Precipitation Simulation of Ni-base Superalloys

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Outline of Presentation

I. Background

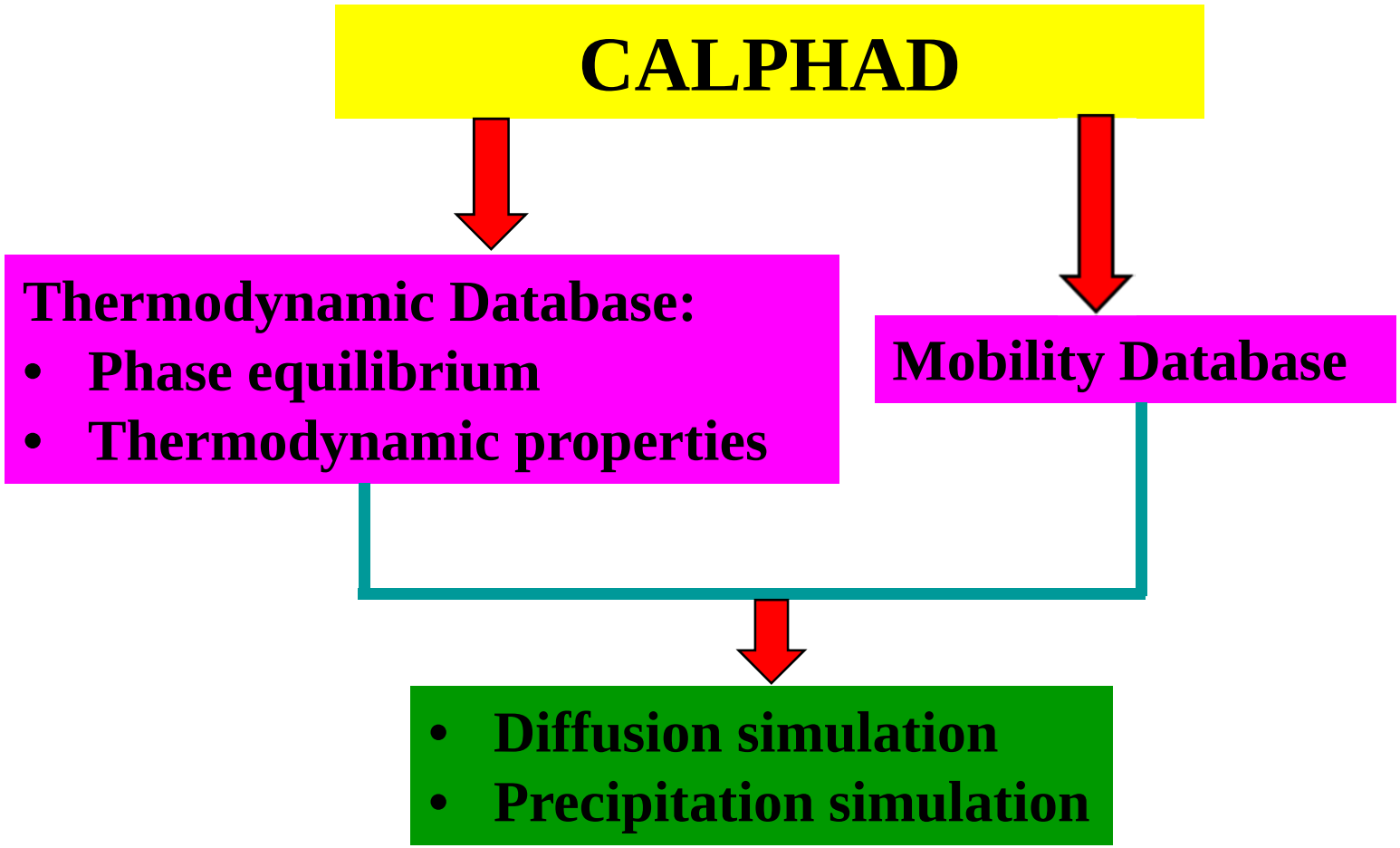
- Extension of the CALPHAD approach
- Precipitation Kinetics

II. Application to Ni-base Superalloys

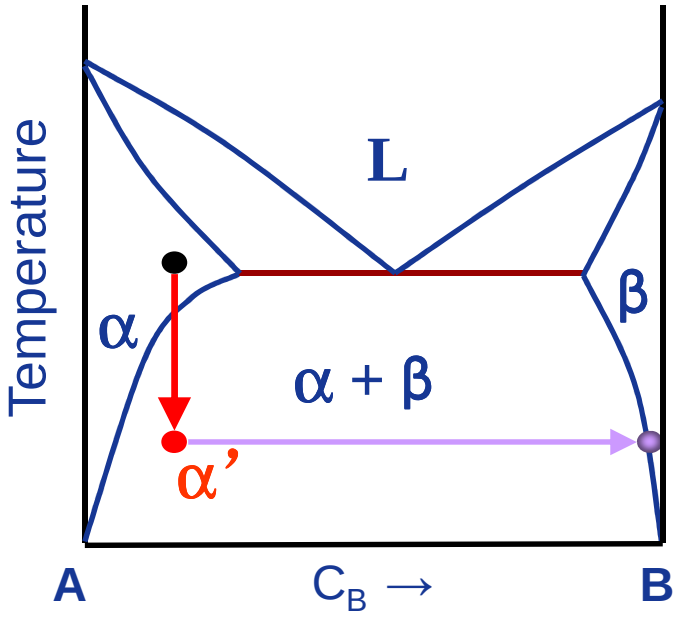
- Ni-Al-Cr system
- Commercial alloys: Rene88, IN100, U720, Alloy718

III. Summary

Beyond Phase Diagrams



Precipitation Simulation

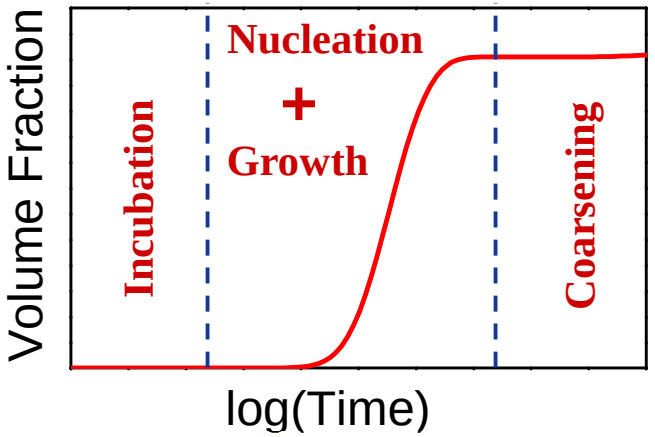


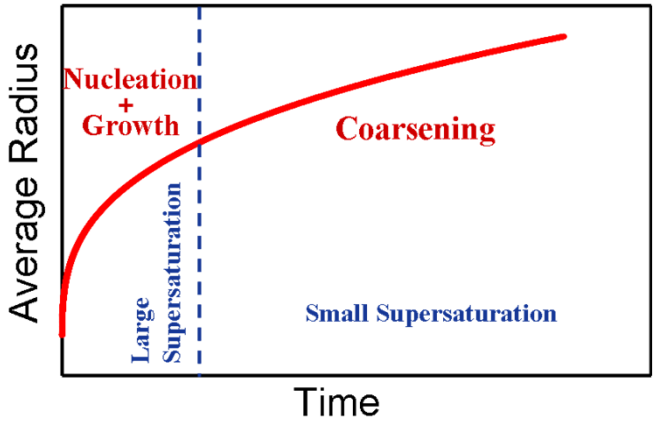
$$\alpha' \rightarrow \alpha + \beta$$

α' : matrix phase (supersaturated)

β: precipitate phase

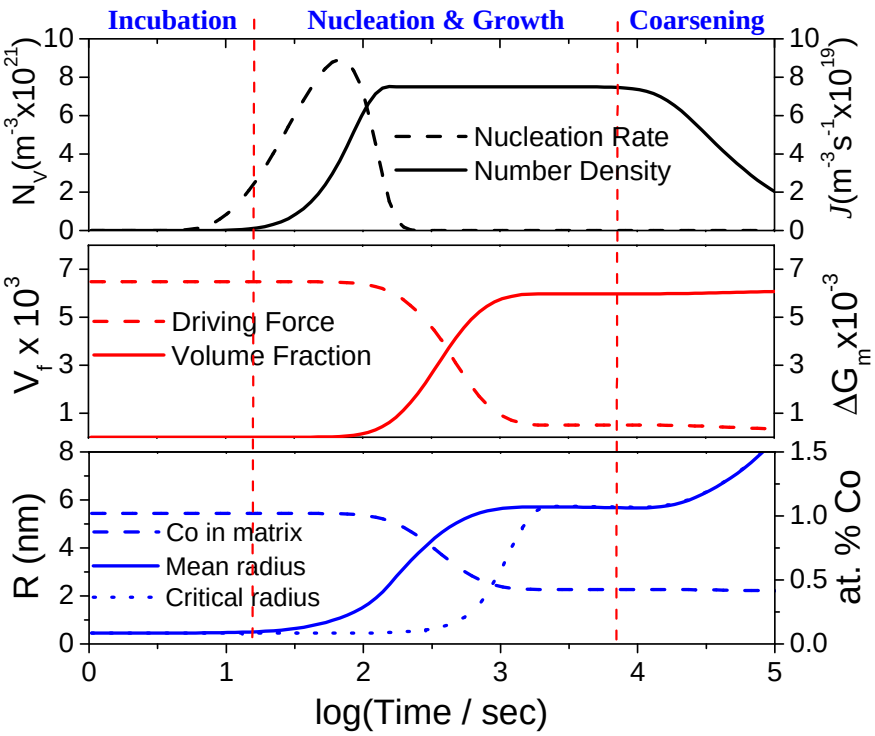
α: stable solid solution



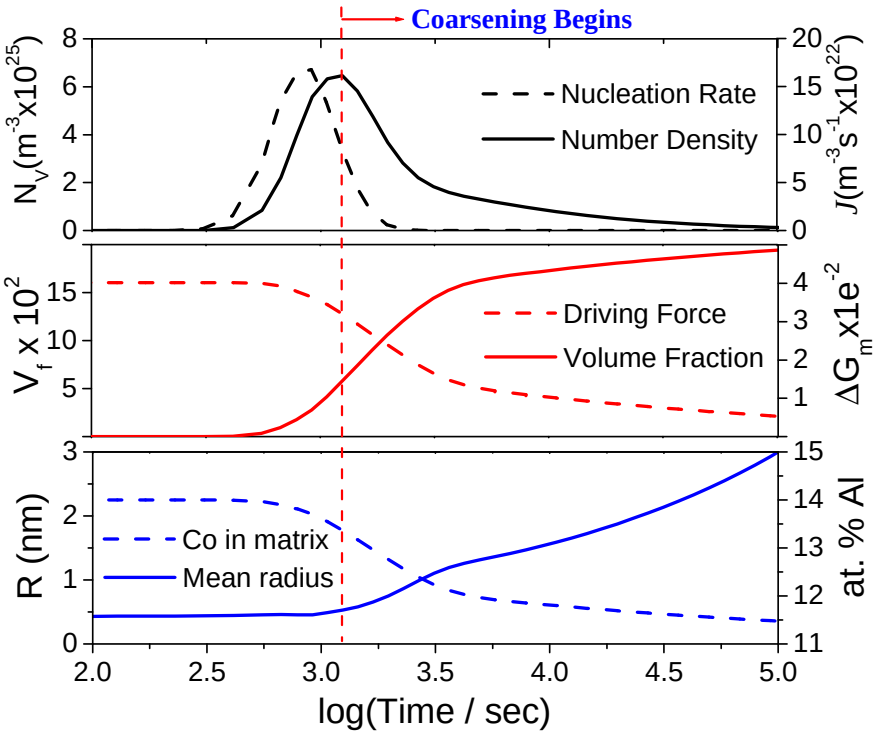


☞ **Smooth integration of precipitation simulation with thermodynamic calculation engine**

