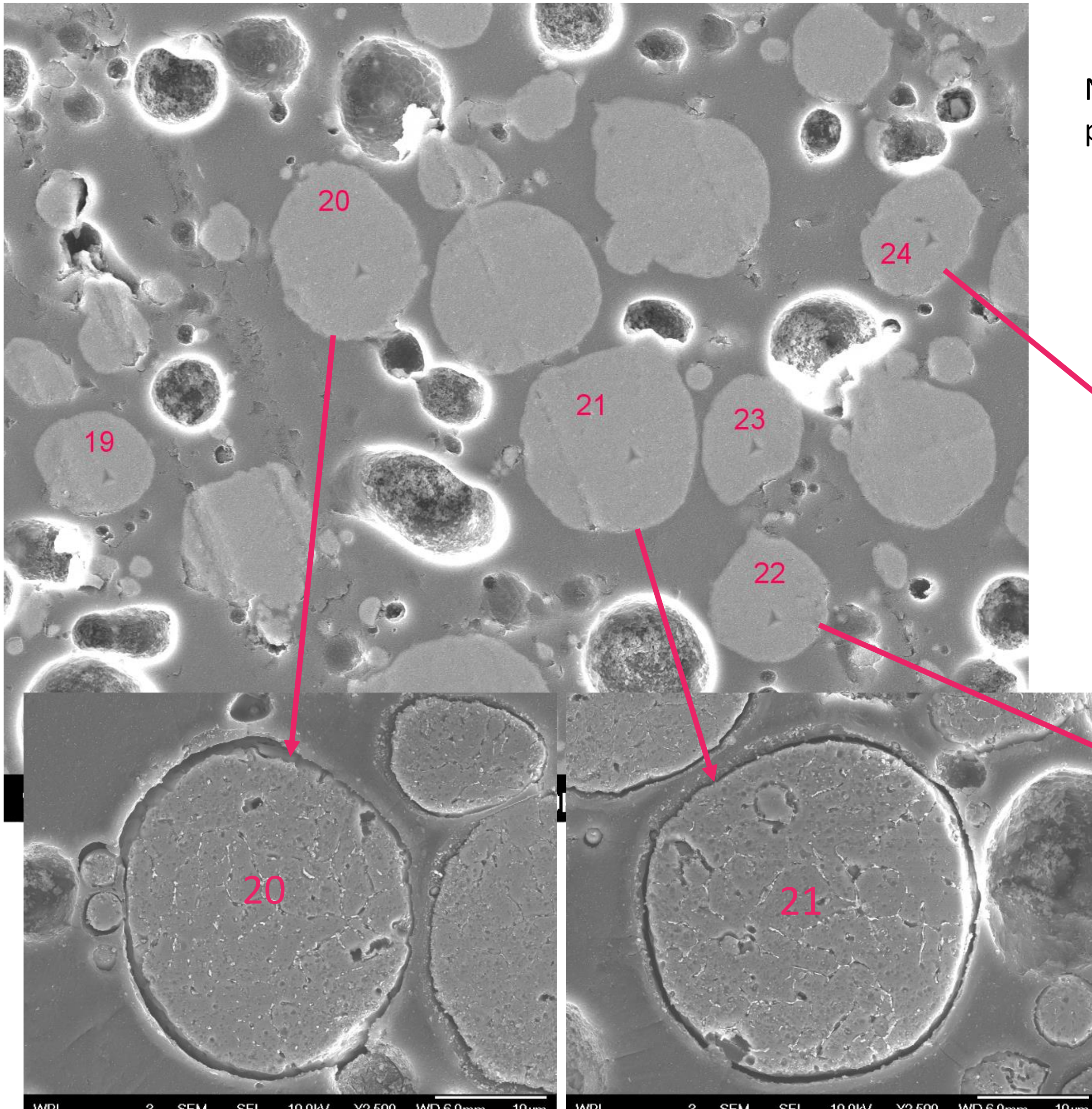


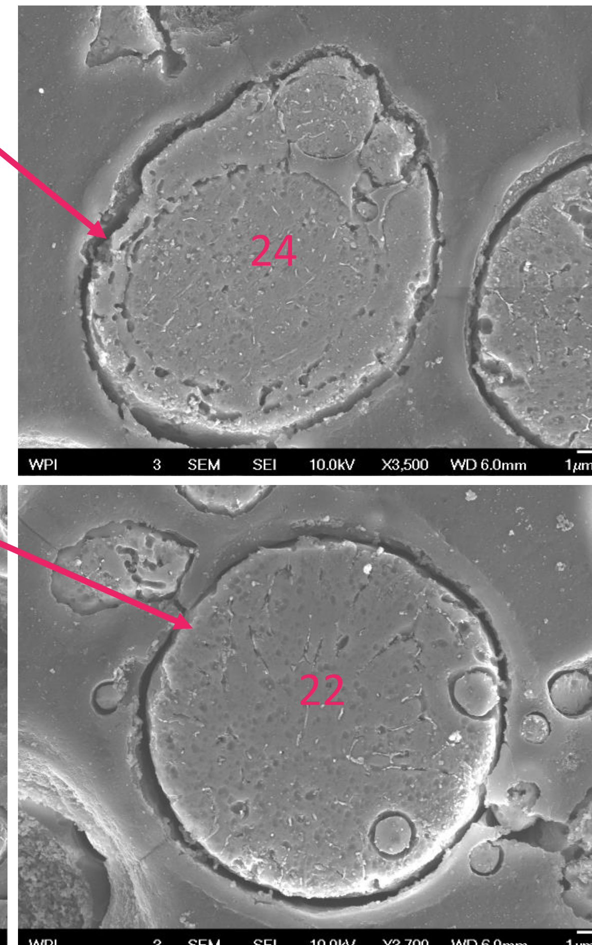


$$\sigma_y = \sigma_0 + \Delta\sigma_{GS} + \Delta\sigma_{CW} + \boxed{\Delta\sigma_{PPT}} + \Delta\sigma_{DS} + \cdots$$

Experimental Hardness Measurements

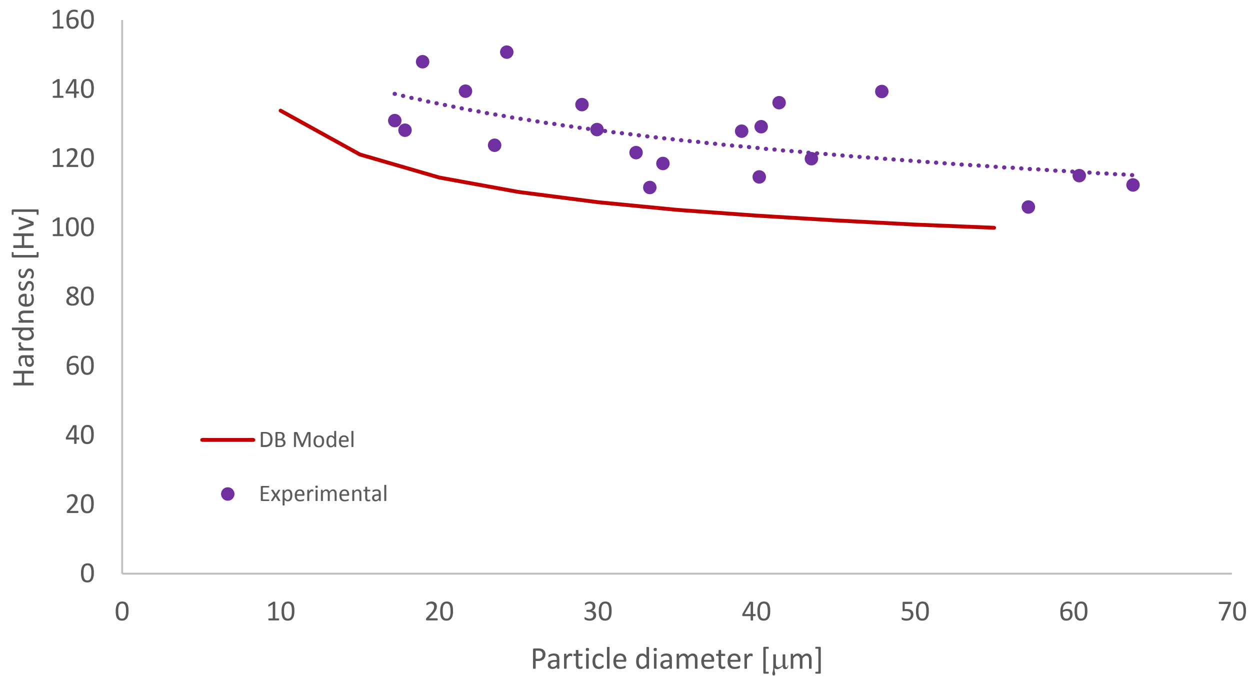
Nanohardness measurements of Al 6061 powder





Model vs. Experimental Results

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



- Model predictions vs. experimental hardness (previous slide).
- Model predictions converted from yield strength.
- Yield strength values used as input into the particle impact model, below.

