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# Development of an Accelerated Insertion of Materials (AIM) System for an Aluminum Extrusion

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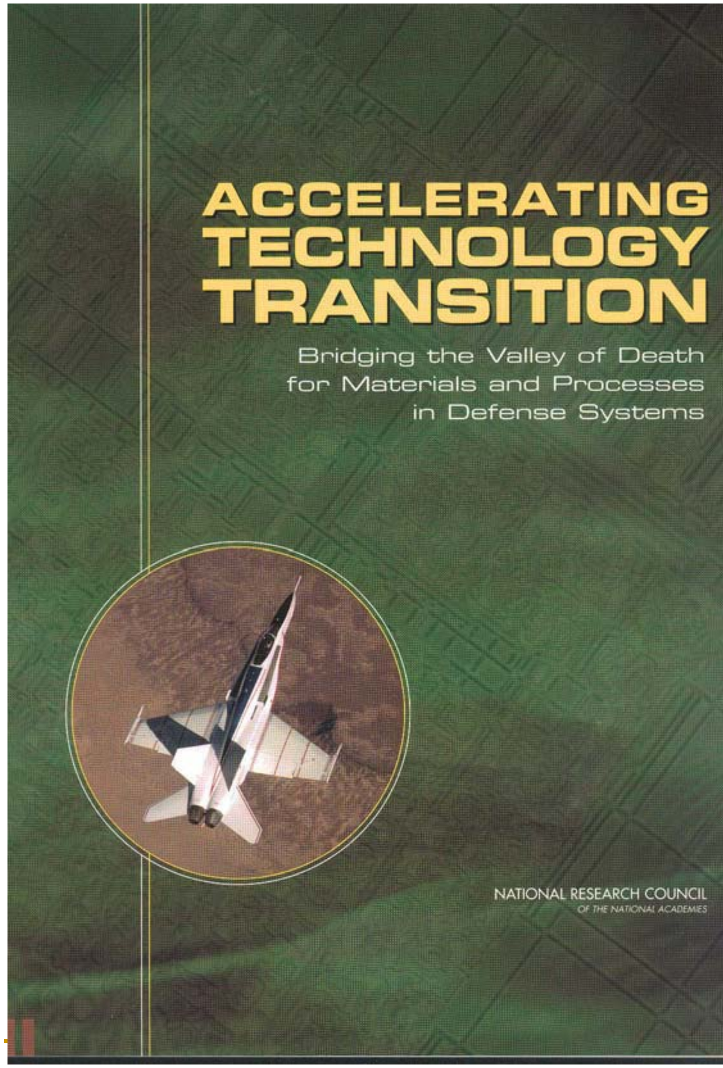
# Overview

- Computational Materials Science:
  A natural and important advance in the evolution of materials technology
  - Accelerated Insertion of Materials
  - Materials Engineering for Affordable New Systems
  - Integrated Computational Materials Engineering
  - Through Process Modeling
- Important to Navy:  developing internal capability
- Insight into development process
  - Appropriate goals for system demonstration/application
  - Commitment to infrastructure (hardware, software, trained personnel)
  - System architecture that makes sense
  - Knowledge base—processing and physical metallurgy

# Technology Transition




Technology transition is a generic problem, including materials technologies

- General need to accelerate the transition from science into engineering practice
- Computational systems are natural approach
- MSE community needs to embrace, develop coherent framework→CICME

**http://www7.nationalacademies.org/nmab/CICME_home_page.html**

# Importance to Navy

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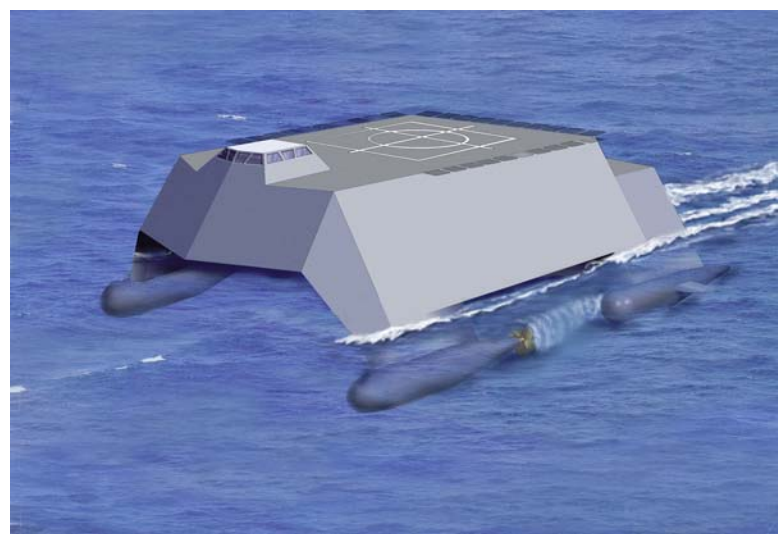
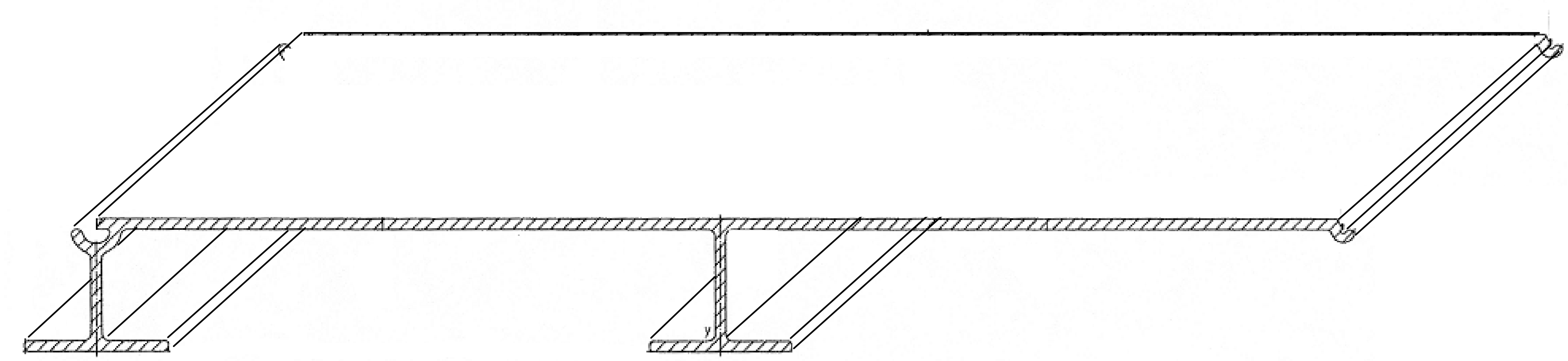
DEPARTMENT OF THE NAVY ONR Science & Technology

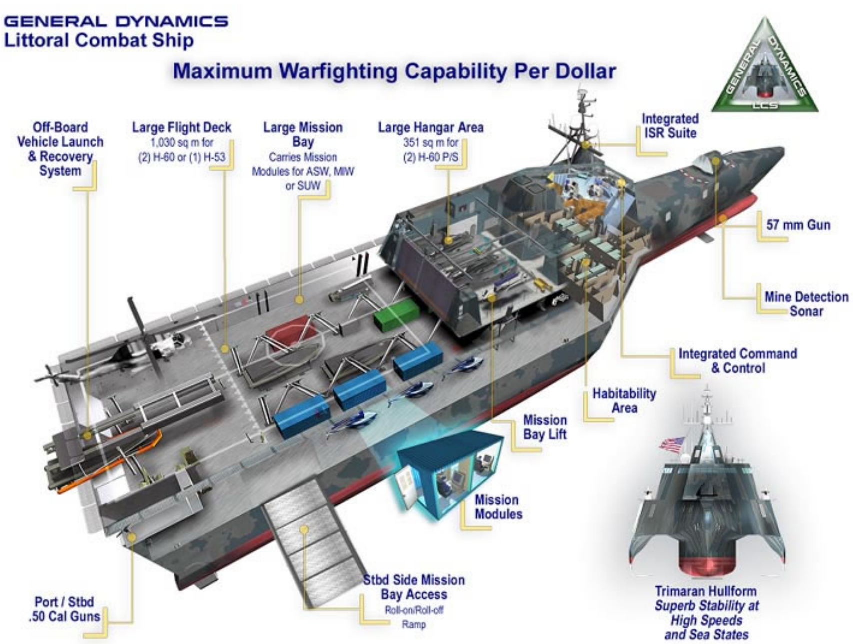
- Reduced cost of testing and evaluation
- Reduced risk
- Rapid insertion: advantages over enemy's systems
    - Mobility
    - Survivability
    - Lethality



# System Demonstration








AA6082 Sidewall Panels for LCS

(1% Si, 0.9% Mg, 0.7% Mn)

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# System Demonstration

Department of the Navy ONR Science & Technology

Issues :