Concurrent Nucleation, Growth and Coarsening



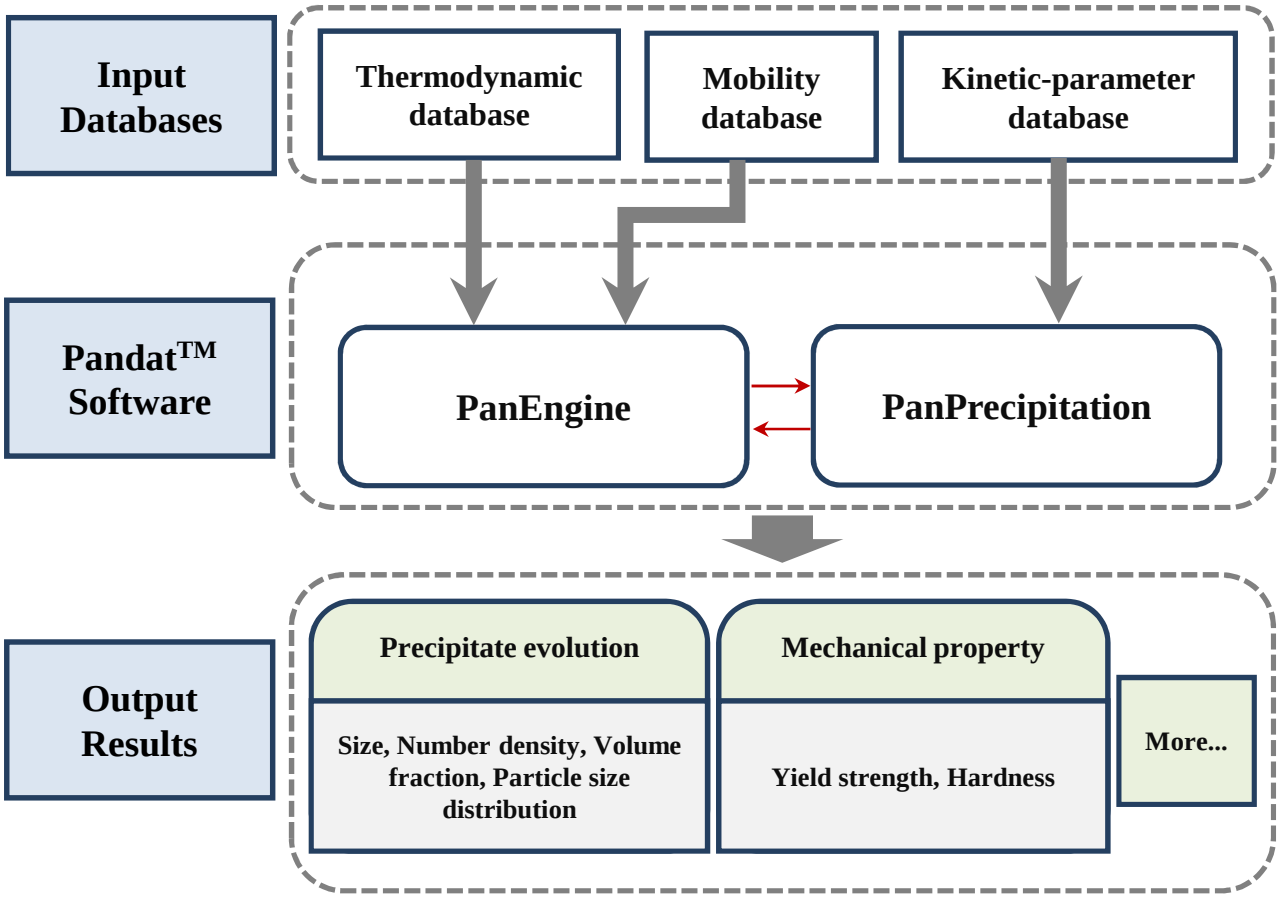
Precipitation evolution of the Cu-1.02 at.% Co alloy ageing at 600°C



Precipitation evolution of the Ni-14 at.% Al alloy ageing at 550°C

☞ **Concurrent nucleation, growth & coarsening**

CALPAHD Tool: Pandat Software



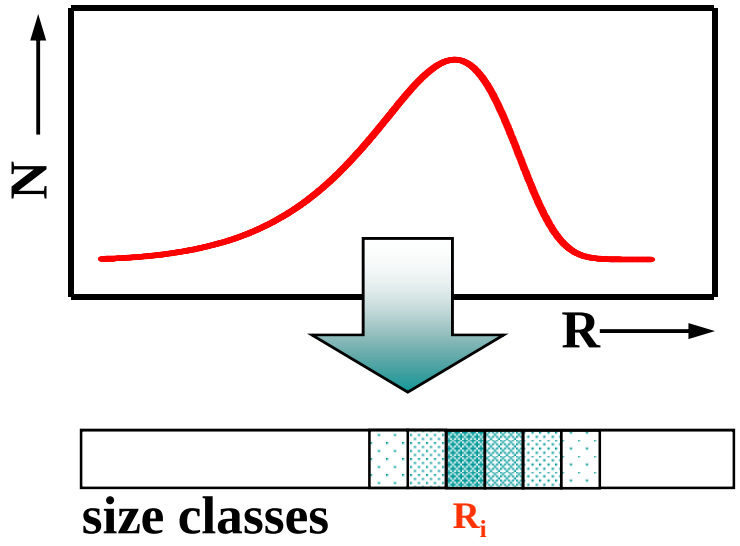
Precipitation Models

- The **JMAK** model (Johnson-Mehl-Avrami-Kolmogorov) for the estimation of the overall transformation rate
- The **Fast-Acting** model based on Langer and Schwartz theory for the simulation of the evolution of particle number density and mean size
- The more advanced **KWN** (Kampmann & Wagner Numerical) model for the predication of the full evolution of the particle size distribution (PSD) in addition to average quantities

Precipitation models: the KWN model

The KWN (Kampmann-Wagner Numerical) Model:

- **Concurrent nucleation, growth and coarsening**
- **Evolution of average quantities: volume fraction, number density, particle size**
- **Evolution of PSD: Particle Size Distribution**
- **Many size classes**



* R. Kampmann and R. Wagner, *Decomposition of Alloys: the early stages*, pp. 91-103 (1984)

Sub-Models: nucleation

Classical nucleation theory:

$$J = N_v Z \beta^* e^{-\frac{\Delta G^*}{kT}} e^{-\frac{\tau}{t}}$$

$$\Delta G^* = \frac{f \sigma^3}{\Delta G_m^2 / V_m^2}$$

Nv : Number of nucleation sites per unit volume

Z : Zeldovich factor accounting for decay of supercritical particles

β^* : Rate of solute atoms joining the critical nucleus

τ : Incubation time

ΔG^*: Activation energy for nucleation

$f = \frac{16\pi}{3}$ for homogeneous nucleation of spherical nuclei

V_m is the molar volume of the precipitate phase

ΔG_m is the molar chemical driving force for nucleation

σ is the interfacial energy of the matrix/particle interface

[1] Svoboda, J., et al., Materials Science and Engineering A, 2004. **385**(1-2): p. 166-174.

Sub-Models: growth

Growth rate of binary alloys

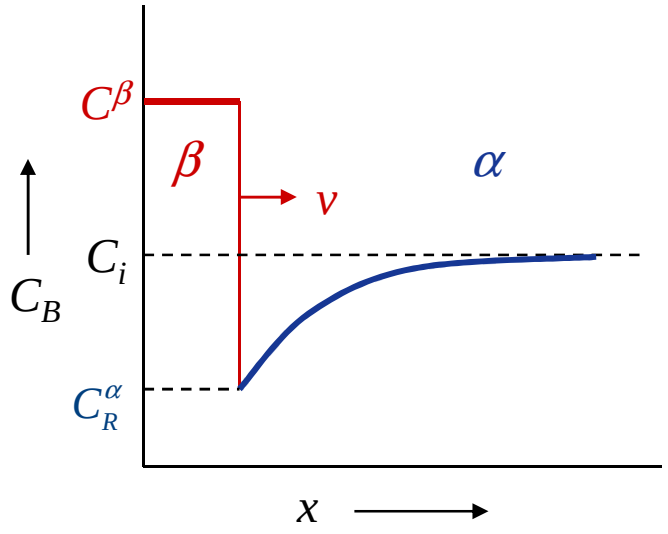
$$v = \frac{dR}{dt} = \frac{D}{R}\frac{C_i - C_R^{\alpha}}{C^{\beta} - C_R^{\alpha}}$$

C_i : instantaneous concentration in the matrix

C^{β}: concentration in the precipitate at the interface

C_R^{α} is the concentration in the matrix at the interface, which is calculated from the equilibrium concentration C^{α} using the Gibbs-Thomson equation:

$$C_R^{\alpha} = C^{\alpha} \exp\left(\frac{2\sigma V_m}{R_g T}\frac{1}{R}\right)$$



Sub-Models: growth

Growth model for multi-component alloys:

- **The Simplified Model: Growth model proposed by Morral and Purdy[1] – very low super-saturation**
- **The SFFK[2] Model for complex systems – the principle of maximum entropy production**
- **Analytical treatment of diffusion in multi-component alloys by Chen[3]**

[1] Morral, J.E. and Purdy, G.R., Scripta Metallurgica et Materialia, 1994. **30**(7): p. 905-908
[2] Svoboda, J., et al., Materials Science and Engineering A, 2004. **385**(1-2): p. 166-174.
[3] Chen, Q., *et al.*, Acta Materialia, 2008. **56**: p. 1890-1896.

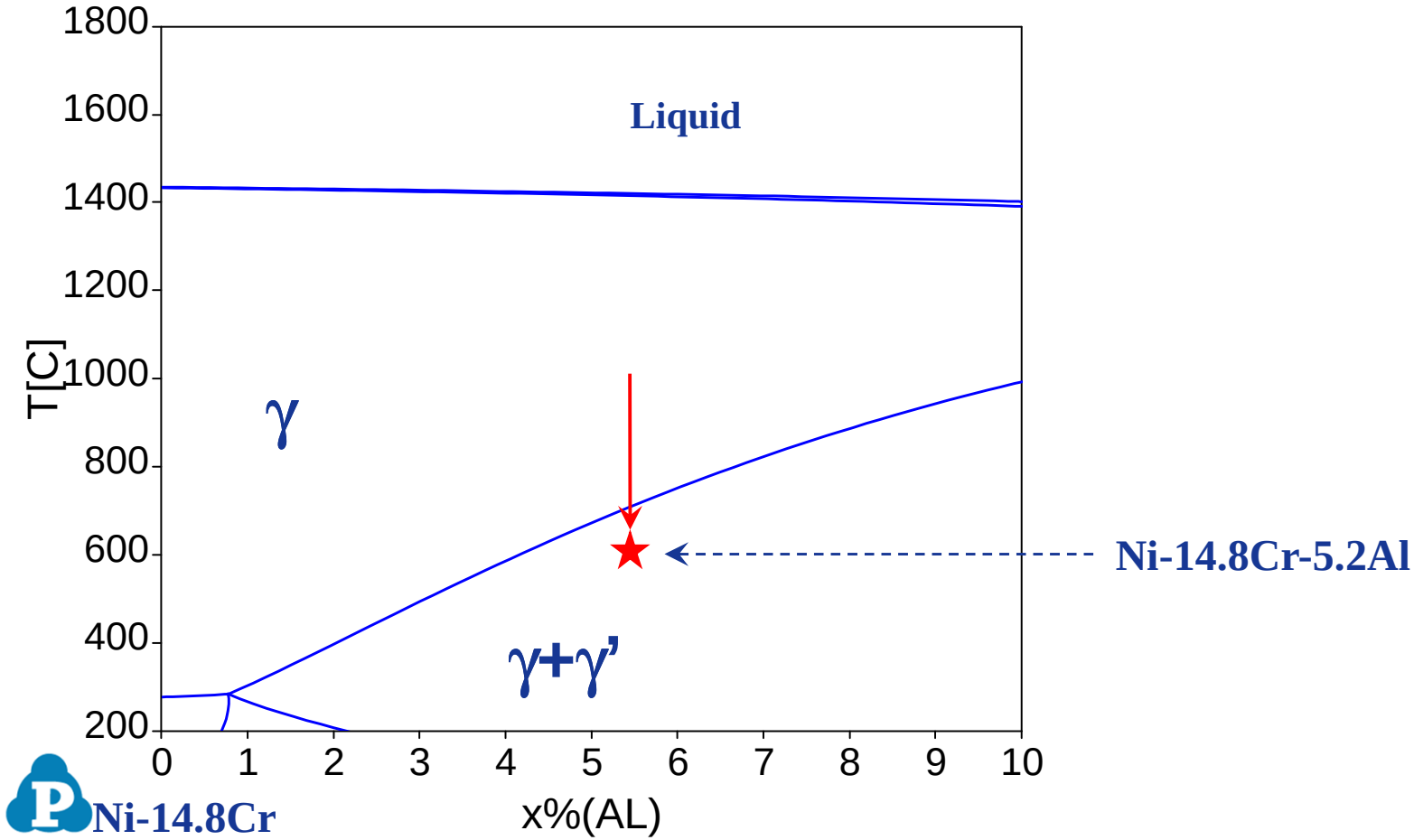
Application to Ni-base Alloys

- **Ni-Al-Cr alloy:**
- **Ni-Al-Cr-W alloy**
- **Rene88DT alloy**
- **IN100 alloy**
- **U720LI**
- **IN718 alloy**