Cold Spray Process Modeling

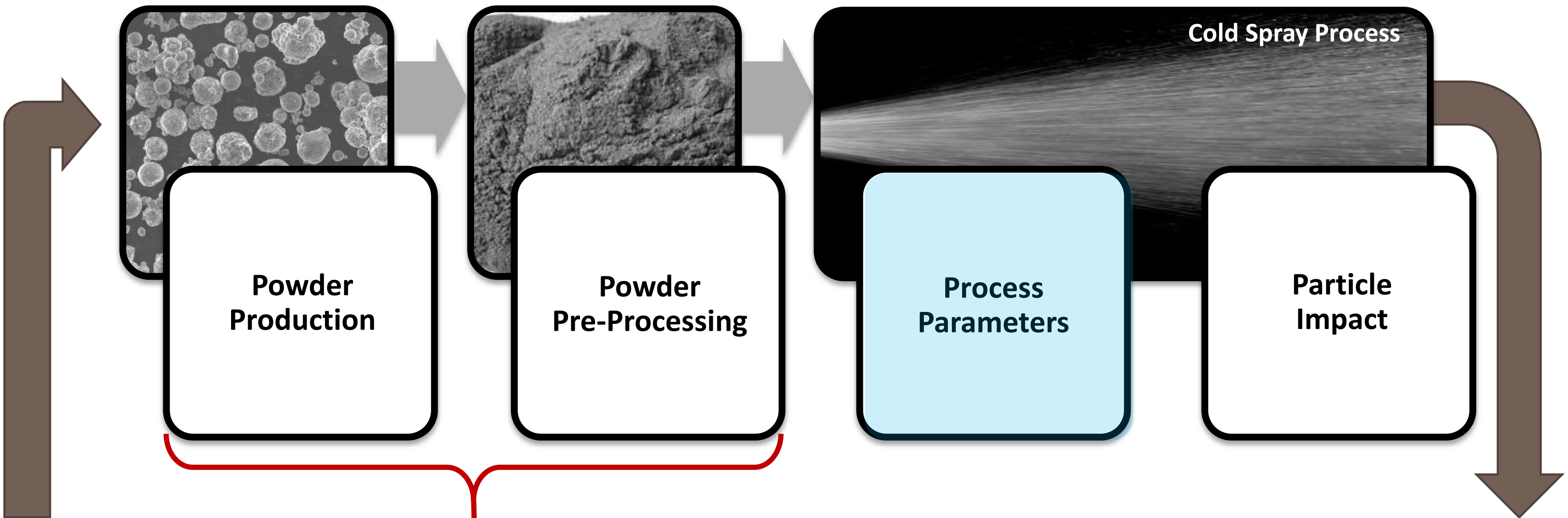
Temperature

Pressure

Feeds

Speeds

Patterns

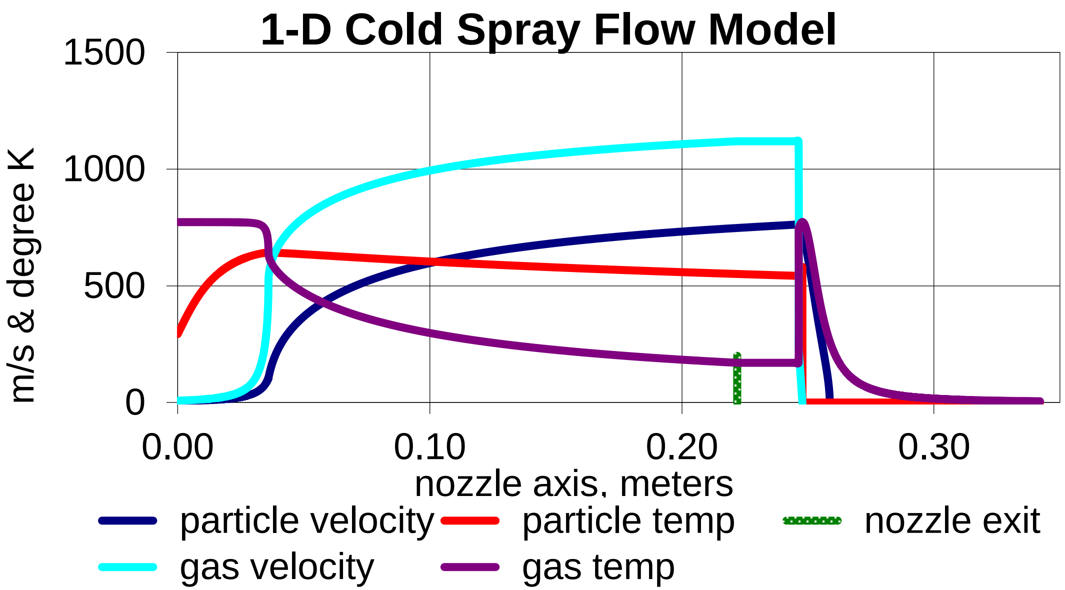


Inputs
- Raw material
- Requirements

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

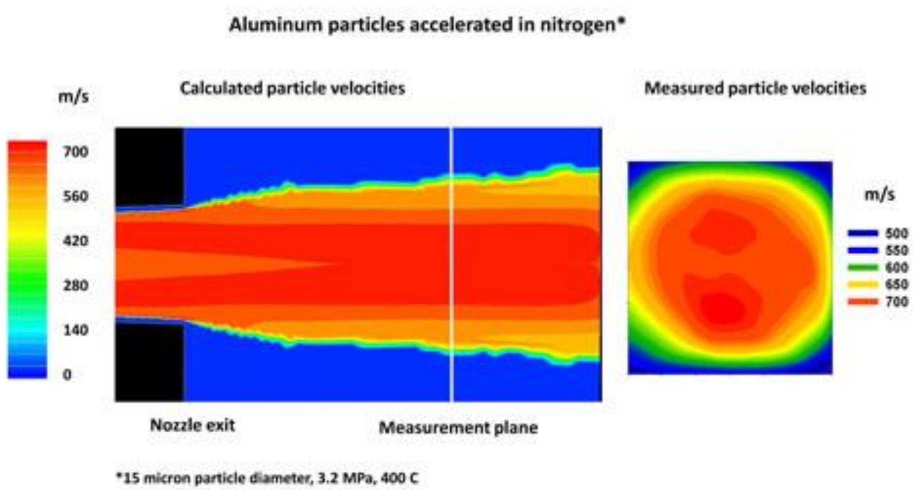
Outputs
- Microstructure
- Mechanical properties

Cold Spray Process Model: ARL



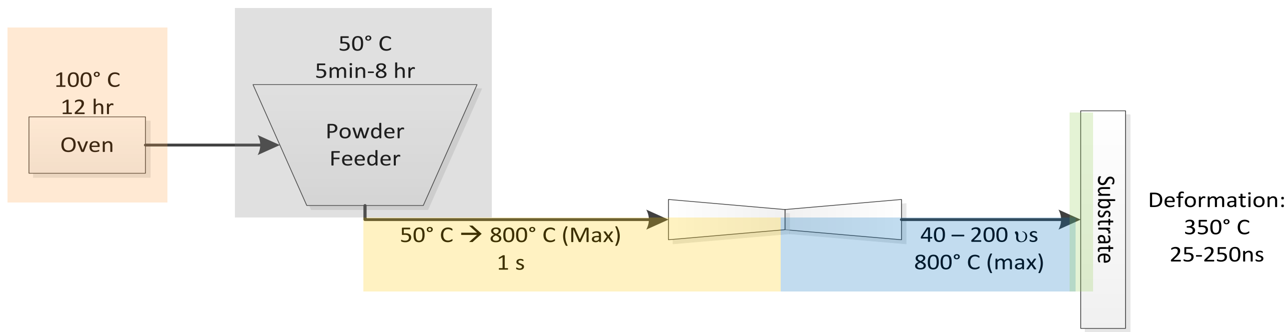
CFD Velocity Profile of Cold Spray Plume