- Tradeoff between enough difficulty to show something substantial, yet easy enough to accomplish in ~2 years
- 6000 series alloy → opportunity to model both extrusion process and microstructural transformations
- Existing data
- Prior or published understanding of physical metallurgy
- Target properties kept simple:  hardness and tensile/yield strength

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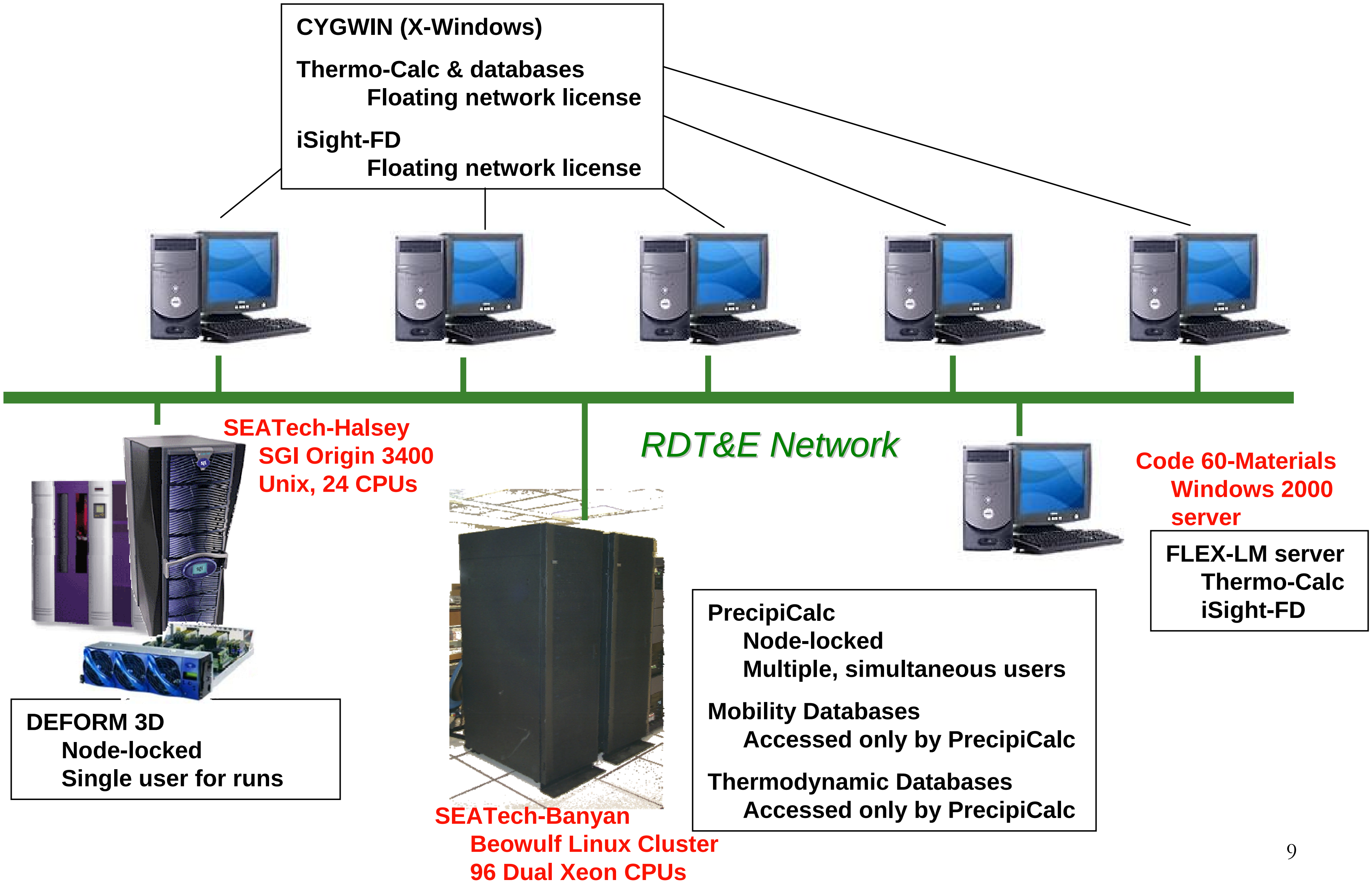
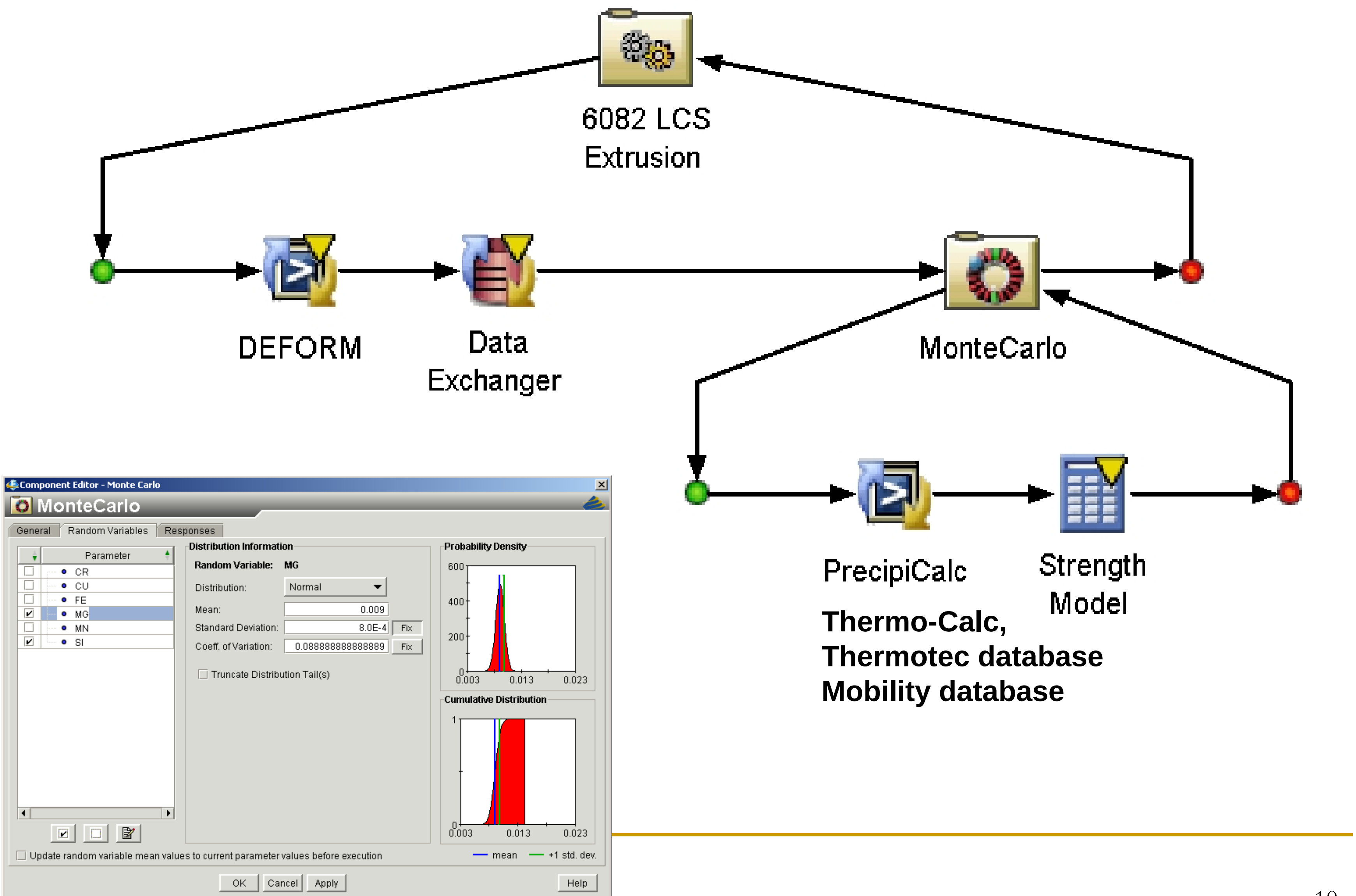
# Infrastructure:
## Minimal Software Configuration

| Software package | Use |
|---|---|
| Thermo-Calc | Thermodynamic phase equilibria |
| MOB2 | Mobility database for kinetics |
| ThermoTec TTAL | Aluminum thermodynamic database |
| PrecipiCalc | NGC of precipitate phases and size distributions |
| DEFORM | Deformation and heat treatment<br>Recrystallization modeling |
| Custom software | Strength model based on microstructure |
| ISIGHT | Process Integration and Design Optimization |

# System Architecture



# Mechanics of Operation



# Knowledge Base

- Compositional variations
- Processing parameters
- Physics of deformation and heat treatment operation
- Recrystallization and precipitation models
- Relationships between microstructure and strength
- Microstructural data (e.g., initial precipitate distribution)
- Microstructural and mechanical data to verify numerical results