Precipitation: Ni-14.8Cr-5.2Al

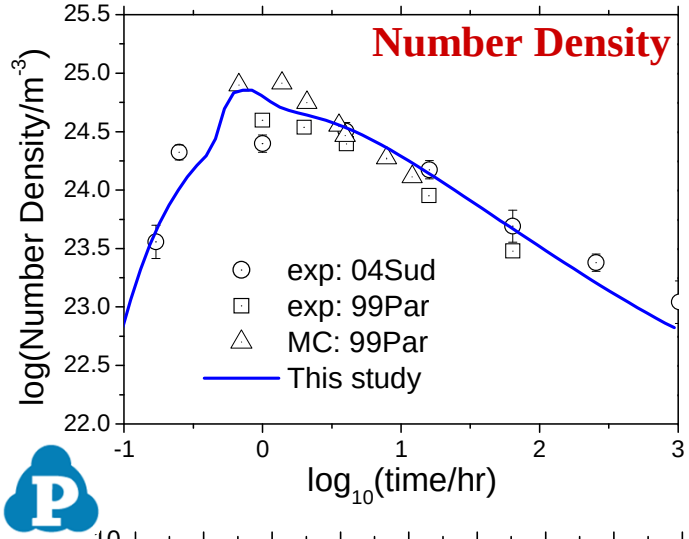
Precipitation simulation

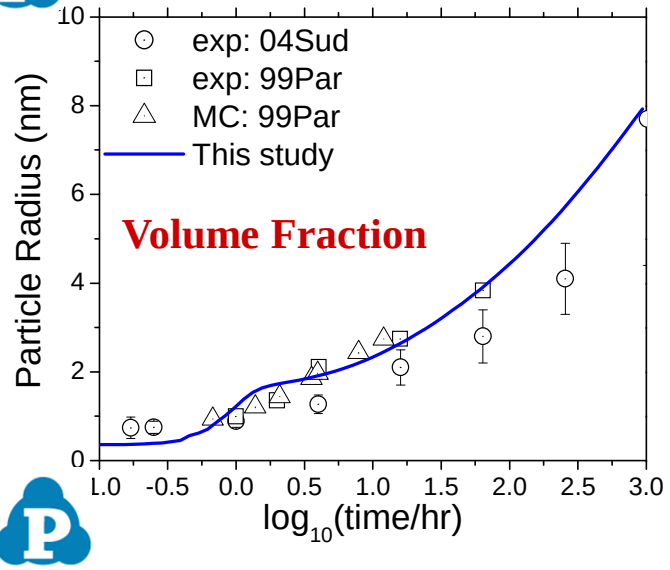
Ni-14.8Cr-5.2Al at.% alloy isothermal annealing at 600°C



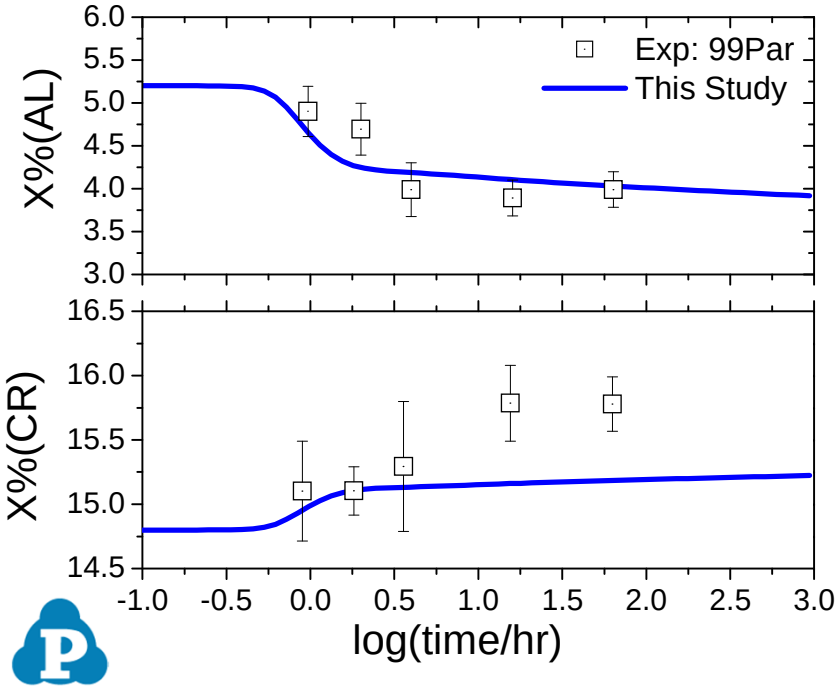
Precipitation: Ni-14.8Cr-5.2Al

Microstructure evolution in Ni-14.8Cr-5.2Al at.% alloy at 600°C
KWN - predictions & experiment





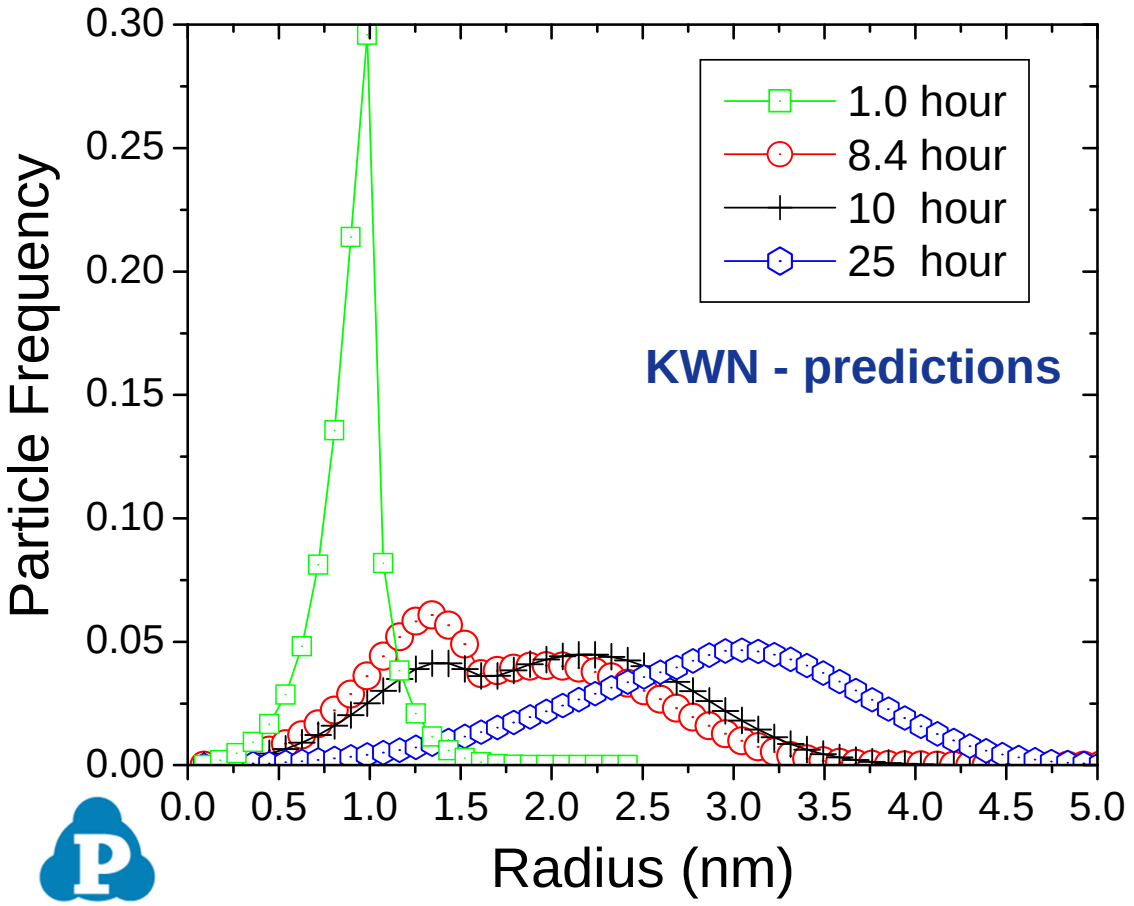
Matrix Composition



Precipitation: Ni-5.2Al-14.2Cr

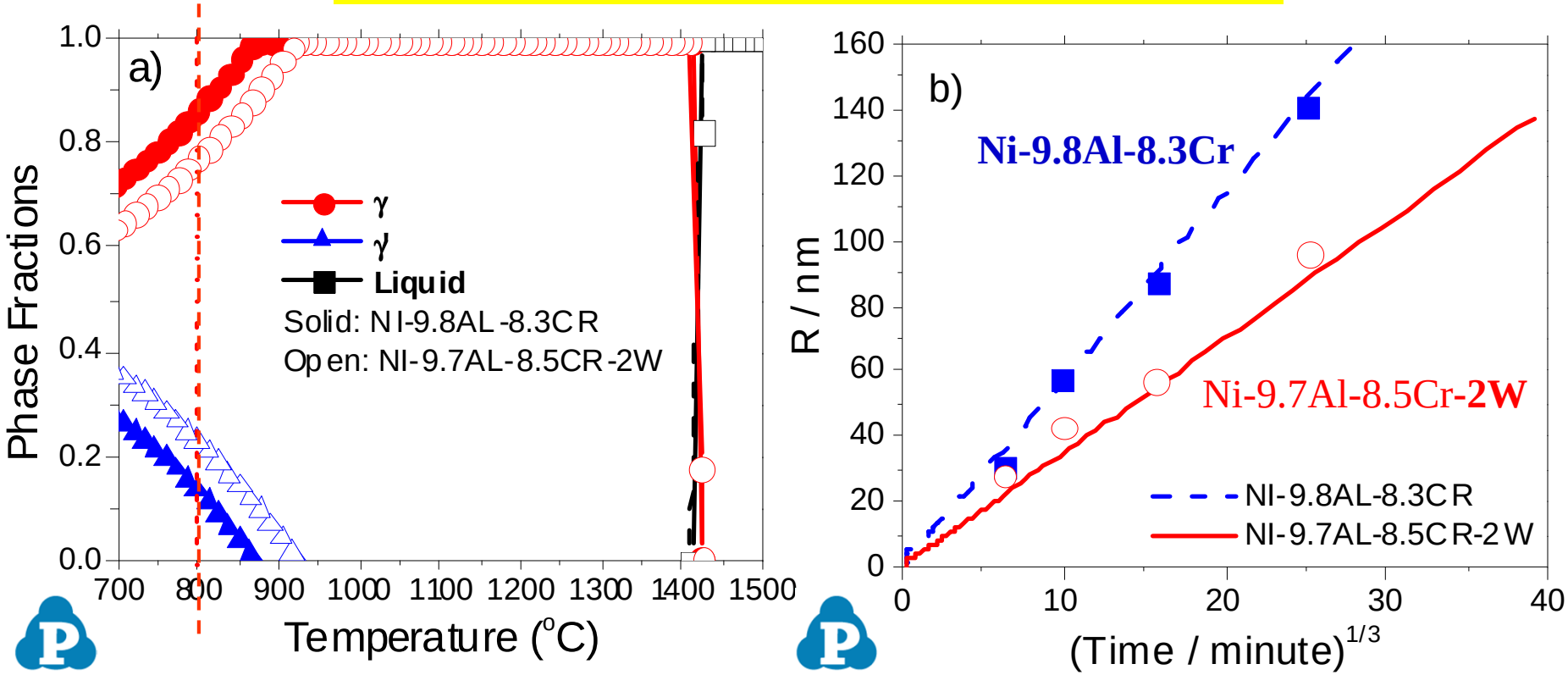
Microstructure evolution in Ni–5.2Al-14.2Cr at.% alloy at 600°C

Particle Size Distribution of γ'