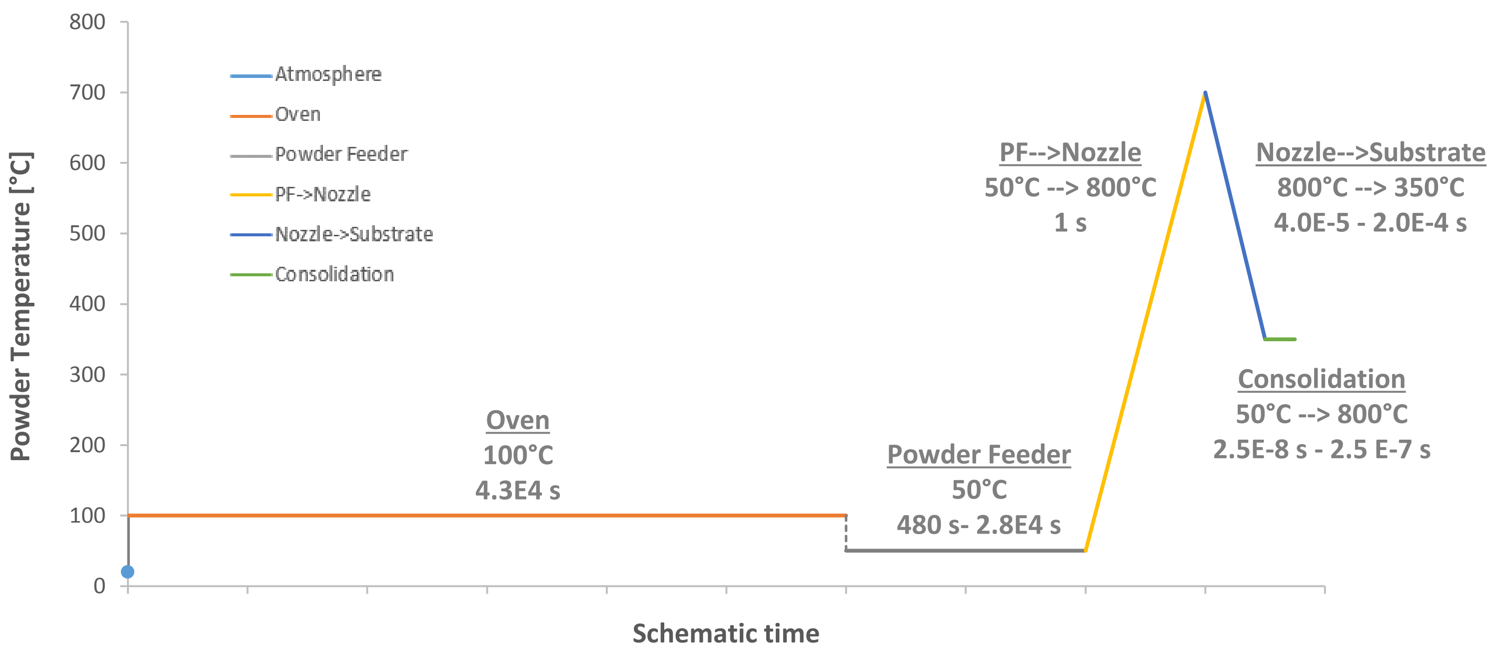
Velocity and Temperature Profile for Gas and Powder from Nozzle to Substrate



Images courtesy of Dennis Helfritch PhD, Army Research Laboratories

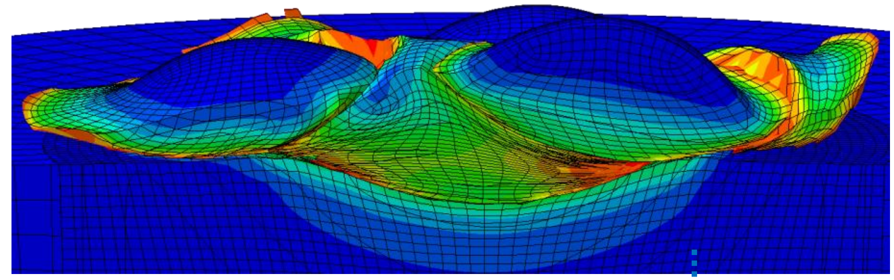
Influence of Process on Material Properties

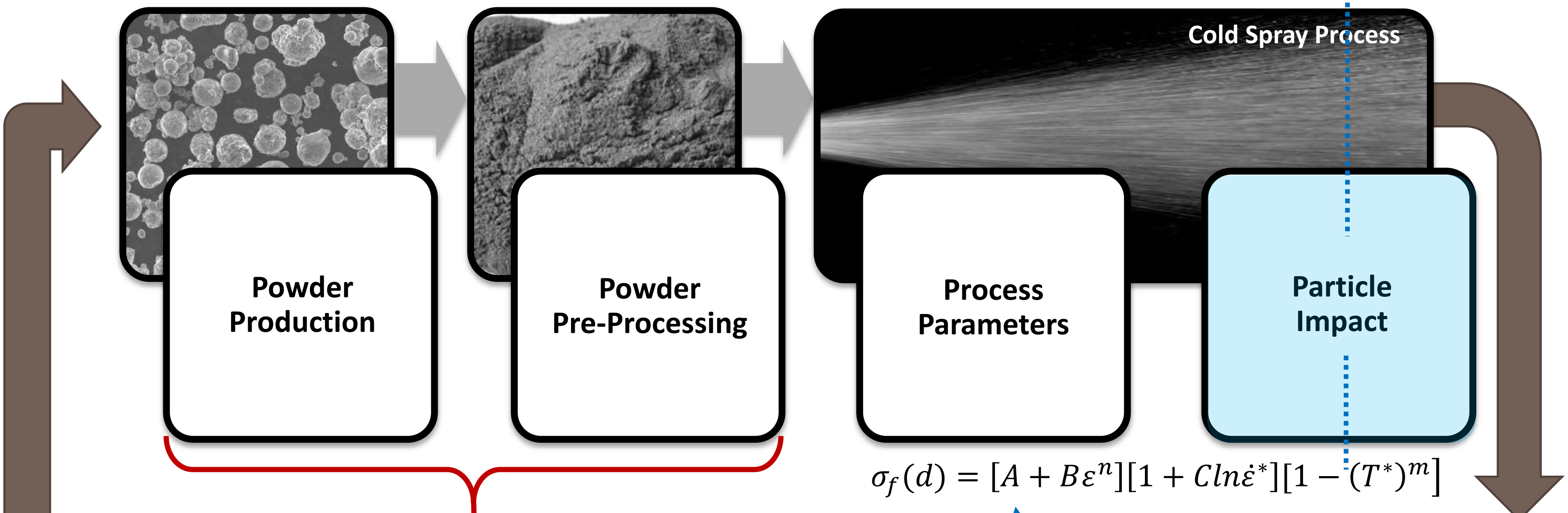




Particle Impact Modeling

Output from Powder Production & Powder Pre-Processing models are used as input to the Particle Impact Model





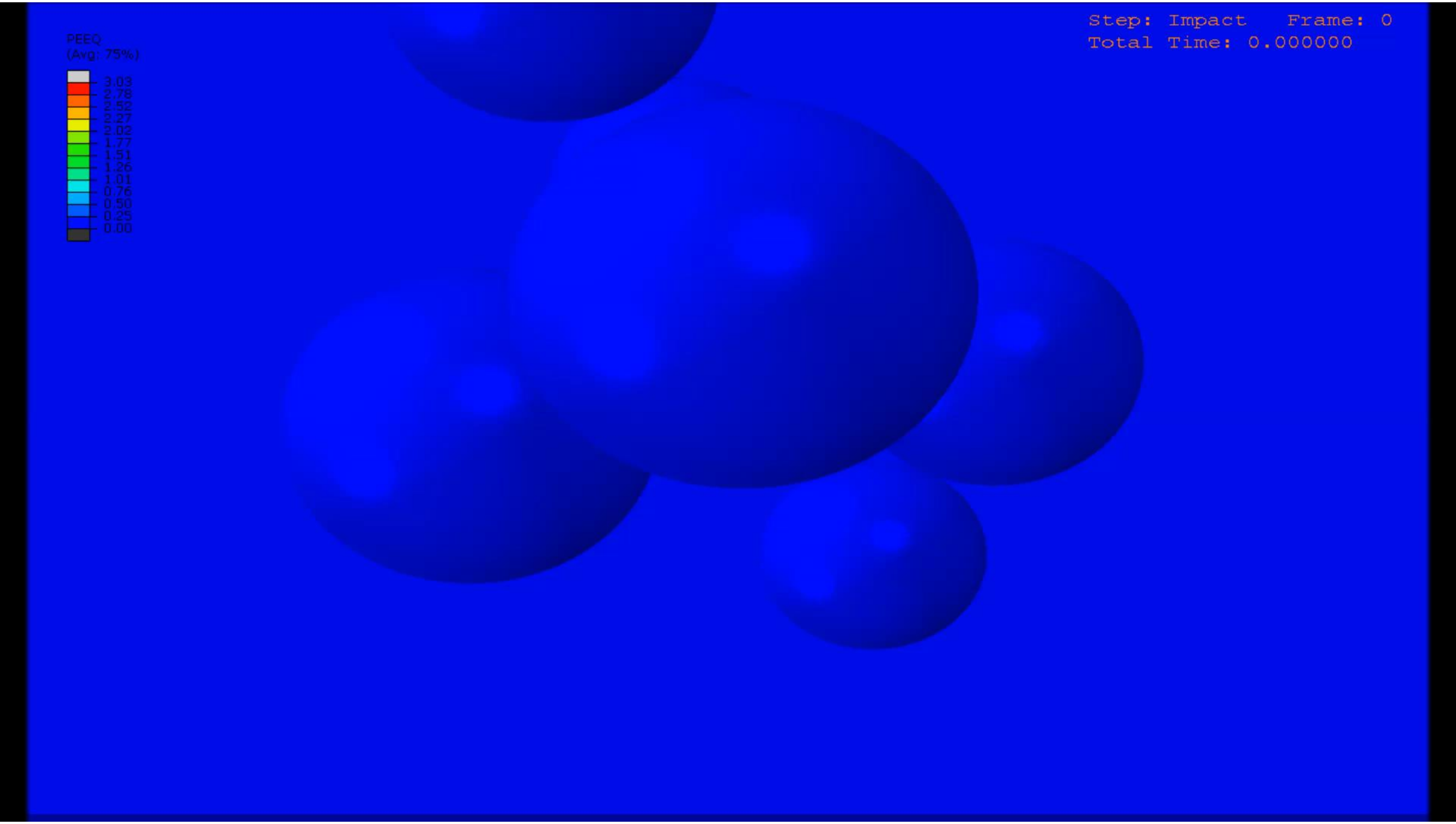
$$\sigma_f(d) = [A + B\varepsilon^n][1 + C\ln\dot{\varepsilon}^*][1 - (T^*)^m]$$