# Knowledge Base
## Process Parameters

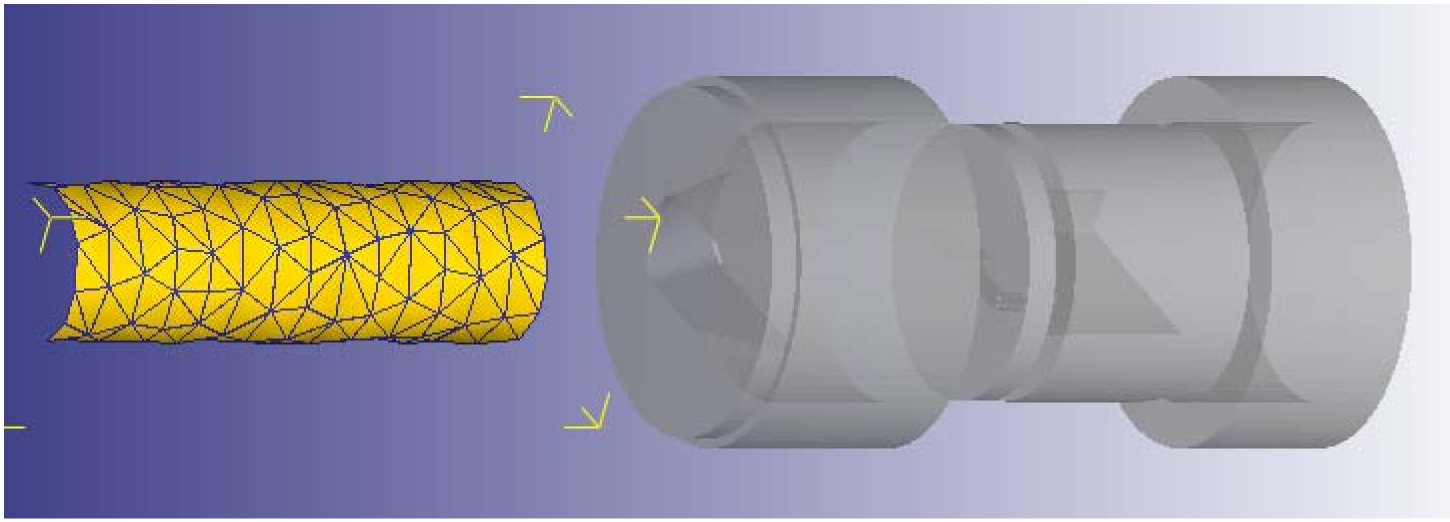
Sensitive information

- Profile drawing
- Die drawings
- Thermal conditions of extruder components
- Billet dimensions and temperatures
- Ram speed
- Quenching rates
- Aging times and temperatures
- Billet microstructure

Material for analysis and validation of models

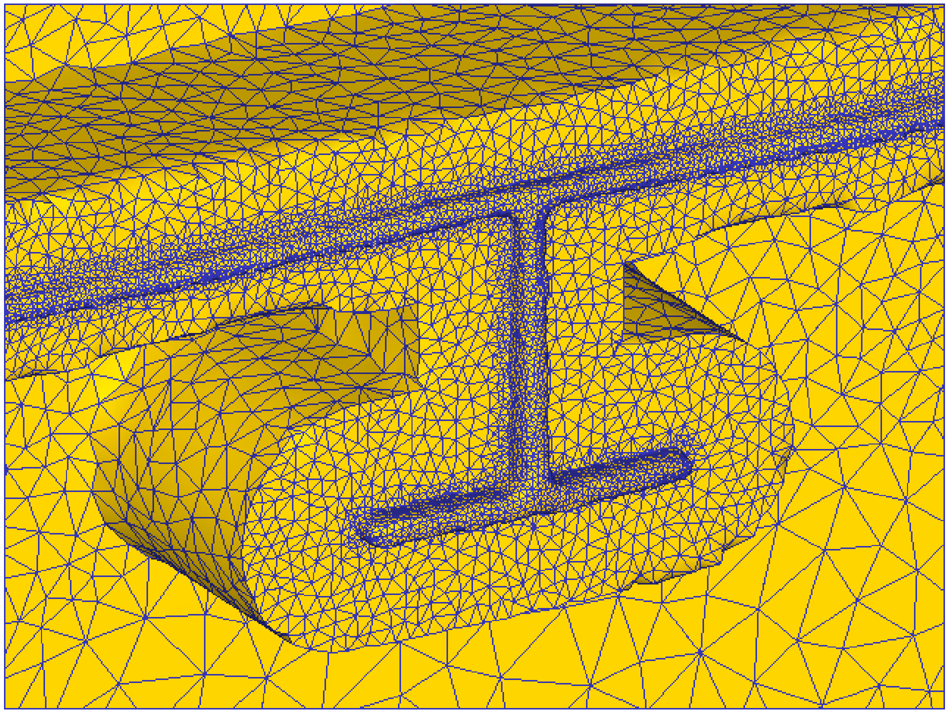
# Extrusion simulation

- 3D problem
- Lagrangian formulation
- > 50:1 reduction
- Work still in progress