Coarsening: Chemistry Effect

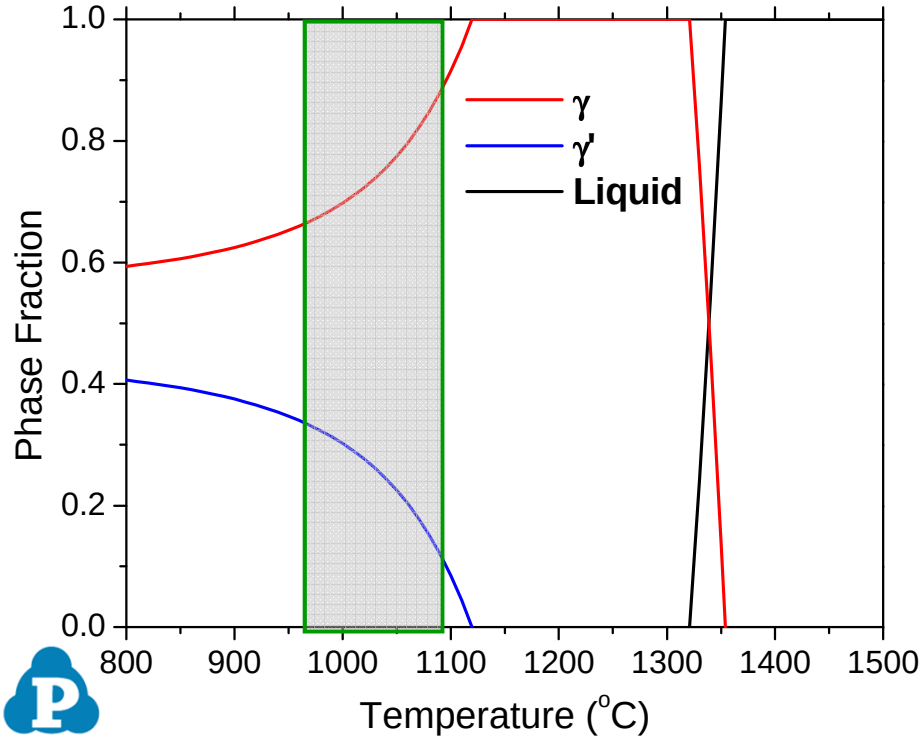
The predicated temporal evolution of mean γ' size in two Nickel Alloys aged at 800ºC: Ni-9.8Al-8.3Cr and Ni-9.7Al-8.5Cr-2W in at%

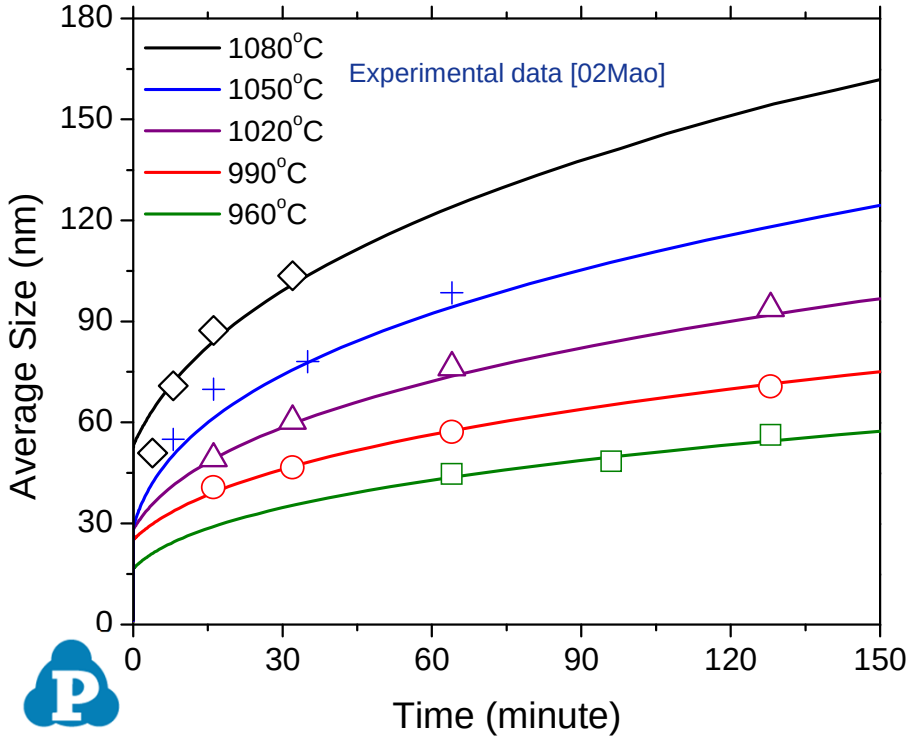


Experimental Data: Sudbrack, C.K., "*Decomposition behavior in model Ni-Al-Cr-X superalloys: temporal evolution and compositional pathways on a nanoscale*", in Department of Materials Science & Engineering, 2004, Northwestern University

Coarsening of Rene88: Temperature Effect

Predicted evolution of average size at different temperatures for commercial alloy Rene88DT with composition: Ni-1.99Al-12.99Co-15.67Cr-4.00Mo-3.88W-3.72Ti-0.70Nb in wt%

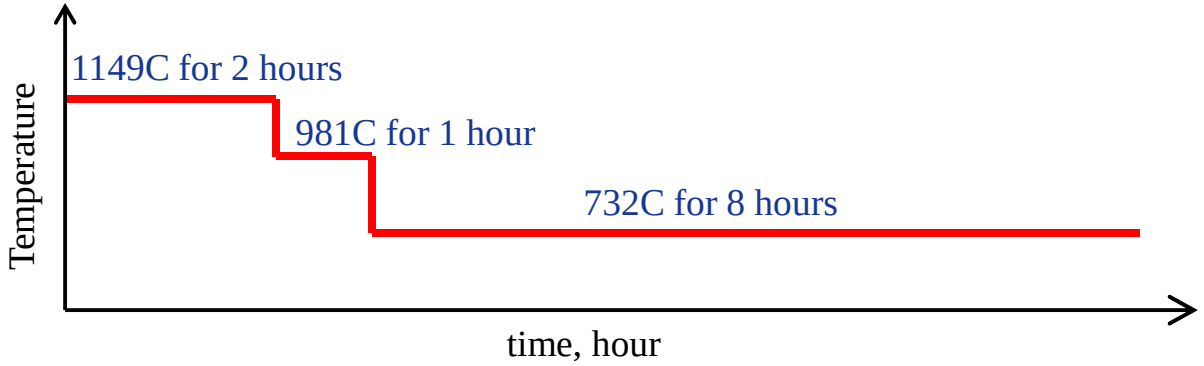




Exp. Data: Jian Mao, "*Gamma Prime Precipitation Modeling and Strength Responses in Powder Metallurgy Superalloys*", in Department of Mechanical Engineering, 2002, West Virginia University

Multi-Step Heat Treatment: IN100

Alloy Chemistry: Ni-4.85Al-18.23Co-12.13Cr-3.22Mo-4.24Ti (wt%).



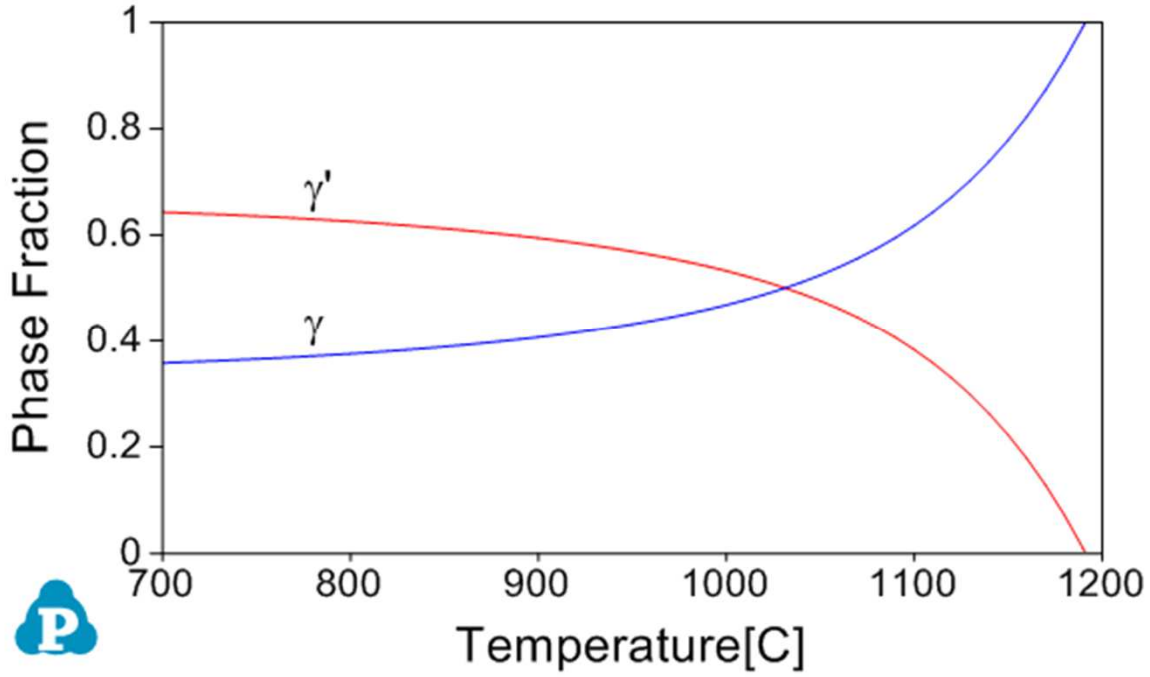
Experimental Data:

By K. Maciejewski, H. Ghonem, Materials Science & Engineering A, 560 (10) (2013), 439-449.

	Primary γ′	Secondary γ′	Tertiary γ′
Size (nm)	**1700**	**208**	**23**
Volume fraction	**20%**	**29%**	**11%**

Thermodynamics of IN100

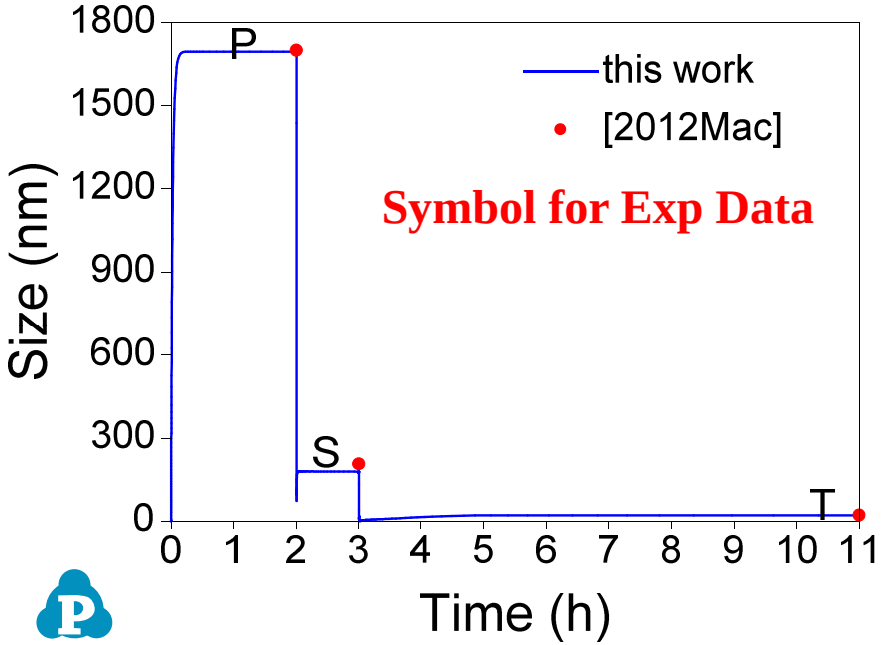
Component	Al	B	C	Co	Cr	Mo	Ti	V	Zr	Ni
wt%	4.85	0.02	0.072	18.23	12.13	3.22	4.24	0.71	0.071	bal

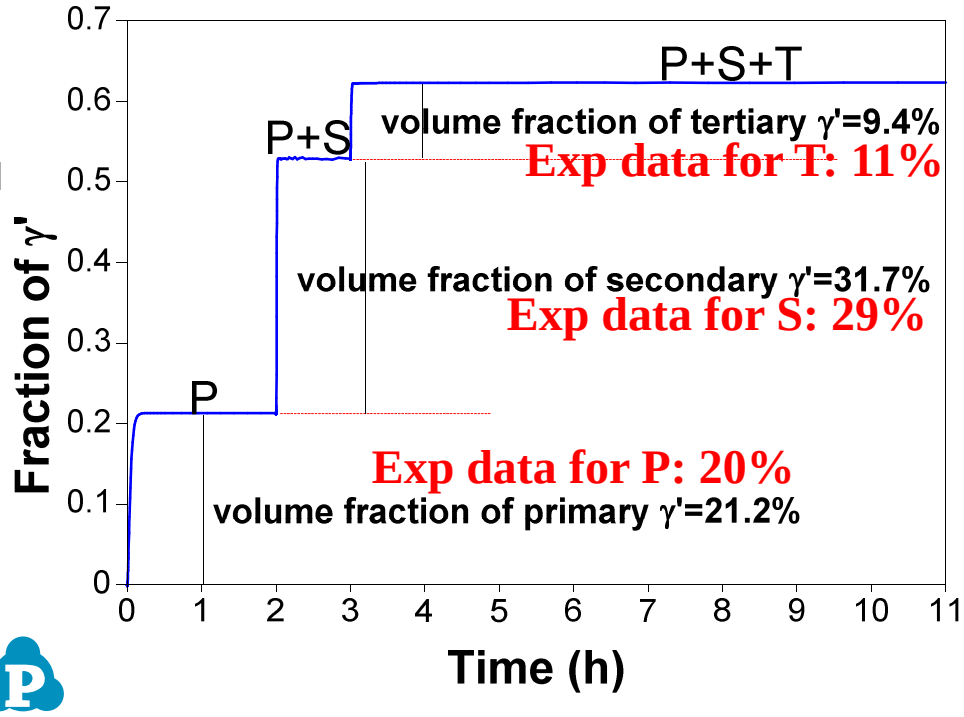


γ′ Solvus:

Calculated: 1191°C
Measured: 1187°C

Multi-Step Heat Treatment: IN100





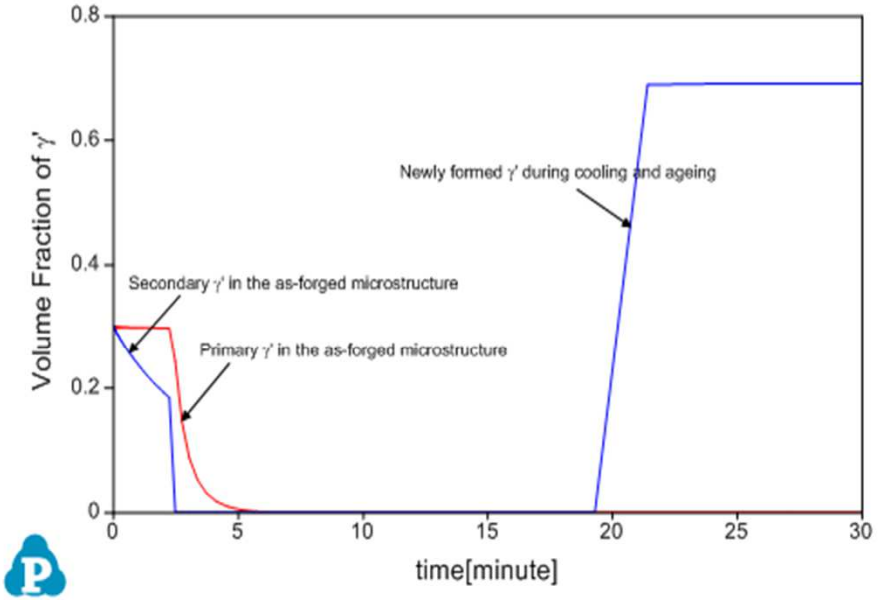
Effect of Initial Microstructure and Heat Treatment Conditions

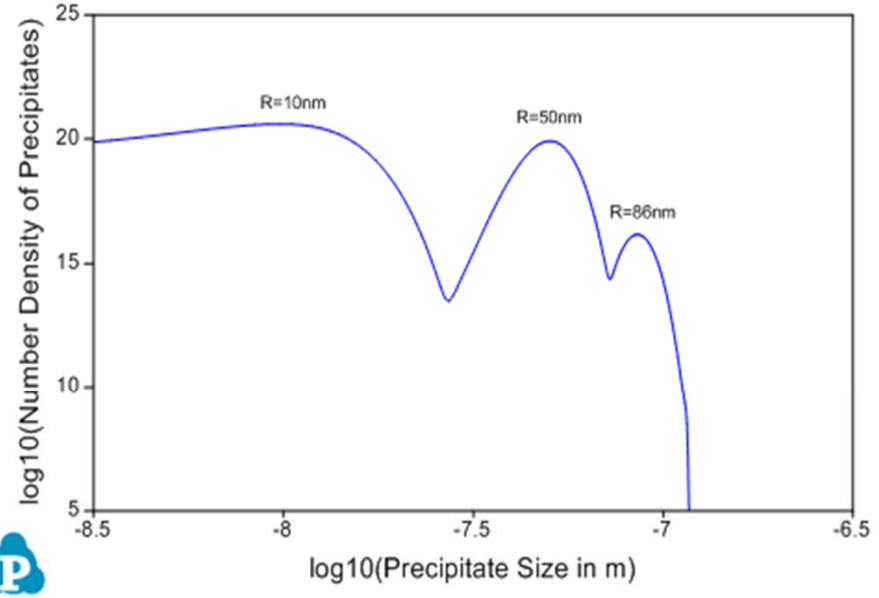
- **Initial microstructure: pre-existing primary and secondary γ'**
- **Supersolvus vs. Subsolvus solution treatment**
- **Long vs. short solution treatment time**

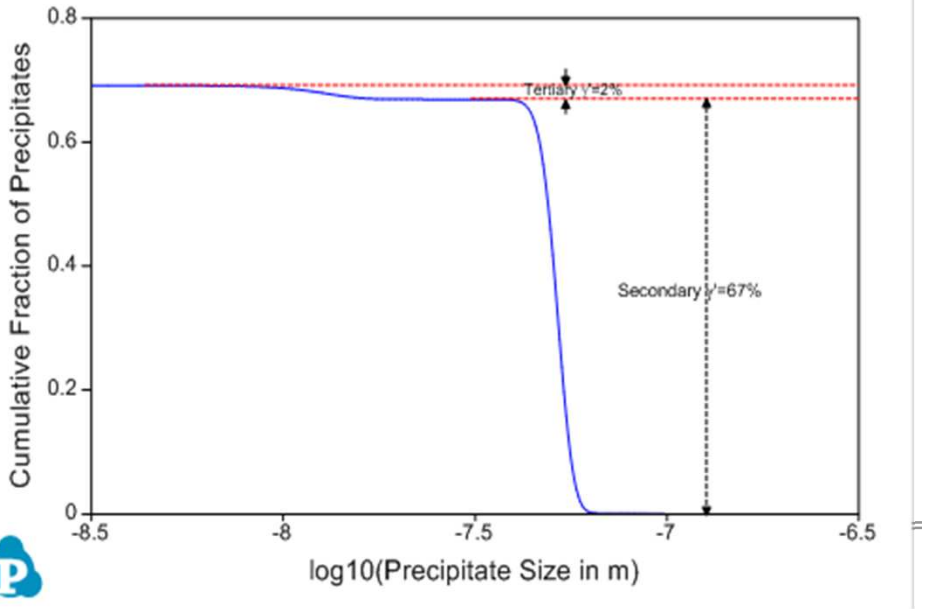
Precipitation of IN100-Supersolvus Solution

Initial microstructure:
30% primary γ′ with average size r=600nm
30% secondary γ′ with average size r=70nm

Heat treatment schedule:
Supersolvus solution at 1200°C for 20min
Cool down to 750°C at 7.5°C/s
Age at 750°C for 6 hours



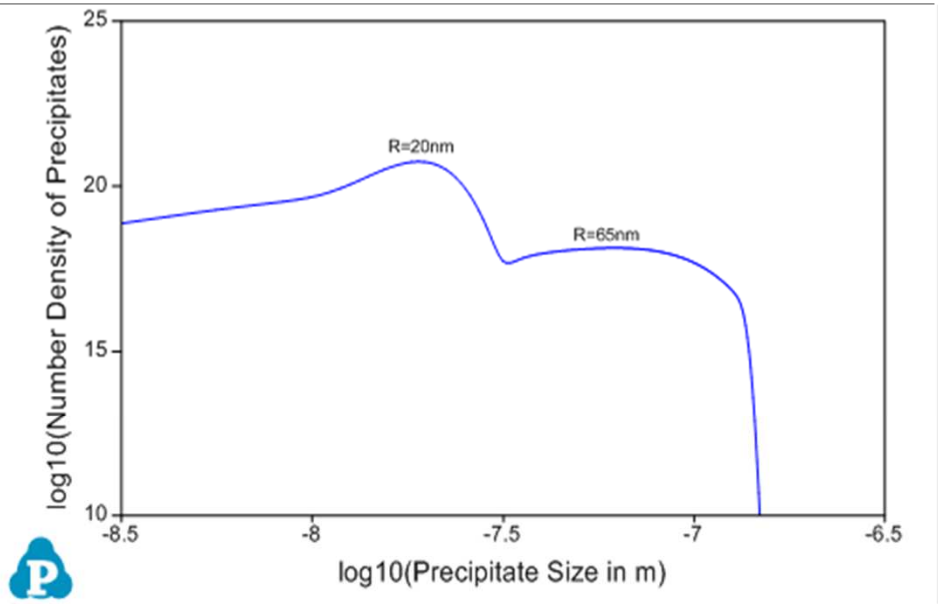


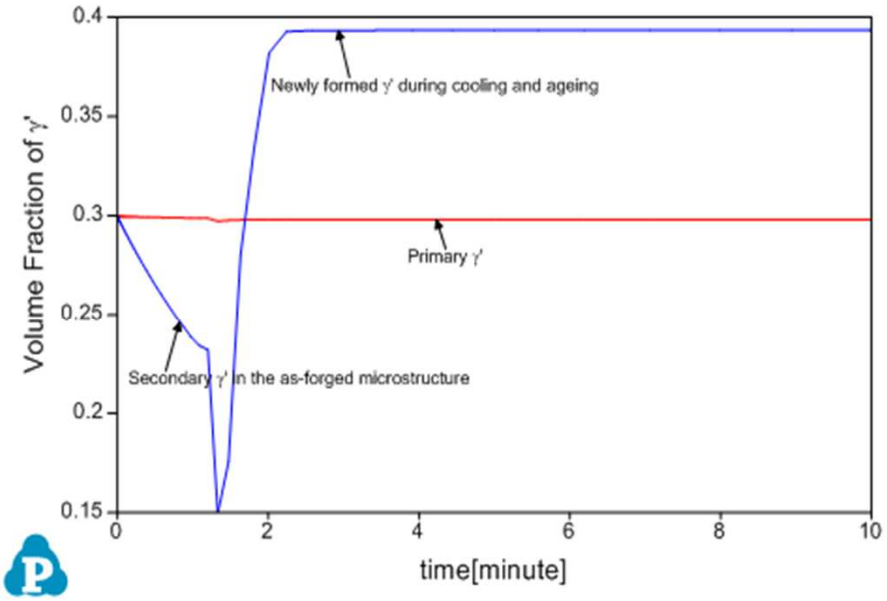


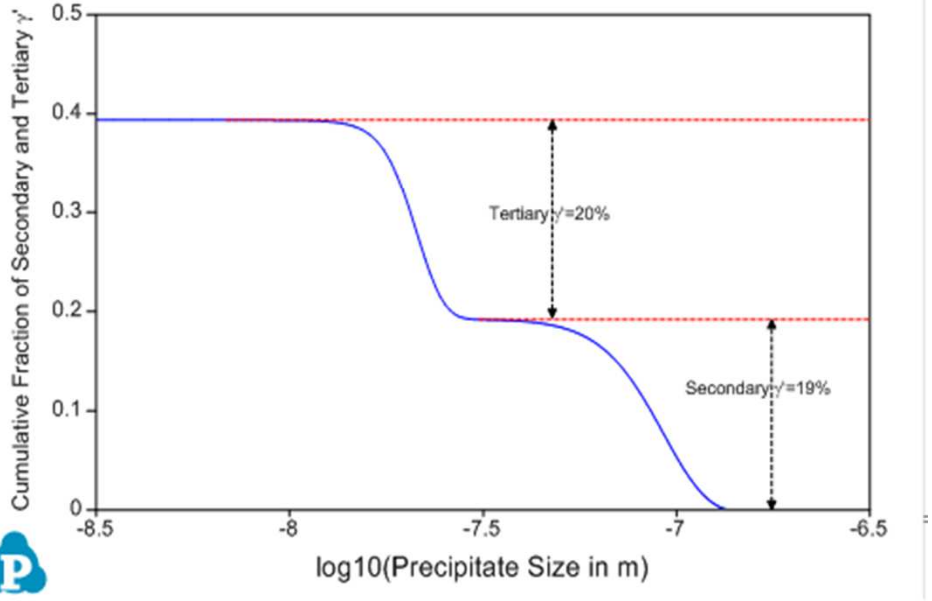
Precipitation of IN100-Supersolvus Solution

Initial microstructure:
30% primary γ′ with average size r=600nm
30% secondary γ′ with average size r=70nm

Heat treatment schedule:
Supersolvus solution at 1200°C for 1min
Cool down to 750°C at 7.5°C/s
Age at 750°C for 6 hours