Inputs
- Raw material
- Requirements

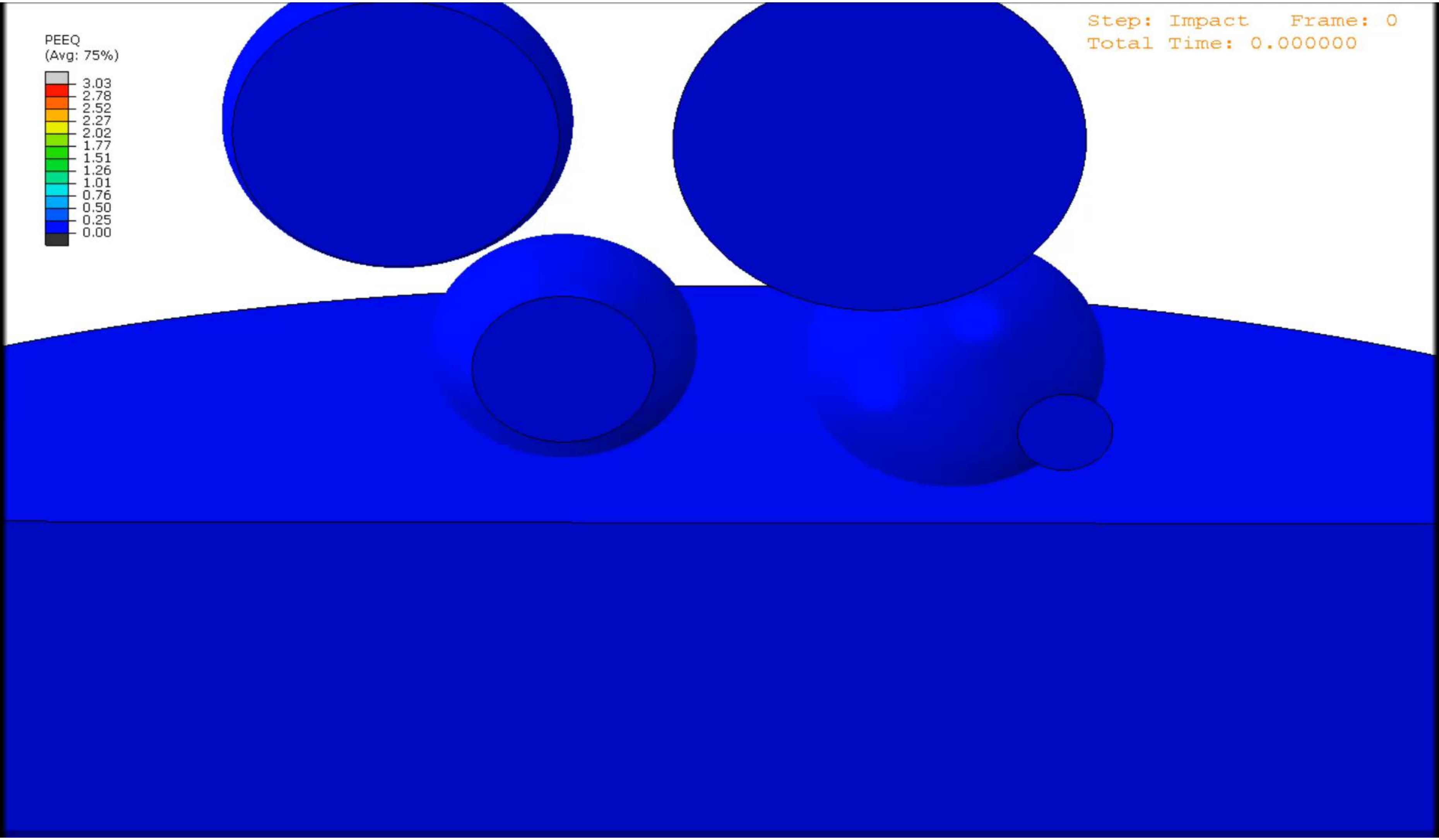
$$\sigma_{YS}(d) = \sigma_o + \Delta\sigma_{ss} + \Delta\sigma_{mic} + \Delta\sigma_{ppt}$$