# Extrusion Simulation



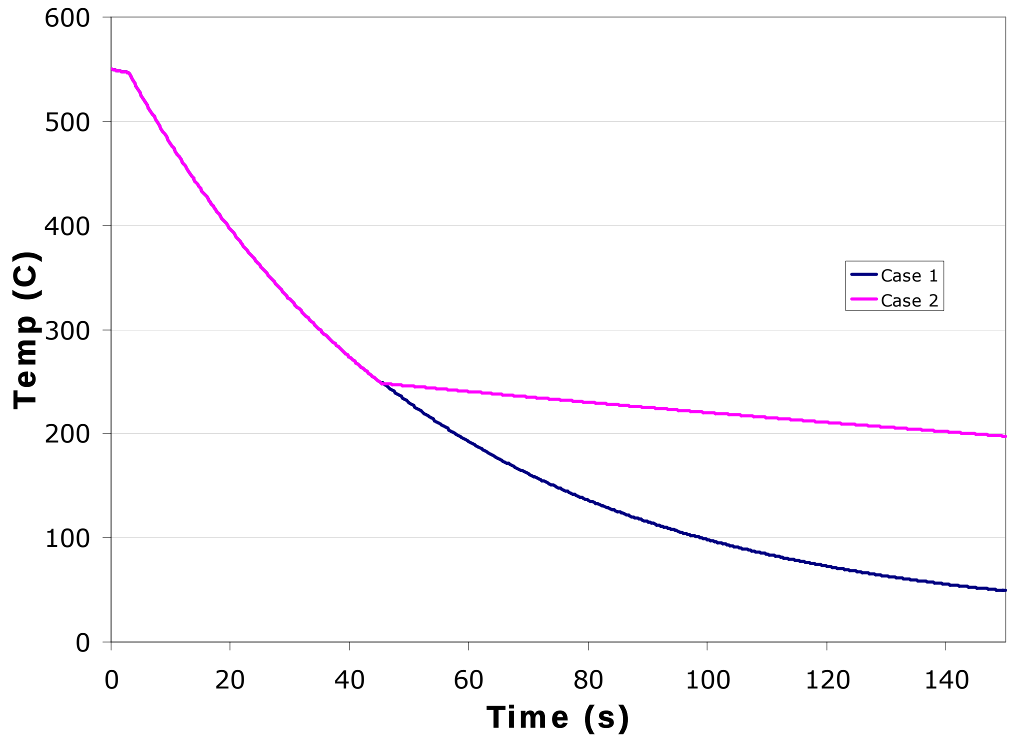


# Thermomechanical Modeling

## Analytic approximation

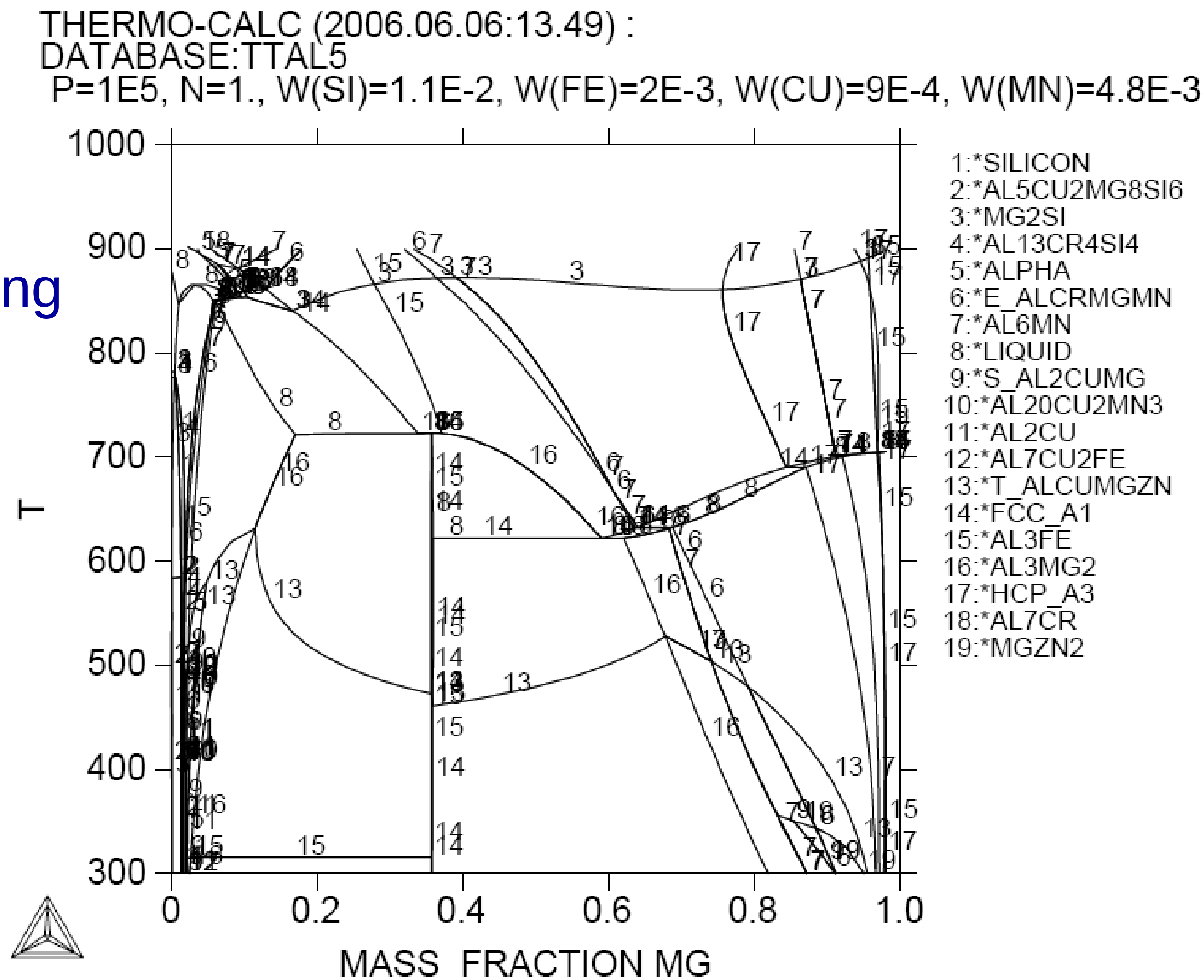
- Small Biot number → constant temperature through thickness
- Stagnant for first few seconds
- Then *h* based on maintaining 7ºC/sec

$$T(x) = (T_o - T_\infty) * \exp(-\frac{h}{\rho C_p w} t) + T_\infty$$



# Thermo-Calc
# ThermoTec TTAL database

- Understanding of phases before precipitation modeling
- Rejected all but:
  - **FCC_A1**
  - **ALPHA**
  - **MG2SI**

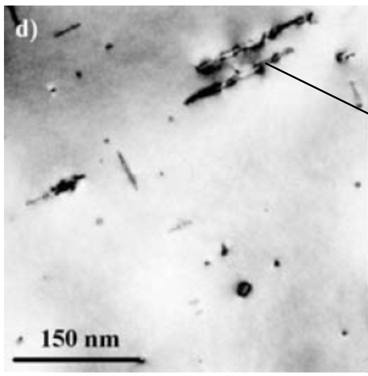


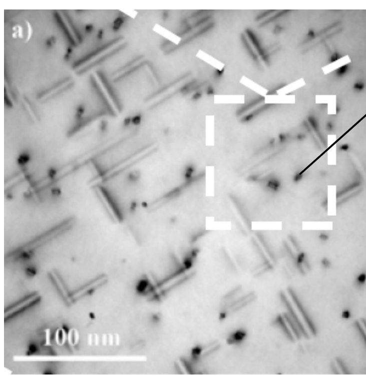
# Thermodynamics

- Aluminum matrix (FCC_A1)
  - 98.9 mole % Al with traces of the other elements in solid solution
- $\alpha$ (ALPHA, aka "Dispersoids")
  - $Al_{72}Si_{11}Mn_{10}Fe_4$
  - High temperature phase—present at all temps up to m.p.
  - Mn is primary dispersoid-former
- $\beta$, $\beta'$, $\beta''$ (MG2SI)
  - Thermodynamically stable below 498ºC

# Thermodynamics

## Actual composition of phases

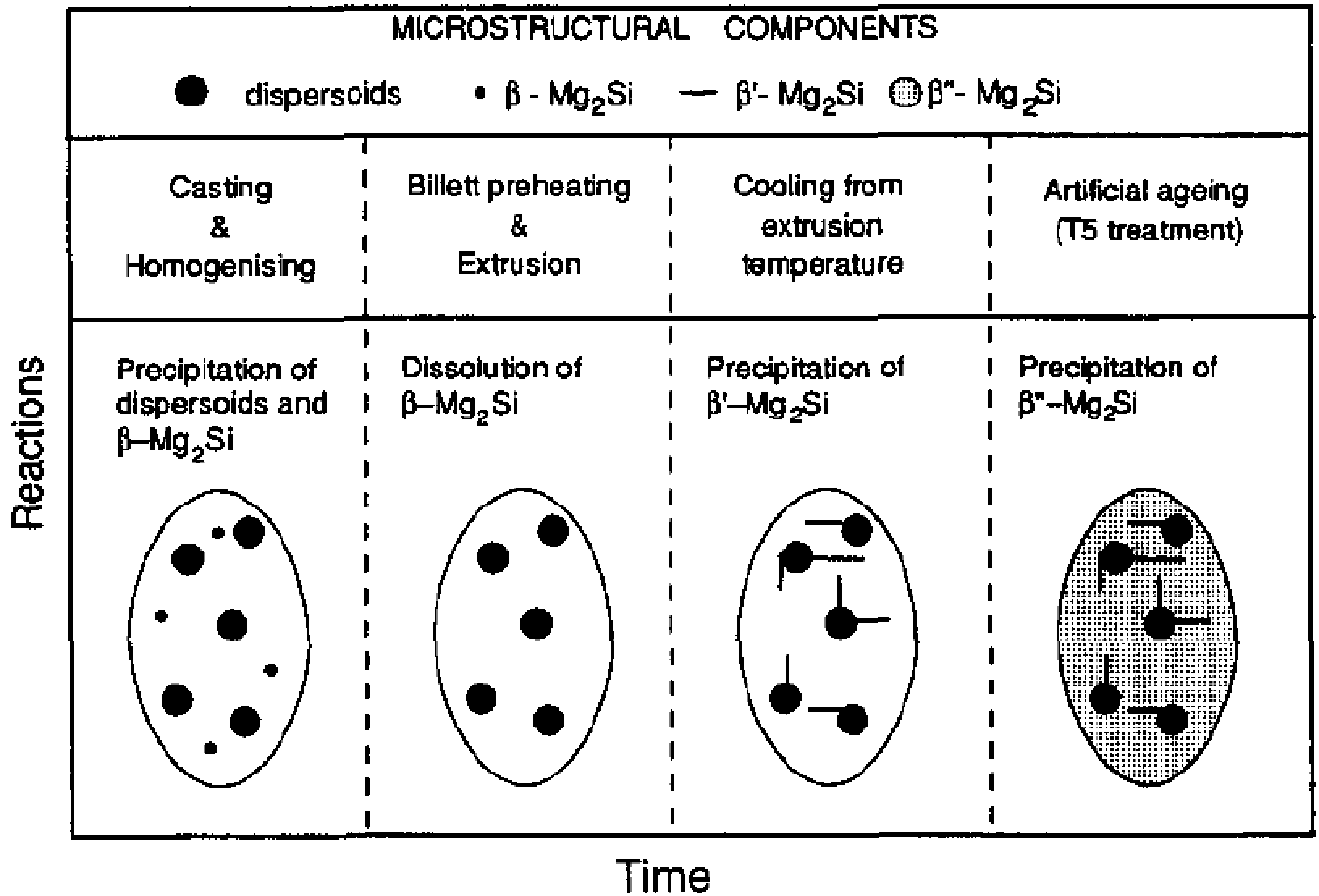



- $\beta$ ($Mg_2SI$)
- $\beta'$ ($Mg_5Si_3$)
  - Not available in ThermoTec database
- $\beta''$
  - $Mg_5Si_6$
  - Various measurements $Mg_{0.8\text{-}1.2}Si$
  - Not available in ThermoTec database

Myhr and Grong, "A Multiscale Modelling Approach to the Optimisation of Welding Conditions and Heat Treatment Schedules for Age Hardening Aluminium Alloys," Graz, 26 May 2005.