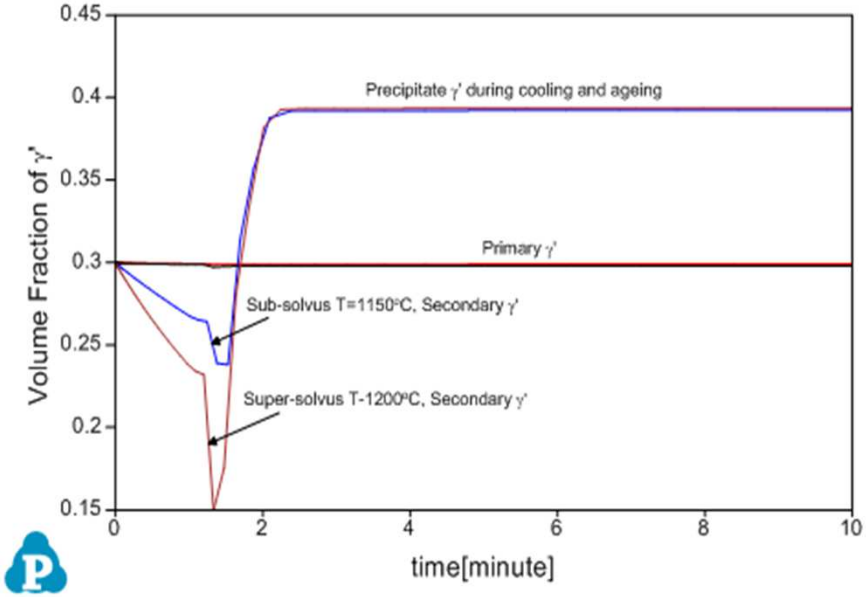


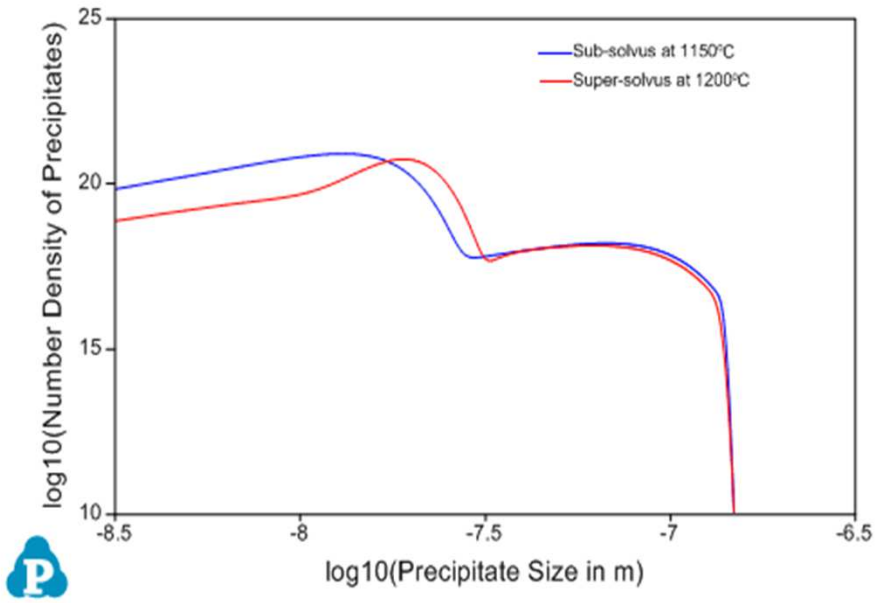


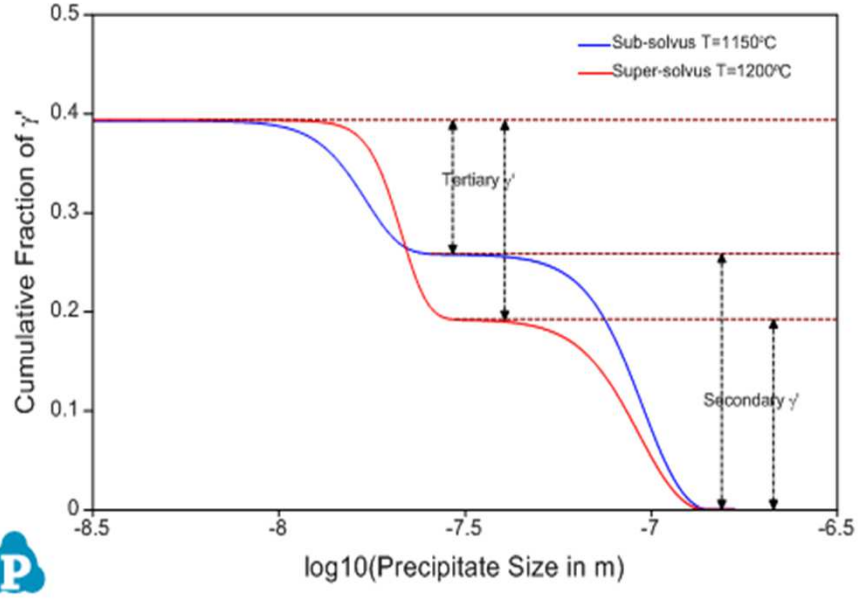
Precipitation of IN100 -Supersolvus vs. Subsolvus Solution

Initial microstructure:
30% primary γ′ with average size r=600nm
30% secondary γ′ with average size r=70nm

Heat treatment schedule:
Supersolvus at 1200°C vs. Subsolvus at 1150°C solution treatment for 1min
Cool down to 750°C at 7.5°C/s
Age at 750°C for 6 hours







Effect of Cooling Rate on the Size Distribution of U720LI

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Multimodal size distributions of γ′ precipitates during continuous cooling of UDIMET 720 Li

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Abstract

The technological properties of many nickel-based superalloys originate in the morphology and distribution of $Ni_3(Al, Ti)$ particles (γ′ precipitates). Starting from the solution-annealed condition, the distribution and the morphology of γ′ precipitates are investigated experimentally during continuous cooling of the nickel-base superalloy UDIMET 720 Li. Characterization of the precipitates is carried out by scanning electron microscopy and energy-filtered transmission electron microscopy investigations. Depending on cooling rate, monomodal, bimodal and even trimodal size distributions are observed. The experimental observations of the size distributions are confirmed by numerical simulations of the γ′ precipitation kinetics. The theoretical background for occurrence of multimodal size distributions during continuous cooling is discussed.

Keywords: Multimodal; Nickel alloy; Precipitation; Nucleation and growth; Phase transformation kinetics

The sample were soaked at 1180°C and then cooled continuously to 400°C at different speed

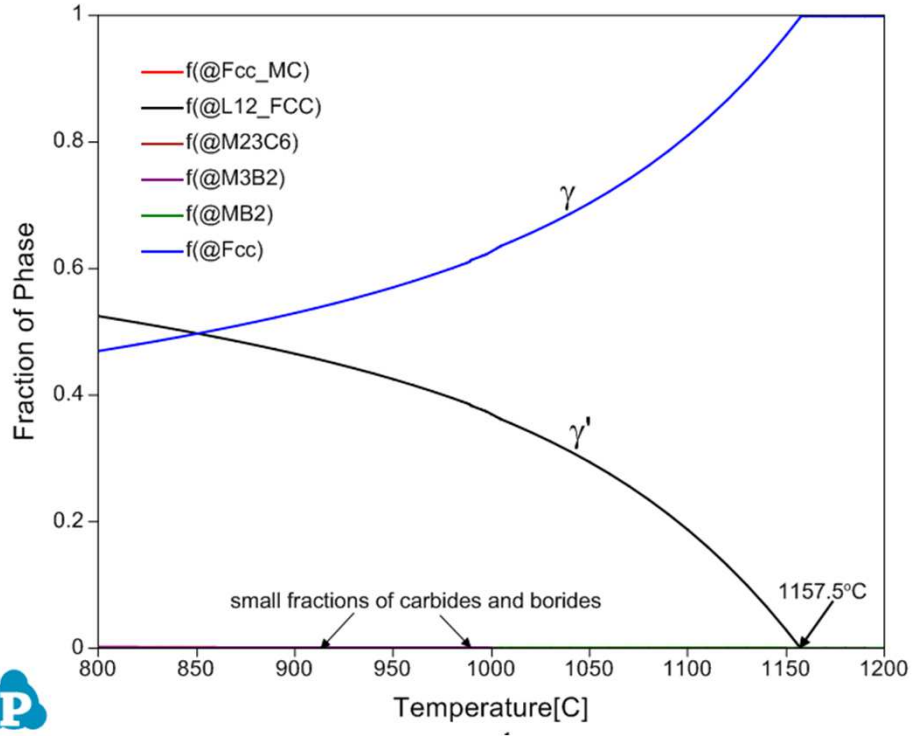
Table 1
Continuous cooling rates of the present investigation.

Sample	Cooling rate (K s^{-1})	Cooling time (s)
1	78	1000
2	19.5	4000
3	6.5	12,000
4	3.25	24,000
5	1.625	48,000
6	0.867	90,000
7	0.433	180,000
8	0.217	360,000
9	0.03333	2,340,000
10	0.01667	4,680,000
11	0.00984	7,920,000
12	0.00619	12,600,000
13	0.00416	18,720,000

Ref: R. Radis et al., "Multimodal size distribution of γ′ precipitates during continuous cooling of UDIMET 720Li", Acta Mat., 57(2009) 5739-5747

Thermodynamics of U720LI

Alloy	Cr	Co	Ti	Al	Mo	W	Zr	C	B	Ni
PM	16.26	14.73	5.05	2.50	3.01	1.27	0.036	0.023	0.018	Bal
C&W	16.06	14.52	5.04	2.54	3.08	1.20	0.047	0.013	0.018	Bal

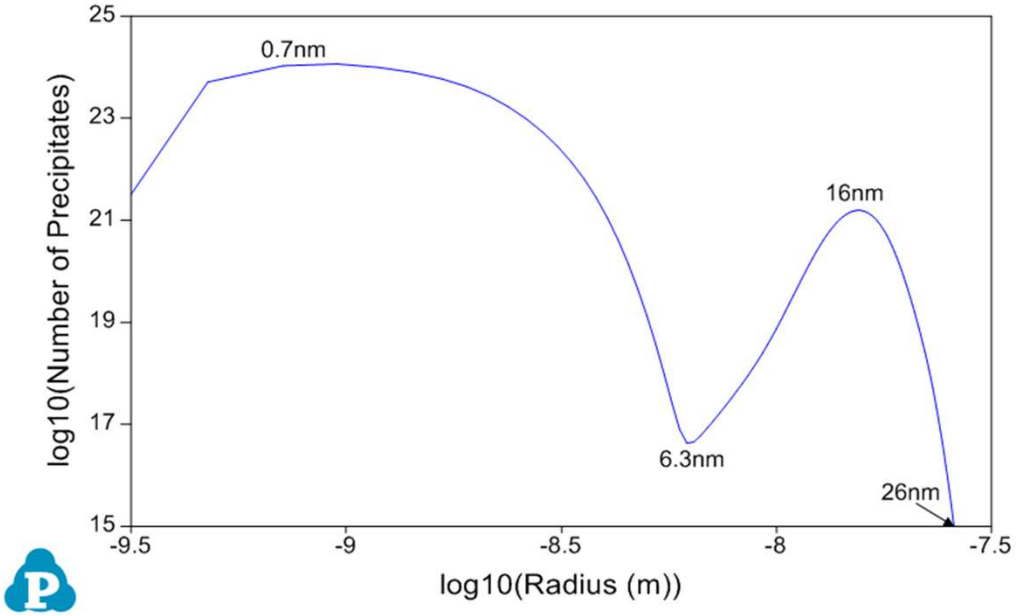


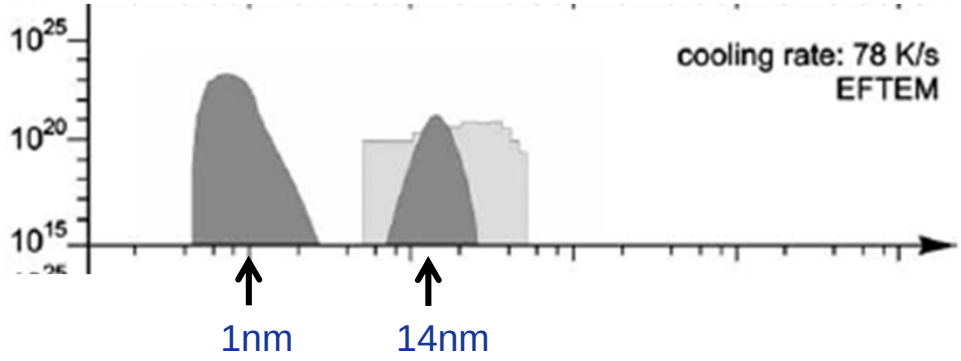
γ′ Solvus:

Calculated: 1157.5°C

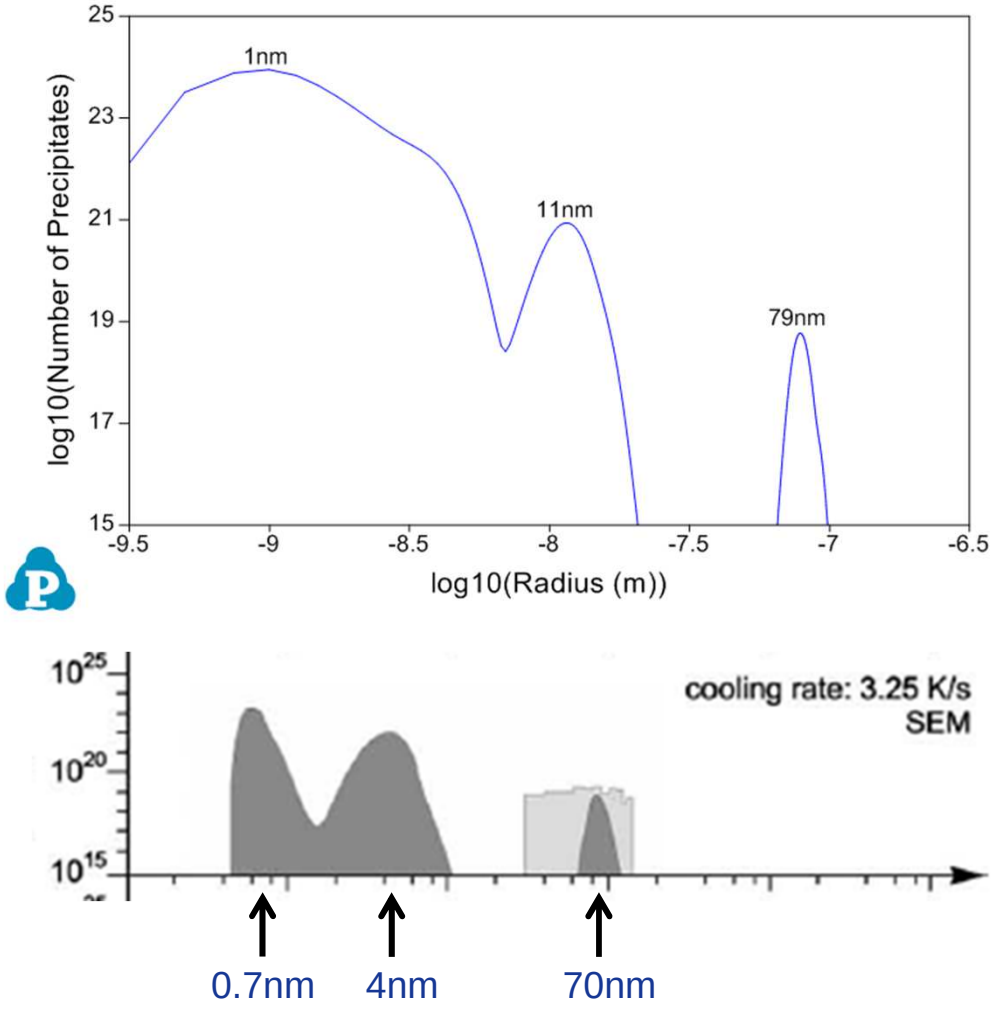
Measured: 1160°C

U720LI: Cooling Effect on Precipitation Fast Cooling

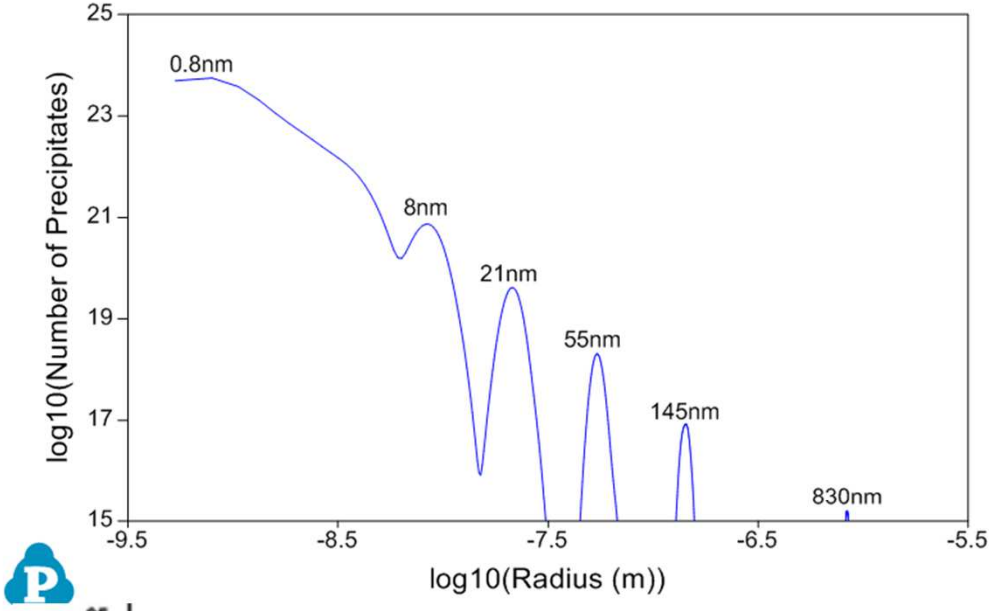


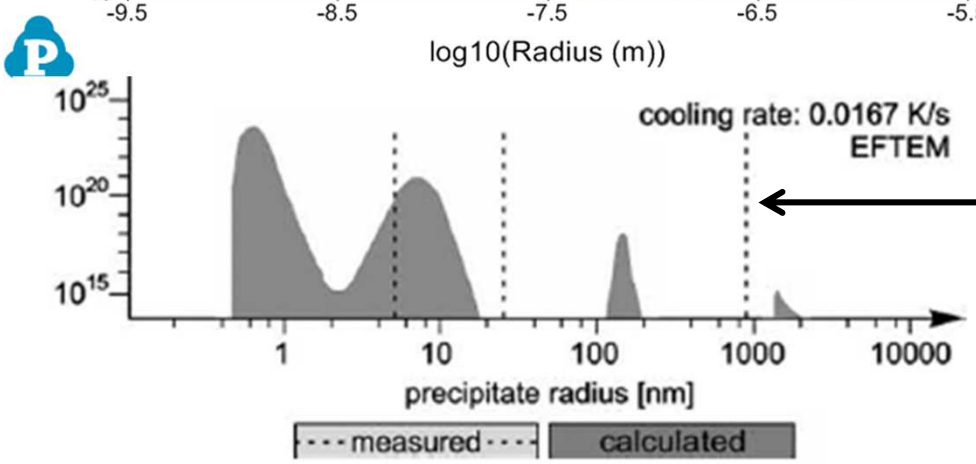


U720LI: Cooling Effect on Precipitation Medium Speed



U720LI: Cooling Effect on Precipitation Slow Cooling

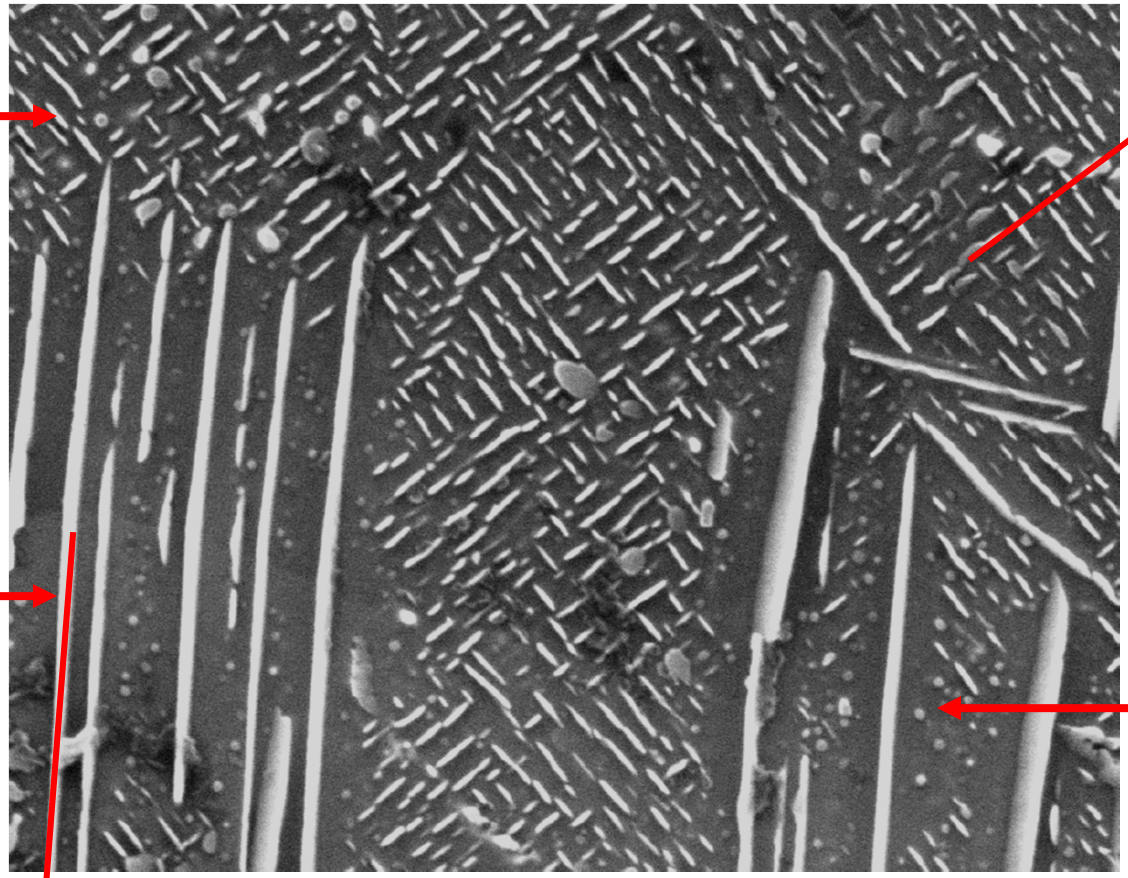




Measured:
790nm
19nm
3nm

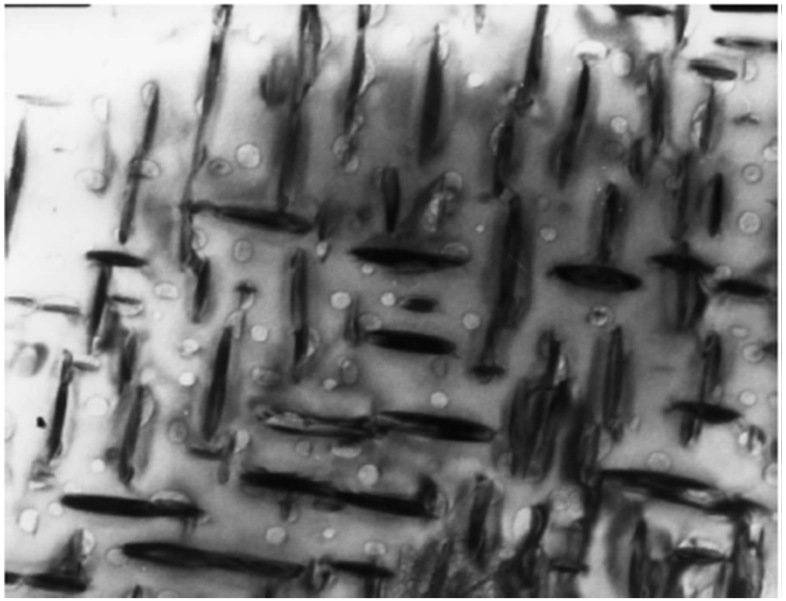
Simulated: 0.4nm 7nm 126nm 1260nm

Alloy 718: Typical Microstructure

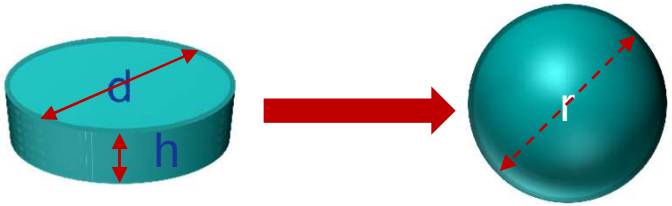


Convert γ” size from the disc to sphere

Our current precipitation simulation module can only handle sphere morphology. Therefore we have to convert the size of disc γ” to the diameter of sphere