Outputs
- Microstructure
- Mechanical properties

Multiple Particle Video

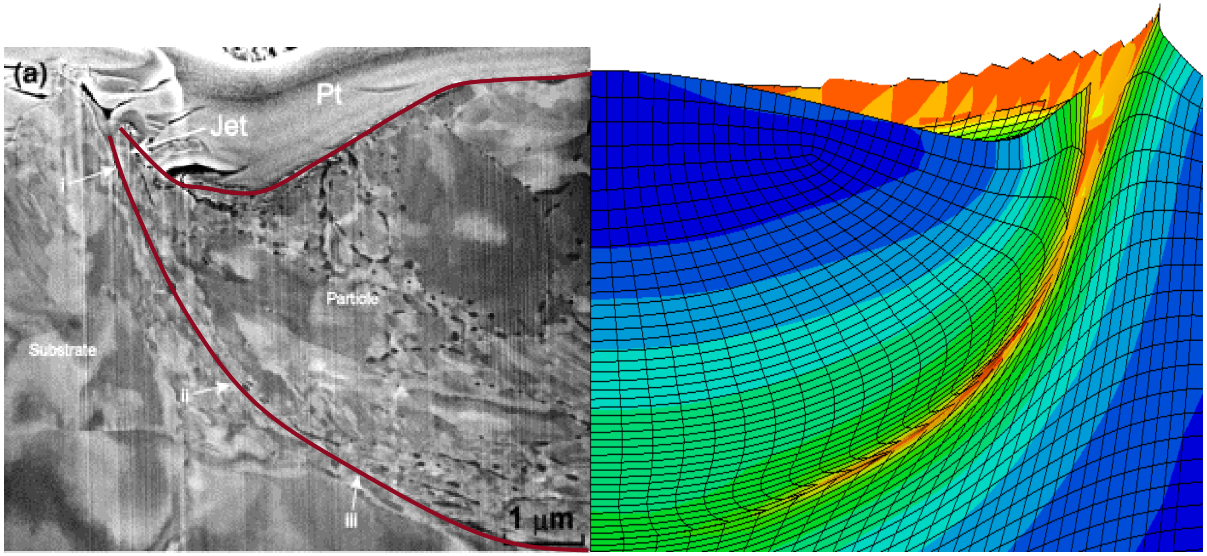


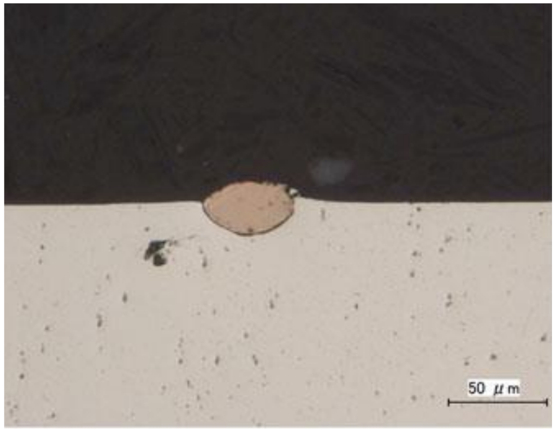
Multiple Particle Video



Deformed Shape Qualitative Validation

Visual comparison of deformed particle to simulation output





Several researchers have taken images of individual deformed particles

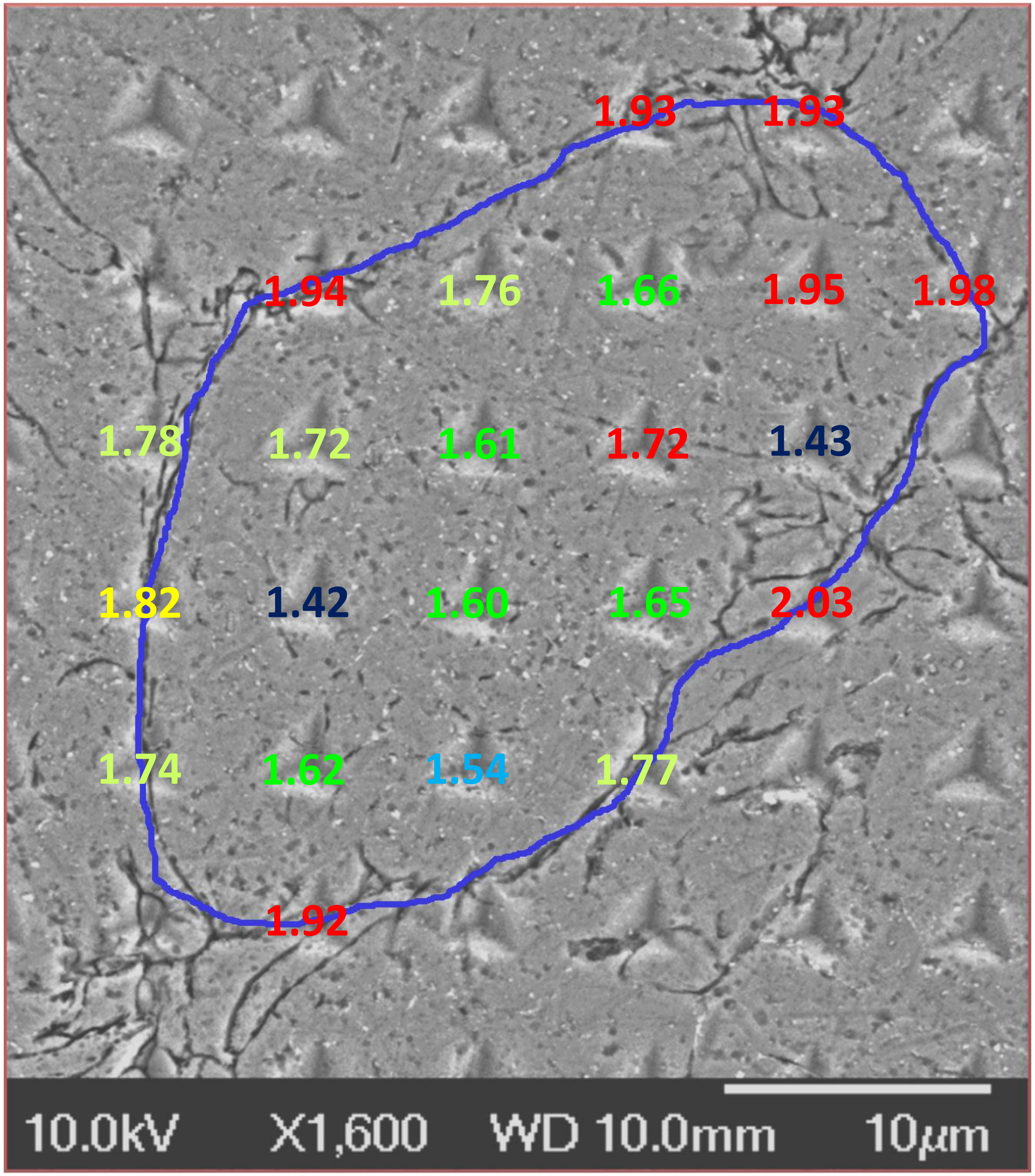
- Simulate scenario described in research
- Compared simulation results to images of deformed particles

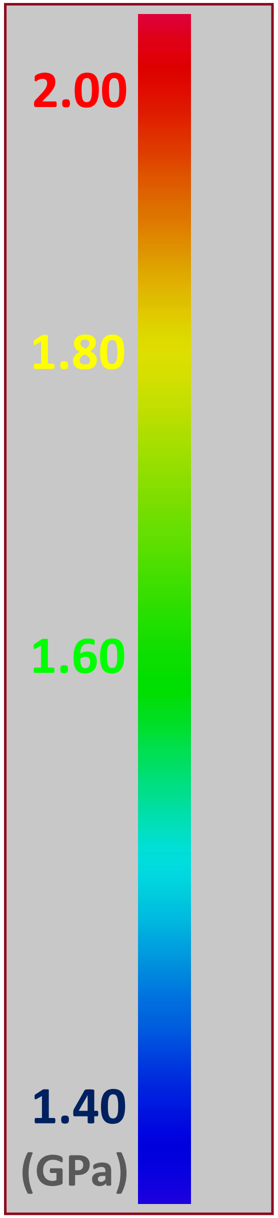
King, P.C., S.H. Zahiri, and M. Jahedi, *Microstructural refinement within a cold-sprayed copper particle.* Metallurgical and materials transactions A, 2009. **40**(9): p. 2115-2123.

Huang, R. and H. Fukanuma, *Study of the Influence of Particle Velocity on Adhesive Strength of Cold Spray Deposits.* Journal of thermal spray technology, 2012. **21**(3-4): p. 541-549.

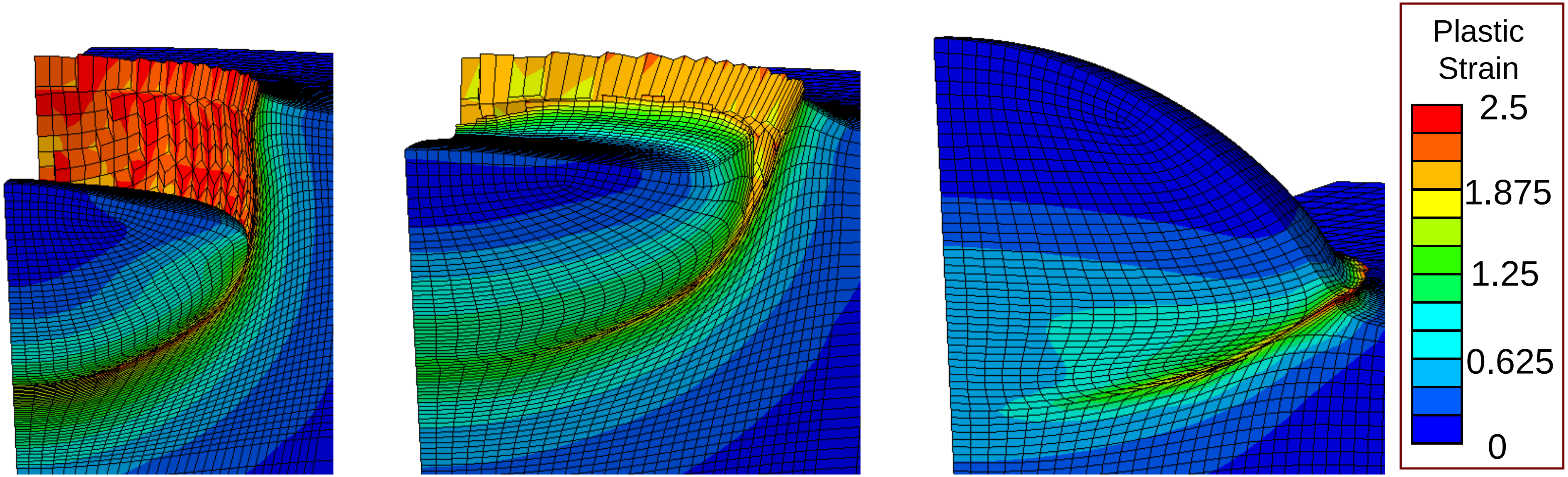
Al 6061 Nanohardness

Spray Direction





Material Behavior



OFHC Copper particle, Al 6061-0 Substrate 600 m/s

316L stainless steel particle and substrate 800 m/s

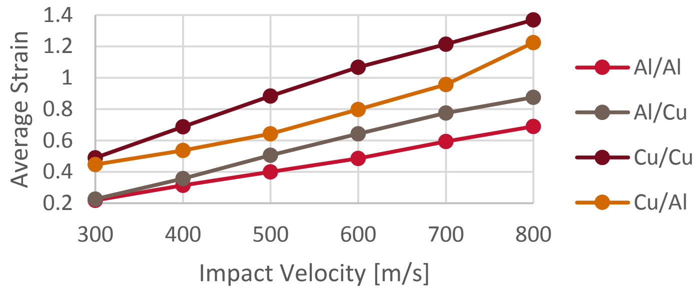
Ti-6Al-4V particle and substrate 800m/s

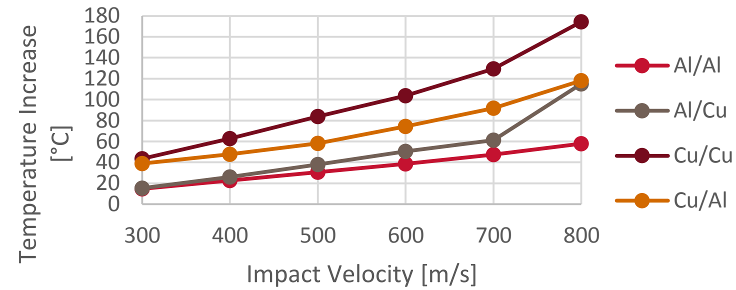
Single Particle Normal Impact

Average Particle Strain

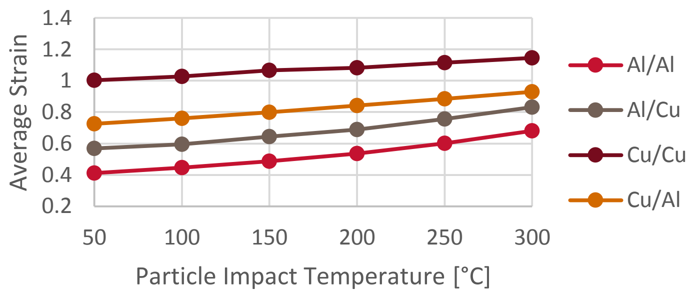
Average Particle Temperature Increase

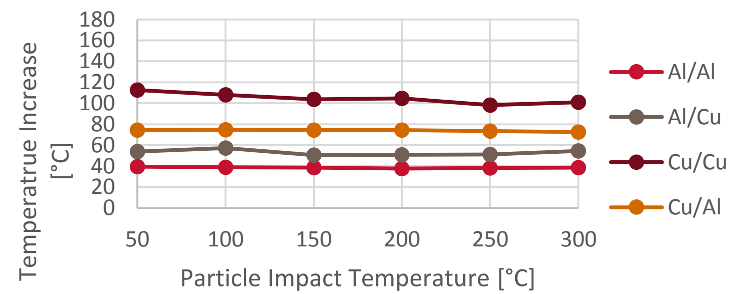
Particle Impact Velocity – 150°C Particle & Substrate