# Precipitation

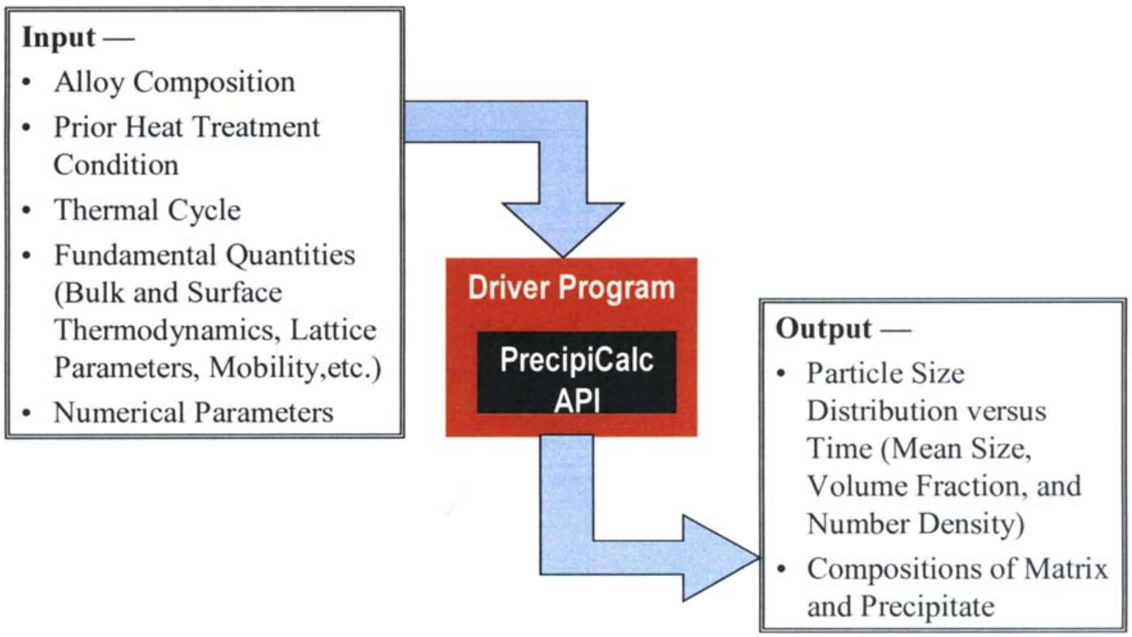



Bratland, et al., Acta Mat., v. 45, No. 1, pp.1-22, 1997.

# Precipitation Modeling

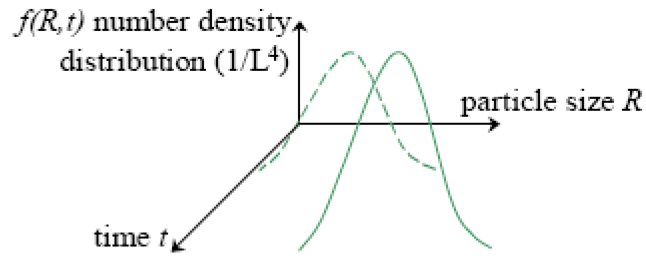
## Using PrecipiCalc to Model Precipitation

### *PrecipiCalc Input/Output*



# Precipitation Modeling

(a)




Continuity : $\frac{\partial f}{\partial t}+\frac{\partial\left(f\frac{dR}{dt}\right)}{\partial R}=e^{-\tau/t}\bar{J}_{SS}$

incubation time τ for transient nucleation

Mass Balance : $C_i^0=\frac{4\pi}{3}\int_0^\infty fR^3\bar{C}_i^\beta(R)dR+C_i^\infty(1-\phi)$ where $\phi=\frac{4\pi}{3}\int_0^\infty fR^3dR$

**Homogeneous nucleation**

**Multi-component interactions via Thermo-Calc**

**$Mg_2Si$**

Surface energy = 0.055 $J/m^2$

Lattice parameter = $4.034\times10^{-10}$ m

Molar volume = $3.9541\times10^{-5}$ $m^3/mol$

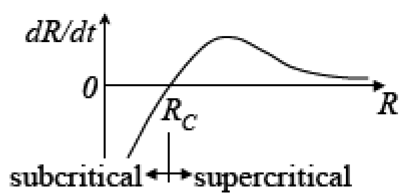
Nucleation dislocation density = $10^{25}$ $/m^3$

(b)

Growth : $\frac{dR}{dt}=\frac{\left(1+R\sqrt{4\pi N_v\langle R\rangle}\right)}{\left(R\Gamma+s(R)\Big/\left(M_0\exp\frac{-Q}{RT}\right)\right)}\left\{\Delta G_m-\frac{2\sigma(R)\bar{V}_m^\beta}{R}\right\}$

where $\Delta G_m=[\Delta C_i]^T\left[\frac{\partial^2\bar{G}^\alpha}{\partial C_i\partial C_j}\right][\Delta C_j^\infty]+[\bar{C}_\infty^\beta]\bullet\left([\bar{\mu}_m^\alpha]-[\bar{\mu}_m^\beta]\right)$

$\Gamma=[\Delta C_i]^T\left[\frac{\partial^2\bar{G}^\alpha}{\partial C_i\partial C_j}\right][D_{jk}]^{-1}[\Delta C_k^\alpha]$




Thermodynamics

Diffusivity

Interfacial Property

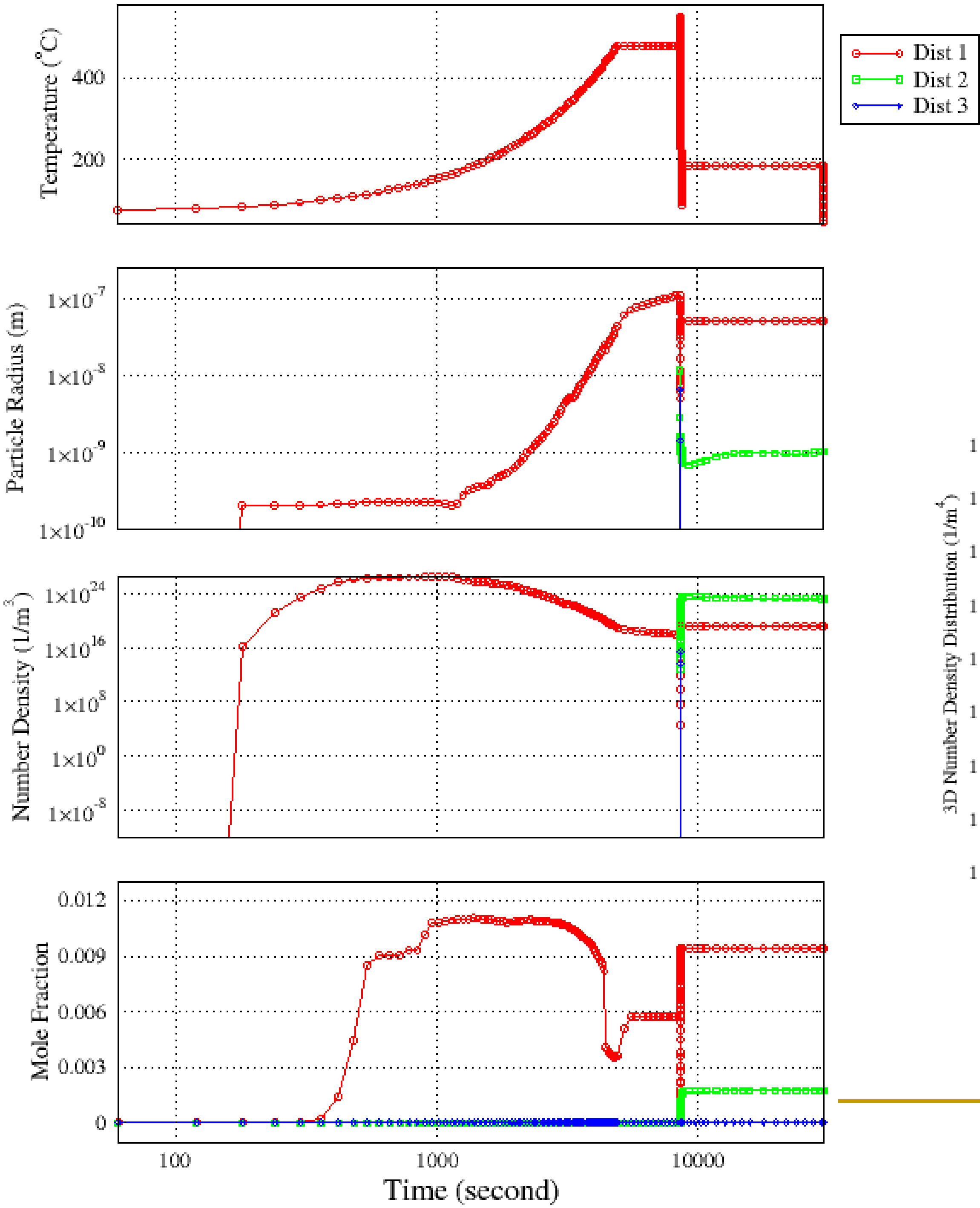
Steady State Nucleation Rate $J_{SS}=Z\beta^*\frac{N_a}{V_m^\beta}e^{\frac{-W_R^*}{k_BT}}=\int_0^\infty\bar{J}_{SS}(R)dR$