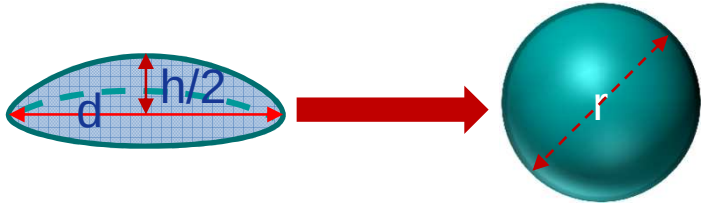


1:



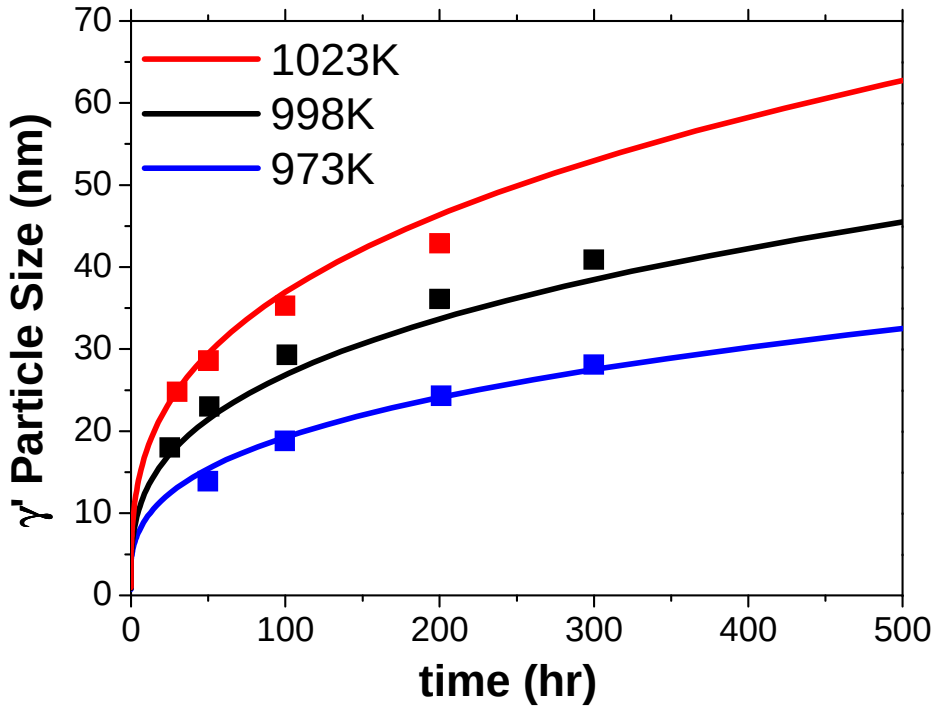
$$V = \frac{1}{4}\pi d^2 h = \frac{4}{3}\pi r^3$$

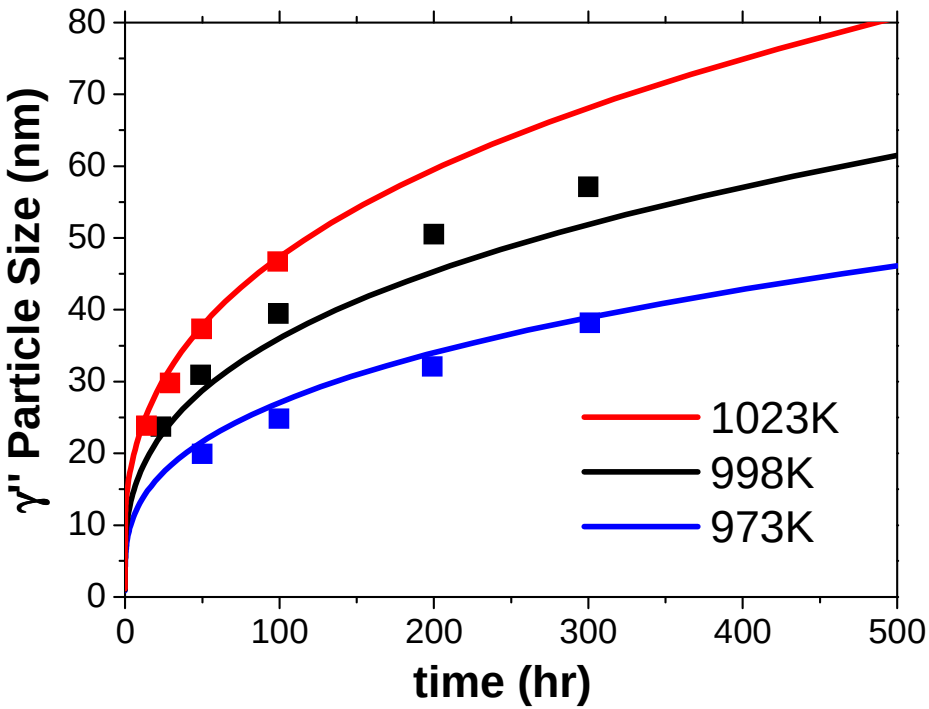
2:



$$V = \frac{1}{6}\pi h\left(\frac{3}{4}d^2 + \frac{1}{4}h^2\right) = \frac{4}{3}\pi r^3$$

Coarsening: Alloy 718 at 973K, 998K and 1023K

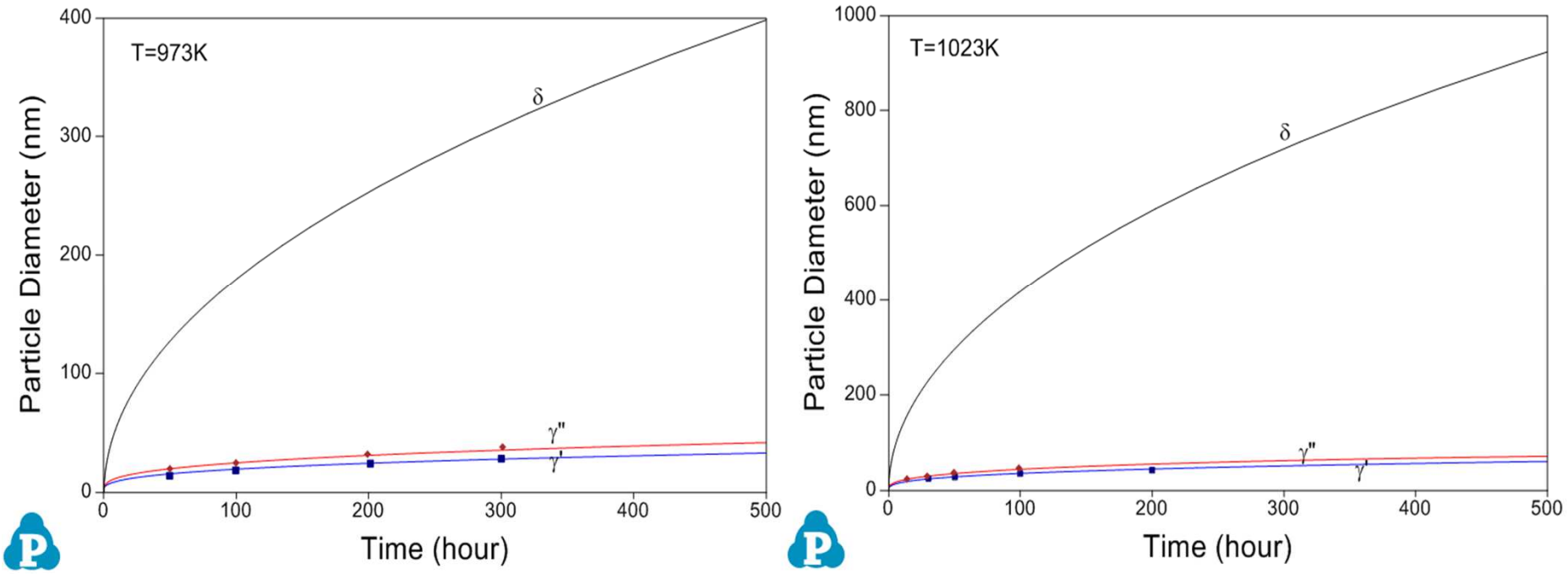




Co-precipitation of γ' and γ'' phases

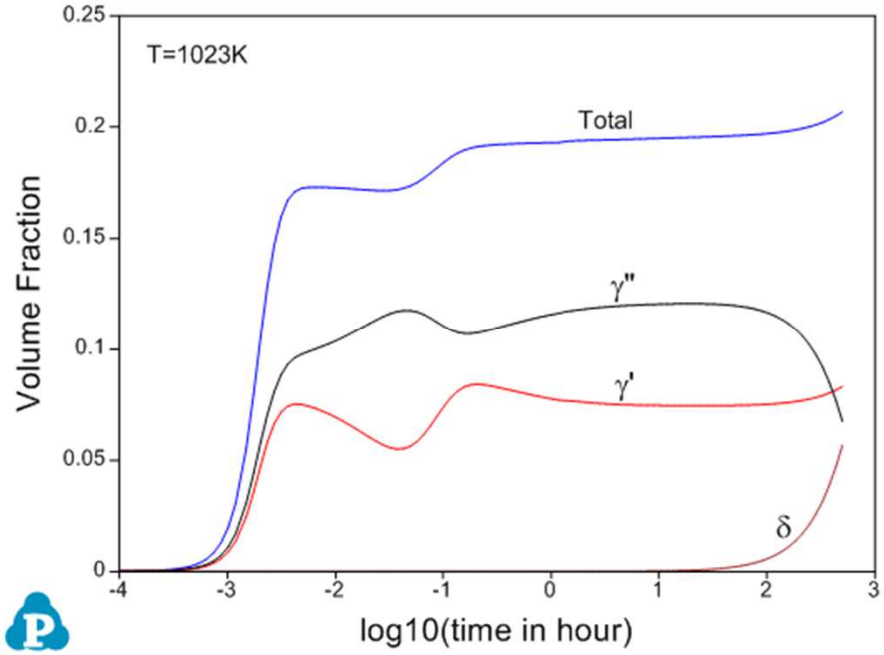
Experimental data: Han, Y.F. et al., *Metal Science*, vol. 16, 1982

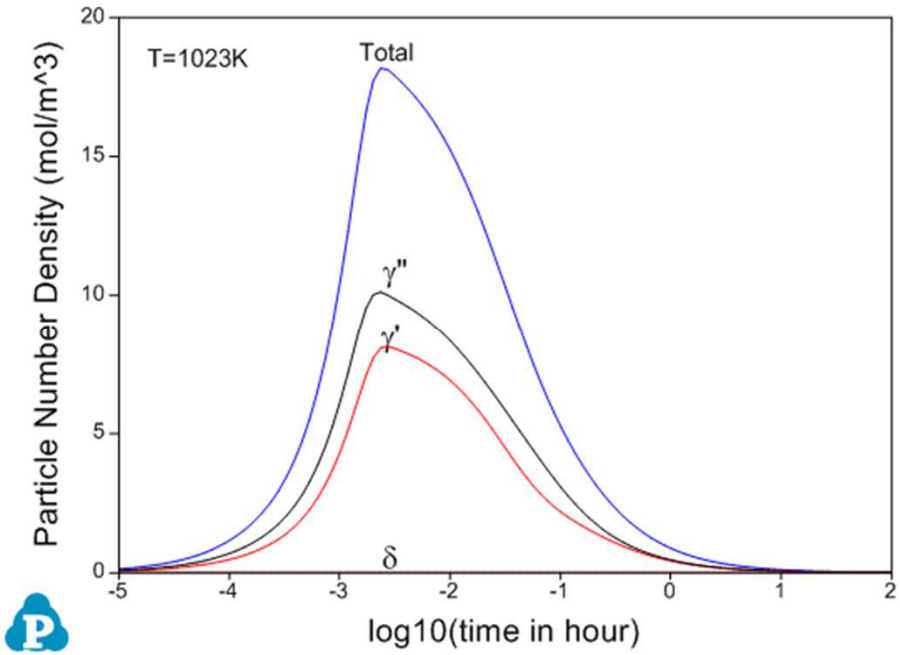
Co-precipitation of γ′, γ″, and δ in Alloy 718



Experimental data: Han, Y.F. et al., *Metal Science*, vol. 16, 1982

Co-precipitation of γ, γ′, and δ in Alloy 718





Summary

- Precipitation simulation is a useful tool to understand the complicated precipitation process;
- To develop a reliable precipitation simulation tool, we need:
  - Good models for nucleation, growth and coarsening
  - Reliable thermodynamic database
  - Reliable mobility database
  - Smooth integration of precipitation module with thermodynamic calculation engine