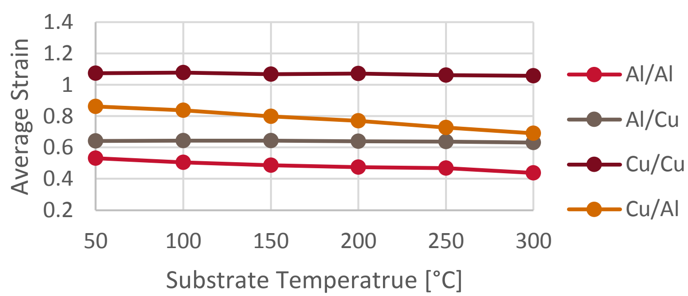


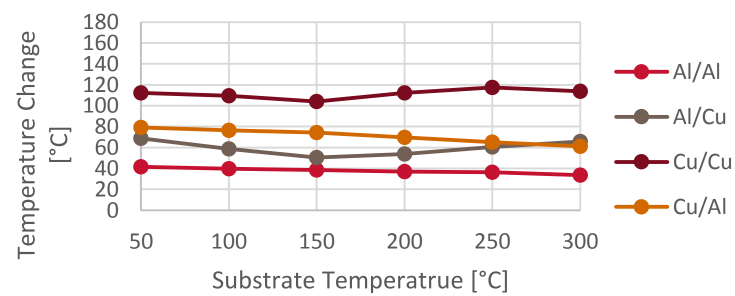
Particle Impact Temperature – 600 m/s, 150°C Substrate





Substrate Impact Temperature – 600 m/s, 150°C Particle

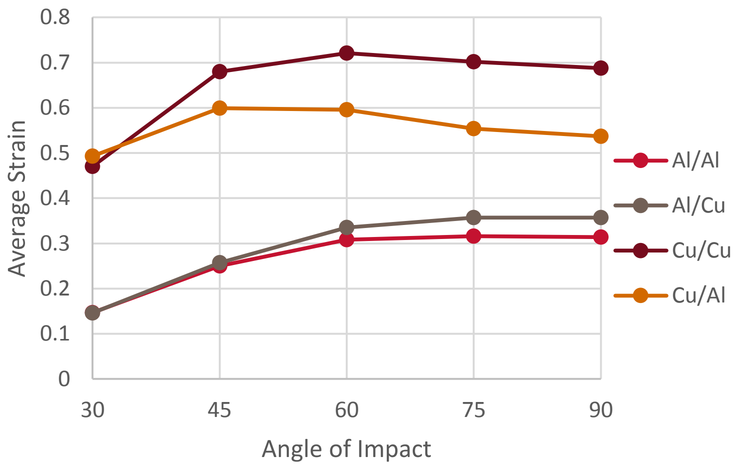




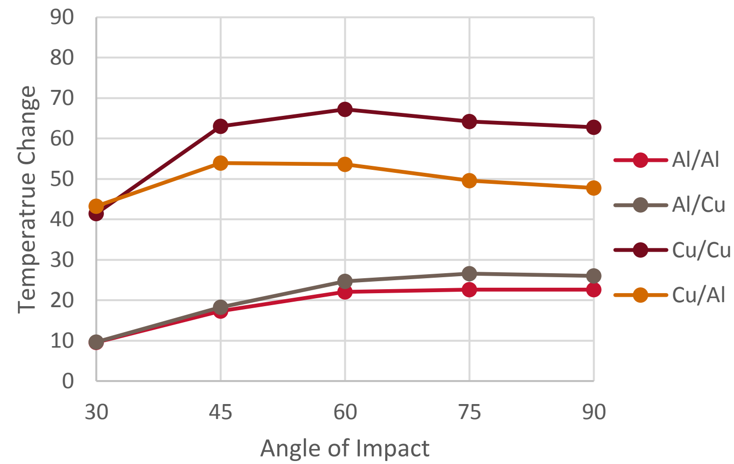
Oblique and Two-Particle Impact

Particle Impact Angle – 400 m/s, 150°C Particle & Substrate

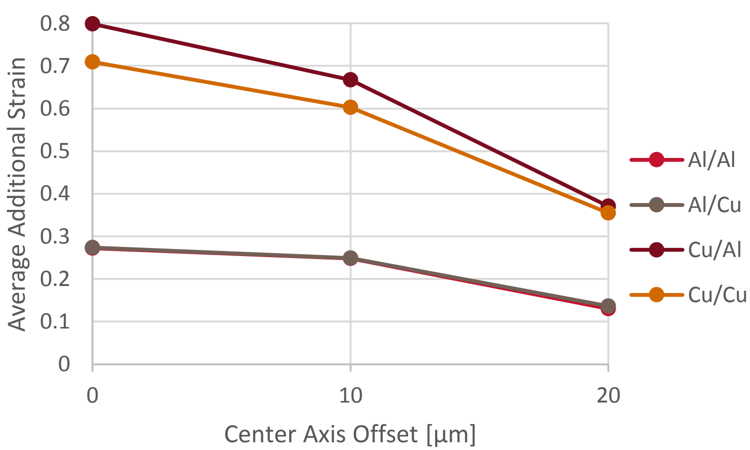
Average Particle Strain

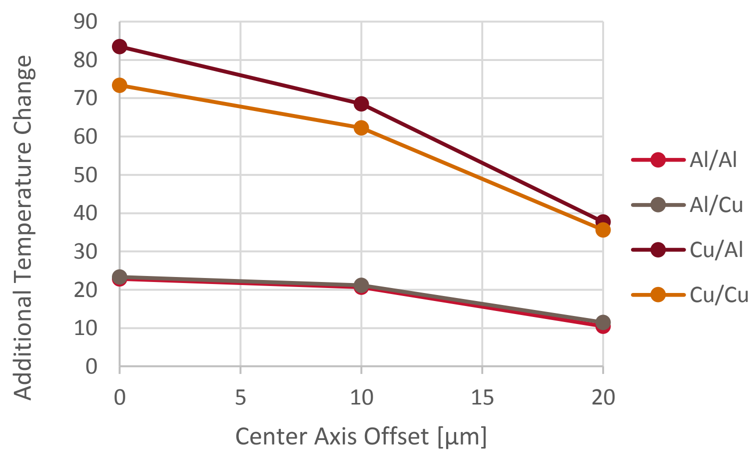


Average Particle Temperature Increase



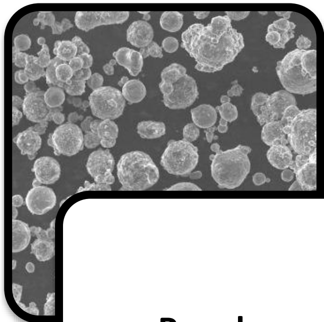
Effect of Second Particle Impact– 400 m/s, 150°C Particle & Substrate





WPI's Vision for the Future

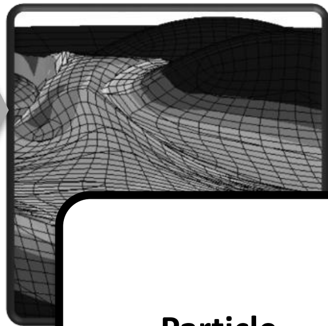
Integrate → Validate → Expand → Utilize



Powder Production

Powder Pre-Processing

Process Parameters



Particle Impact

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

$$\sigma_f(d) = [A + B\varepsilon^n][1 + C\ln\dot{\varepsilon}^*][1 - (T^*)^m]$$

Inputs/Outputs

- Microstructure
- Mechanical properties
- Raw material
- Requirements

Questions?