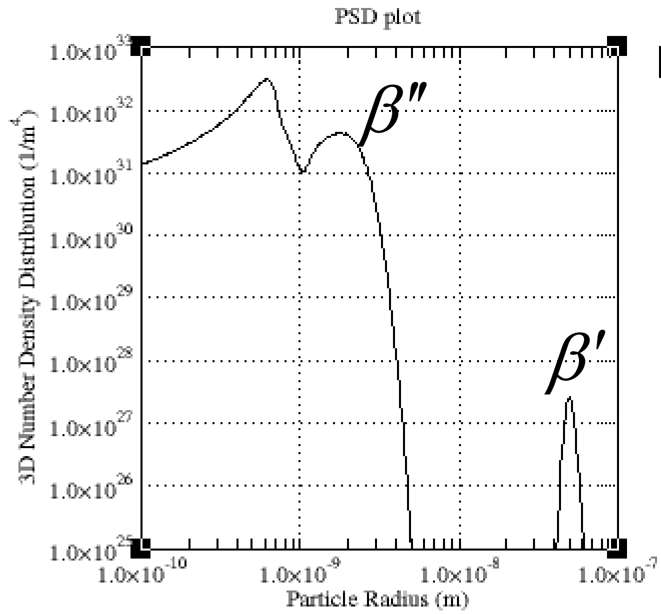
Incubation Time $\tau$ calculated from

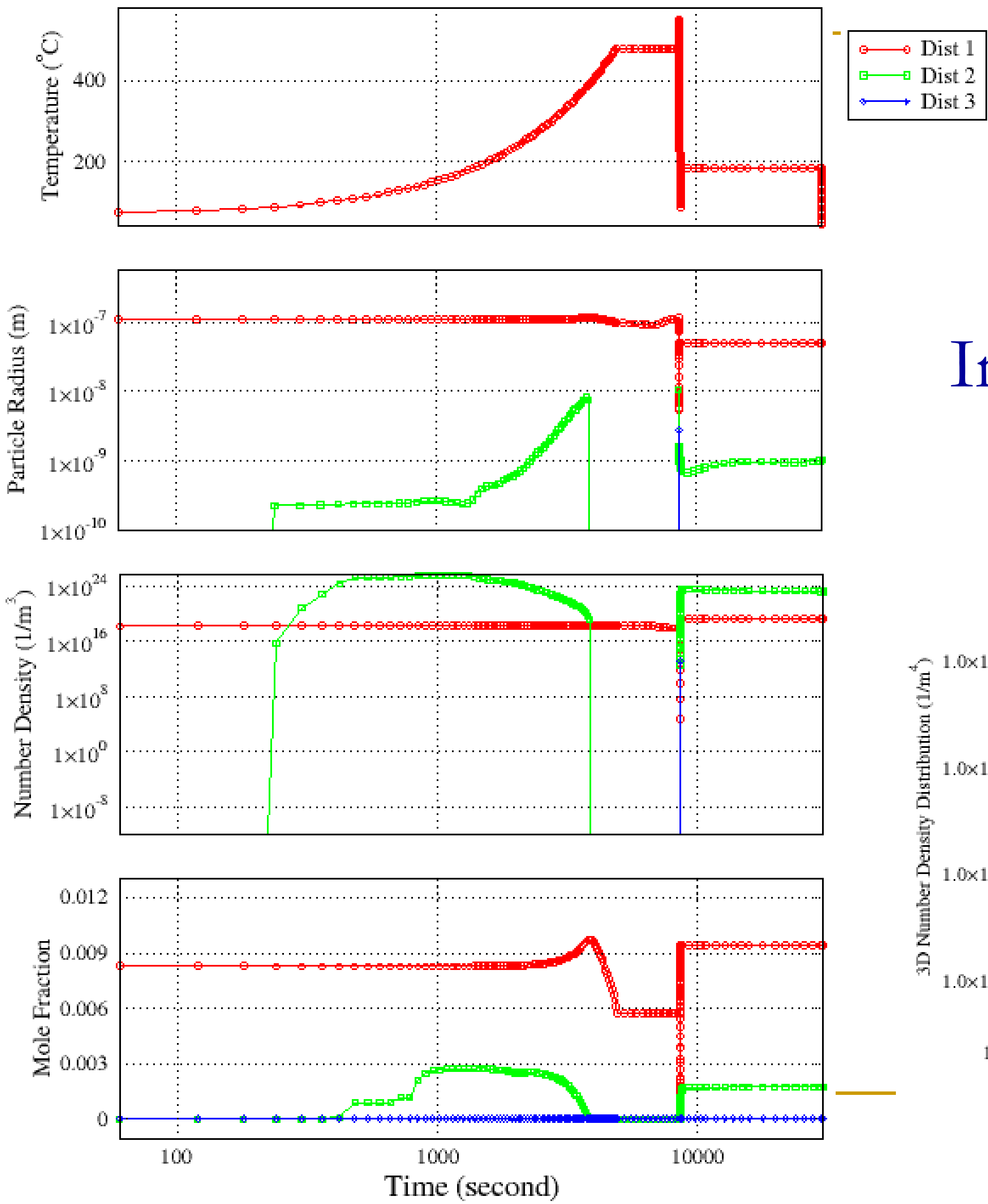
$$\begin{cases}\int_0^t\beta^*(t')dt'=\frac{1}{\theta Z(t)^2}, & \text{if } \tau<t\\ \int_0^\tau\beta^*(t')dt'+\beta^*(t)(\tau-t)=\frac{1}{\theta Z(t)^2}, & \text{if } \tau>t\end{cases}\text{, where } 2<\theta<4\pi$$

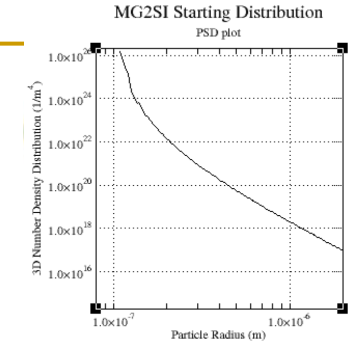
which gives $\tau=\frac{1}{\theta\beta^*Z^2}$, at isothermal conditions.

# Exemplar Result

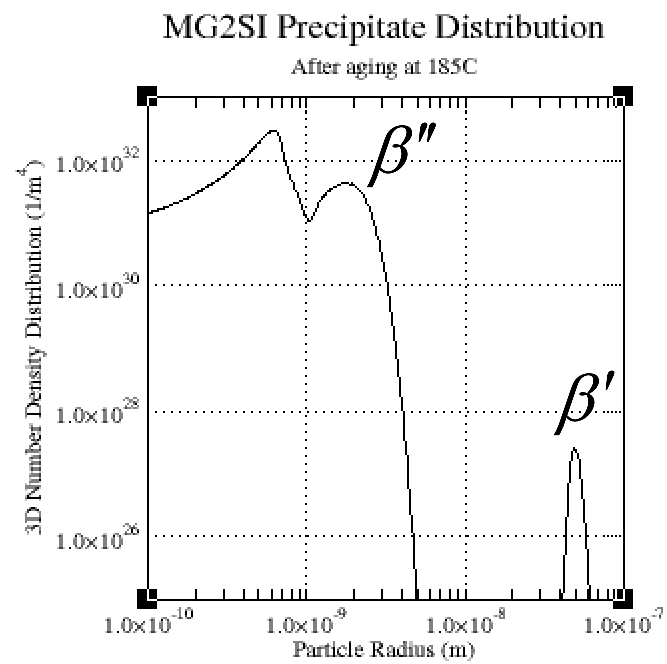


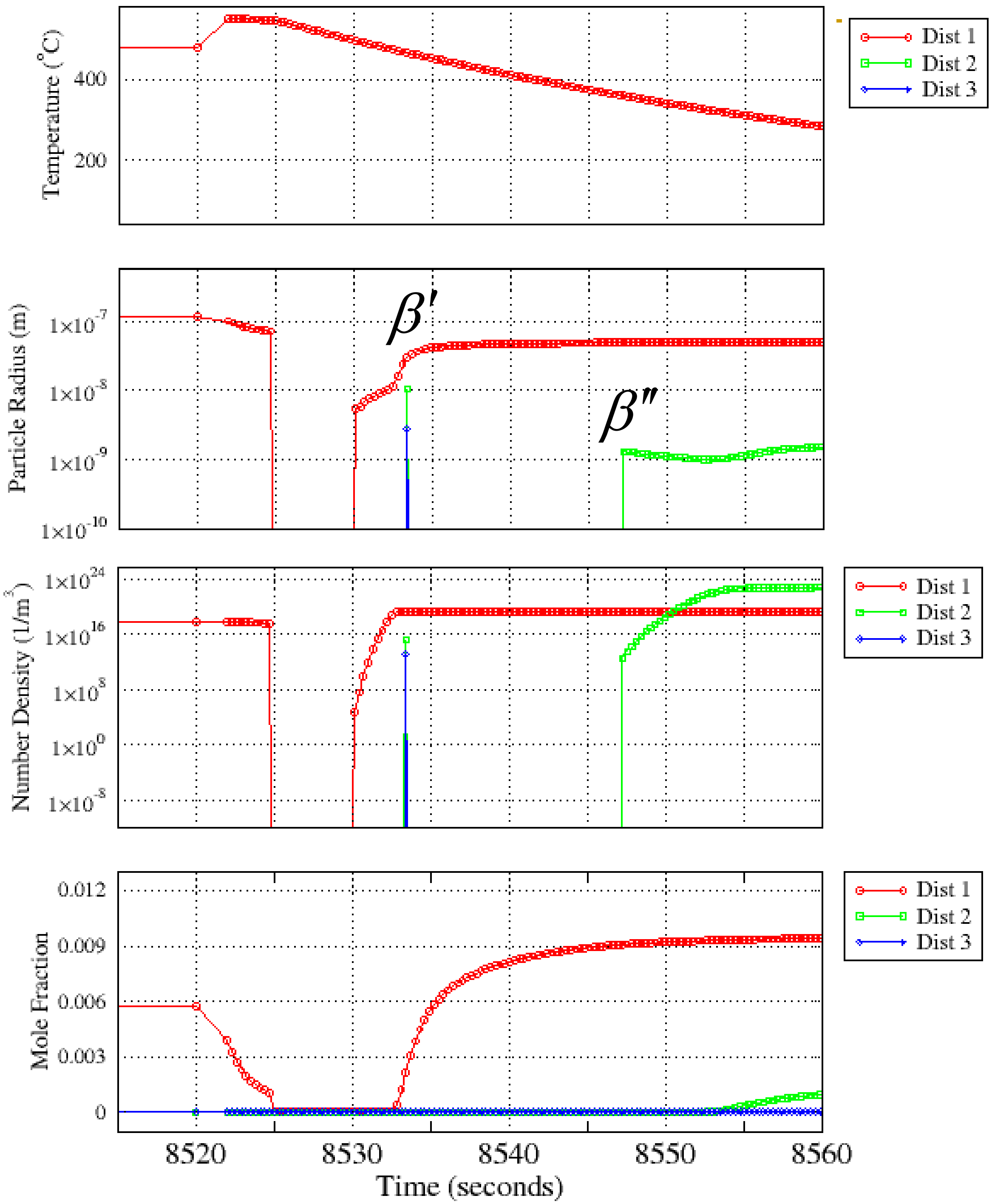



# Initial Distribution Specified

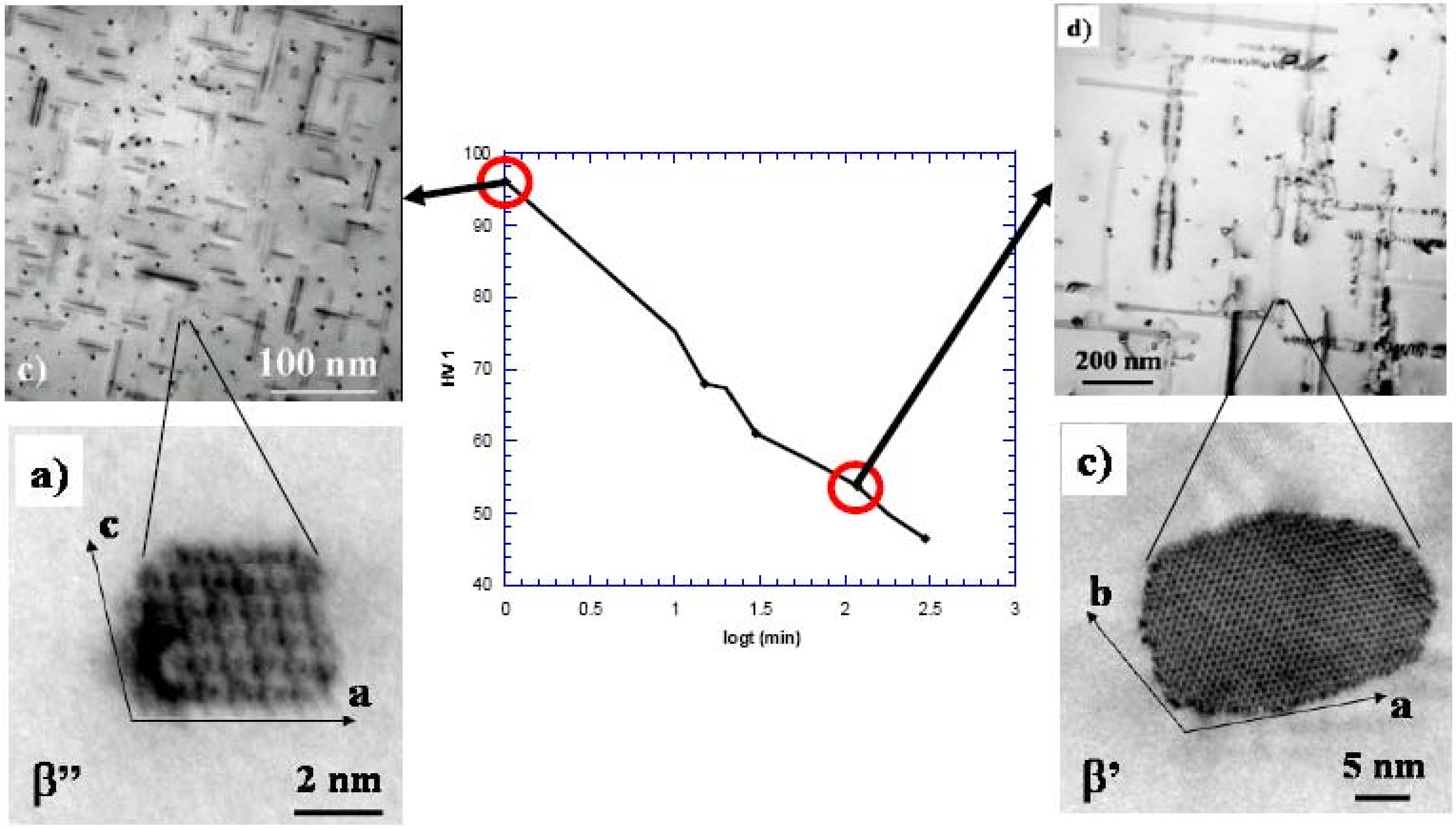


# Quench



Temperature (°C)
400
200
Dist 1
Dist 2
Dist 3
Particle Radius (m)
1x10^-7
1x10^-8
1x10^-9
1x10^-10
β′
β″
Number Density (1/m^3)
1x10^24
1x10^16
1x10^8
1x10^0
1x10^-8
Dist 1
Dist 2
Dist 3
Mole Fraction
0.012
0.009
0.006
0.003
0
Dist 1
Dist 2
Dist 3
8520
8530
8540
8550
8560
Time (seconds)

# Precipitation




Hardness curve (middle) shows the dissolution/transformation of a β" microstructure (left) into β' (right). The material softens because the β' rods are less efficient in opposing dislocation movement due to their incoherent interface with the matrix.