Aaron Birt
ambirt@wpi.edu

Worcester Polytechnic Institute

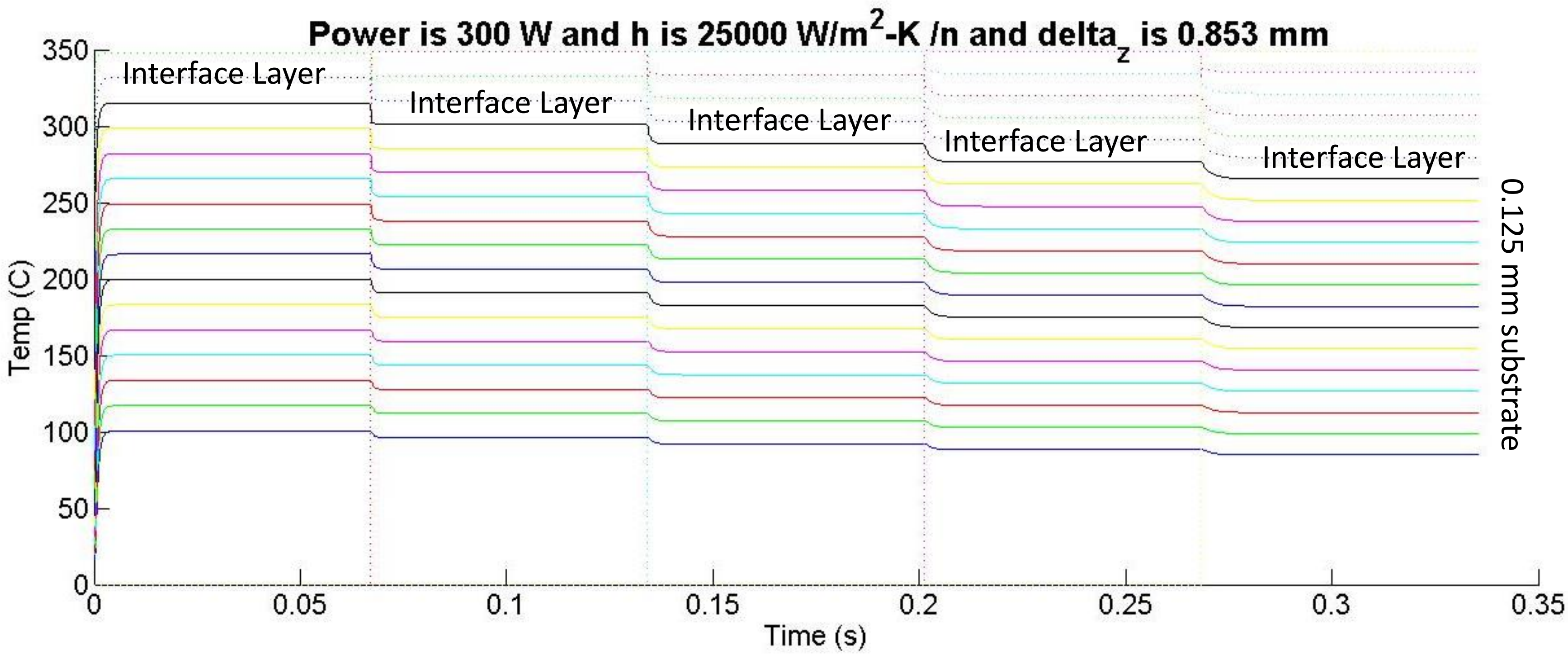
U.S. Army Research Laboratory
Contract #W911NF-10-2-0098

Danielle Belsito
dbelsito@wpi.edu

Baillie McNally
bamcnally@wpi.edu

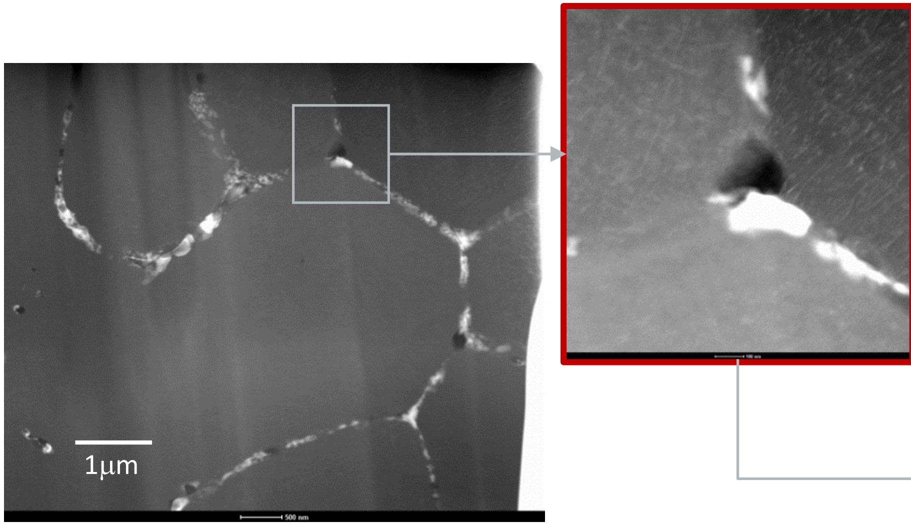
Thank You

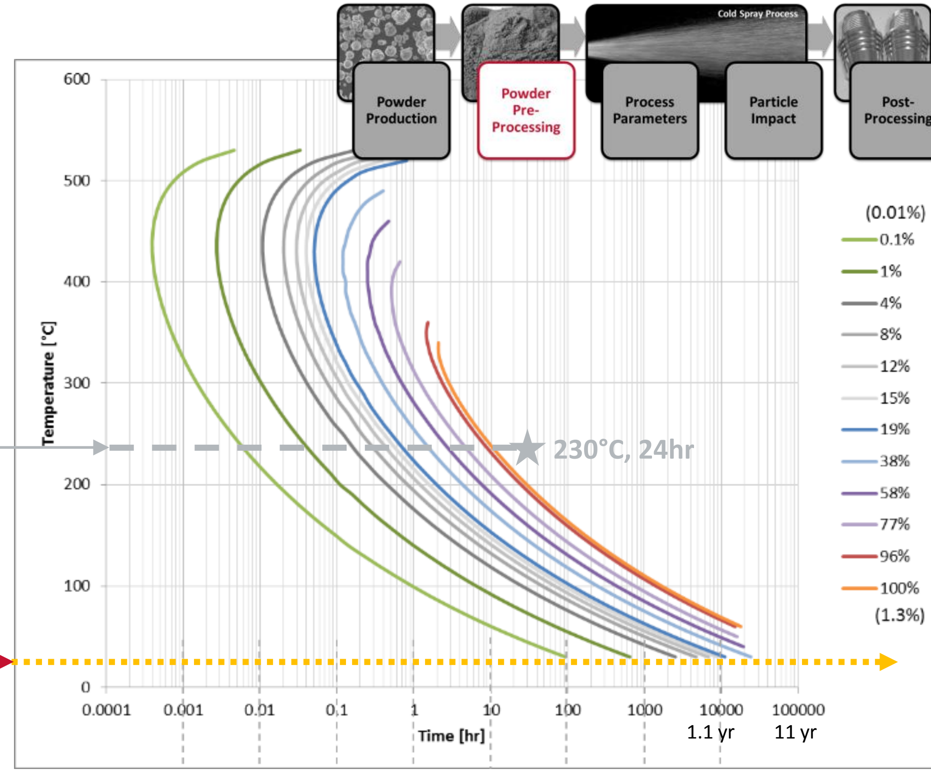
LACS Modeling: Ongoing Work



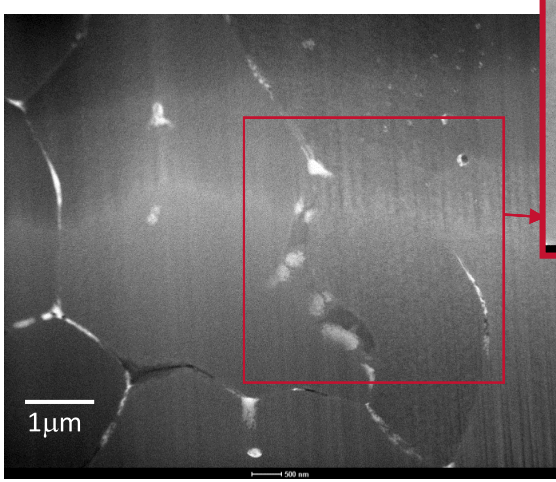
- 1D Laser Heat Flux Model
- Provides Temperature of Substrate/Deposited Material Over Time

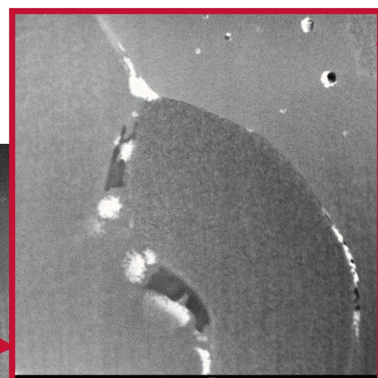
Powder Pre-Processing: Heat Treatment





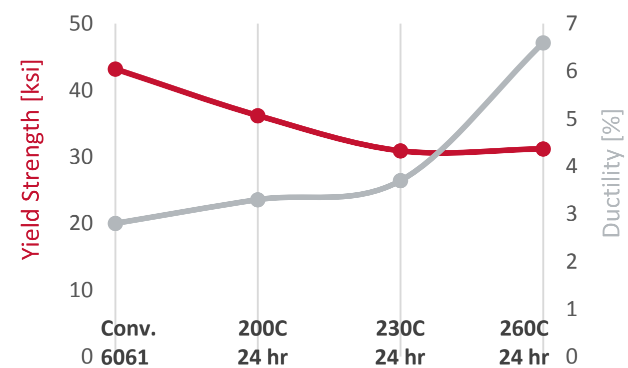
TEM of Al 6061 powders
<u>Above</u>: Heat treated at 230C, 24 hr
<u>Below</u>: No heat treatment