www.sintef.no/static/mt/images/precipitation.pdf

# Strength Model

$$\sigma_y = \sigma_i + \sigma_{ss} + \sigma_p$$

$$\sigma_p = \frac{M}{b\bar{r}}\left(2\beta G b^2\right)^{-1/2}\left(\frac{3f}{2\pi}\right)^{1/2}\bar{F}^{3/2}$$

$$\bar{F} = \frac{\sum_i N_i F_i}{\sum_i N_i}$$

Shearable particles, $r_i < r_c$

$$\bar{F}_i = 2\beta G b^2\left(\frac{r_i}{r_c}\right)$$

Strong, non-shearable particles, $r_i > r_c$

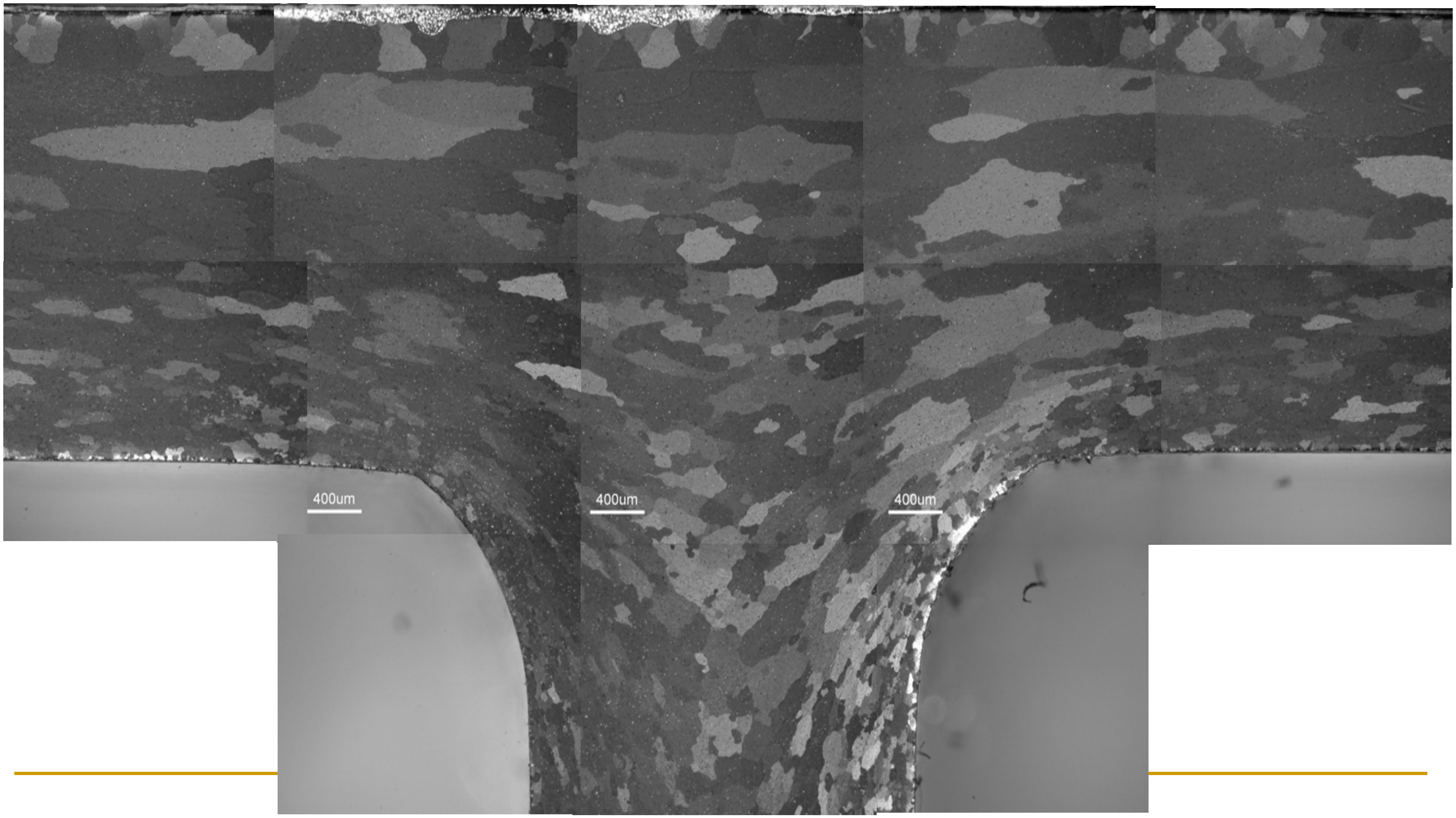
$$\bar{F}_i = 2\beta G b^2$$

| | |
|---|---|
| $M$ | Taylor factor, 3.1 |
| $r_c$ | critical radius, $5 \times 10^{-9}$ m |
| $b$ | Burgers vector, $2.84 \times 10^{-10}$ m |
| $G$ | shear modulus, $2.7 \times 10^{10}$ N/m$^2$ |
| $\beta$ | constant, 0.36 |
| $f$ | volume fraction |
| $\bar{F}$ | mean interaction force between dislocations and particles |

Myhr, et al., "Modelling of the Age Hardening Behaviour of Al-Mg-Si Alloys," Acta Materialia, 49 (2001) 65-75.

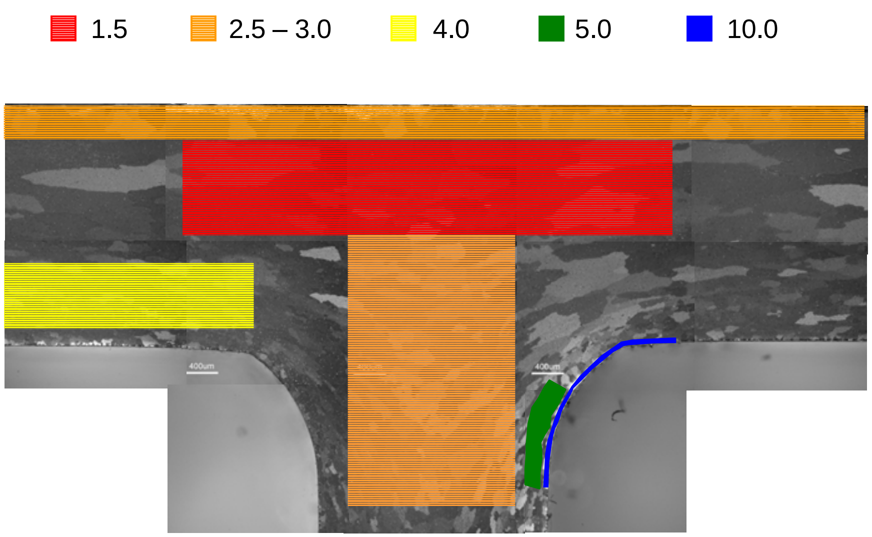
# Metallography

**Grain size differences indicate influence of strain history**

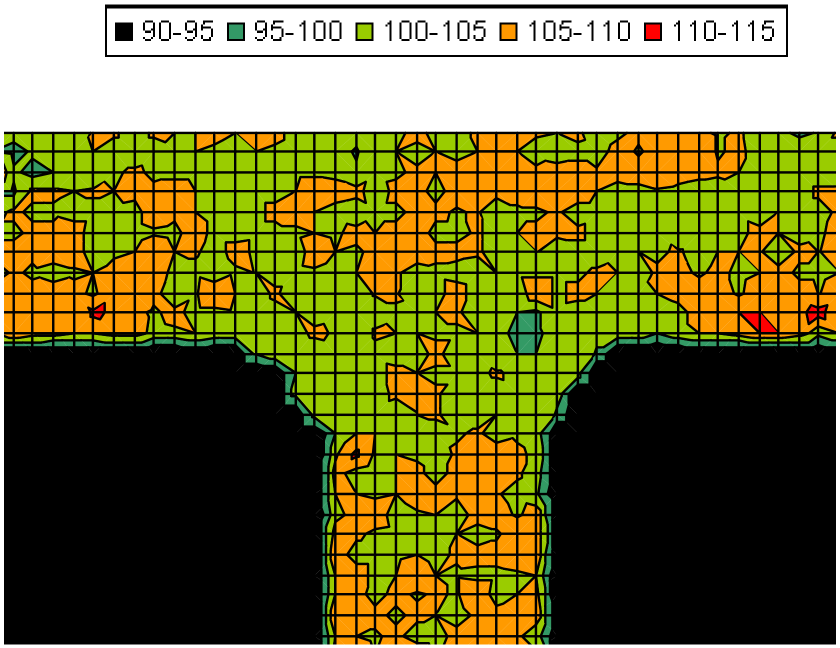


# Metallography

**No correlation between grain size and hardness (HV)**




**Grain size map (ASTM numbers)**




**Hardness map (HV)**

# Remaining Work

- Complete DEFORM development
  - Vary speed, quench conditions
- Integrate DEFORM using iSight-FD
- Complete strength model and verify against published data (tune PrecipiCalc)
- Reconcile hardness variation with model results
- Fully-coupled runs, generate response surface

# Summary

- Computational Materials Science: important advance
- Navy committed to developing capability
- Application balances difficulty vs. substantial result
- Built infrastructure with iSight, Thermo-Calc, PrecipiCalc, DEFORM 3D, Custom microstructure model, databases
- Networked system based on available resources
- Thermal history, extrusion process→precipitate distribution
- PrecipiCalc can predict realistic $\beta'$ *and* $\beta''$ distributions
- Precipitate size distribution influences strength
- Actual part shows strength variations to be reconciled with models

# Sponsors

**Dr. Julie Christodoulou, ONR Code 332**

**NSWCCD Code 61 Technology Enterprise**

**NSWCCD Code 0020 Bid & Proposal**