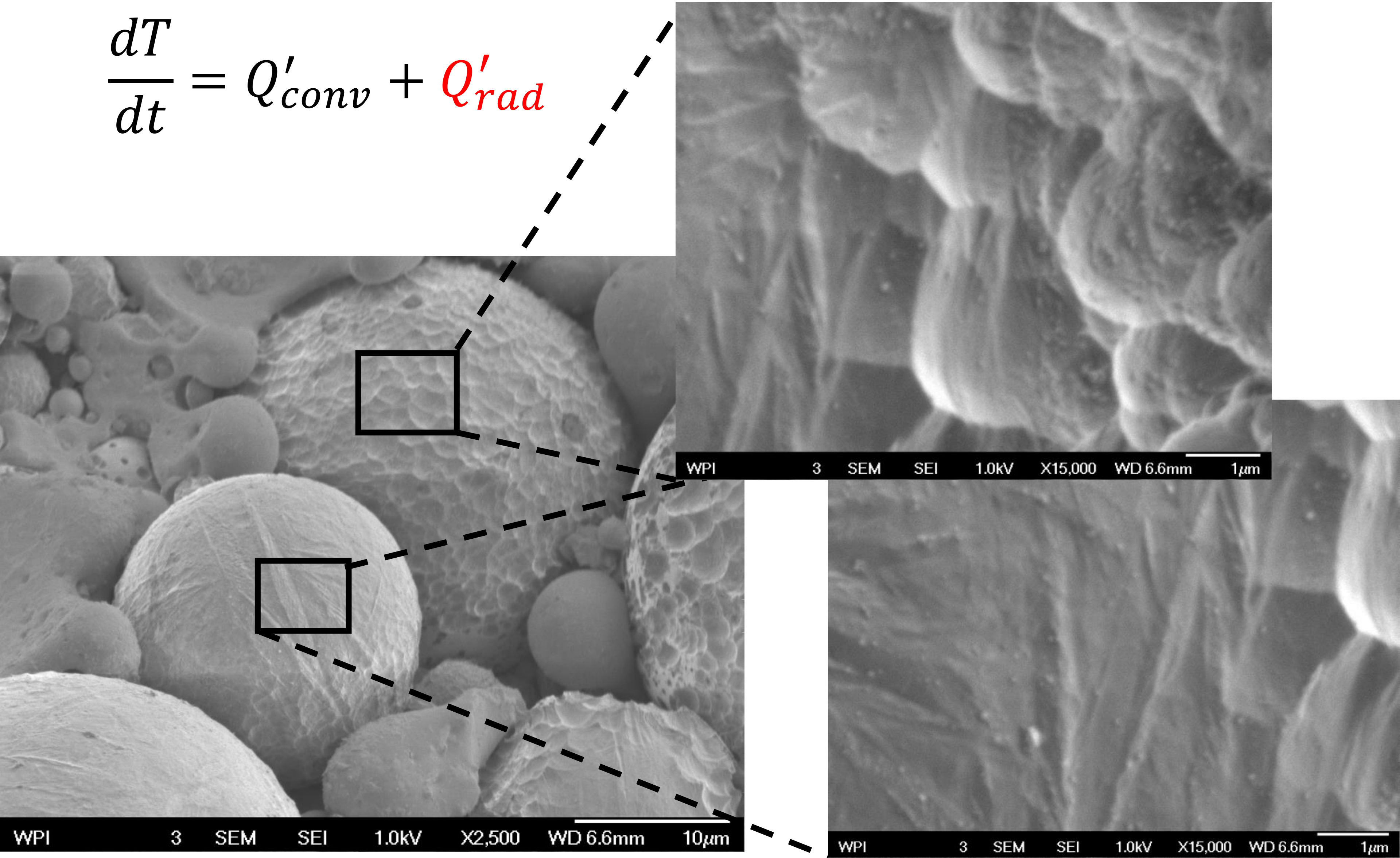
Metastable Mg2Si Phases

Heat treating powder increases rate of stable Mg2Si formation



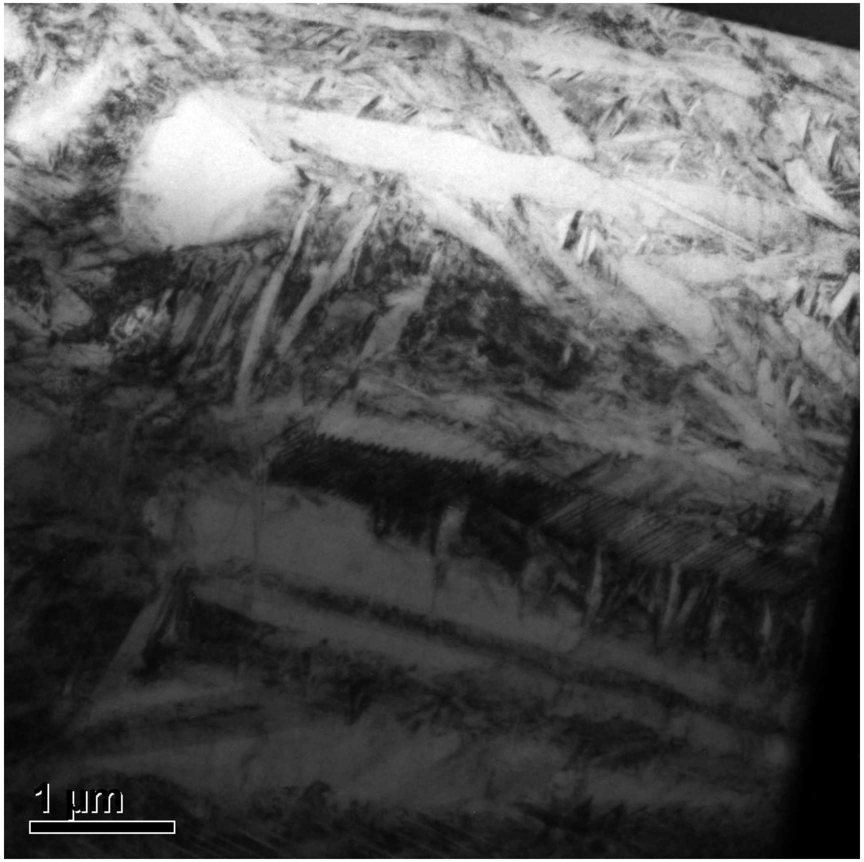
Plasma Atomized Ti-6Al-4V Etched Powder

$$\frac{dT}{dt} = Q'_{conv} + Q'_{rad}$$

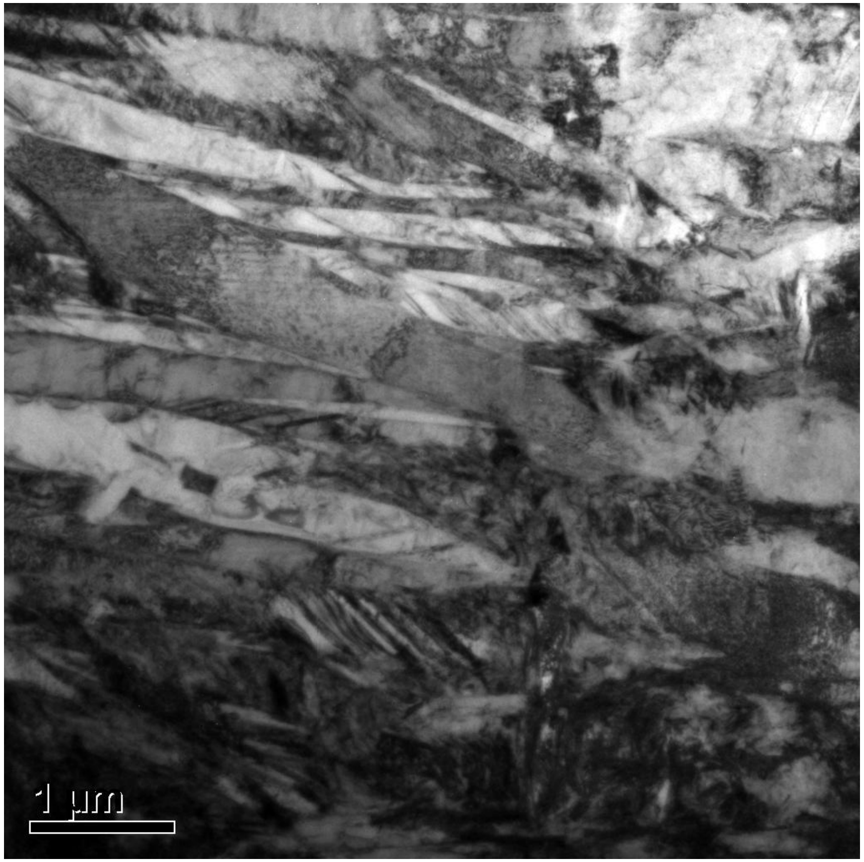


Additive Hardness Model: Additional Terms

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



- 33 micrometer
- Plasma Atomized
- Ti-6Al-4V



- 14micrometer
- Plasma Atomized
- Ti-6Al-4V