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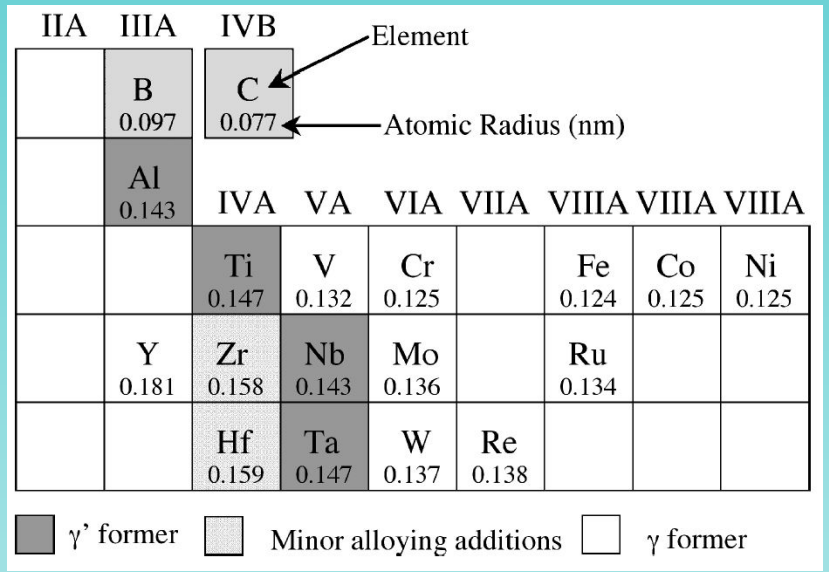
Modeling of microstructure evolution and properties for Ni-based superalloys

Content

- Brief overview of Ni-based supealloys
- Computational model development
- Microstructure modeling during specified heat treatments
- Calculation of mechanical properties based on predicted microstructure

Brief overview of Ni-based supealloys

Composition of superalloys

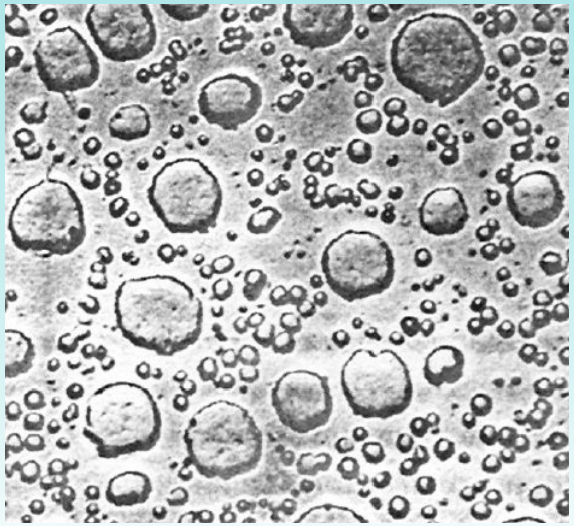


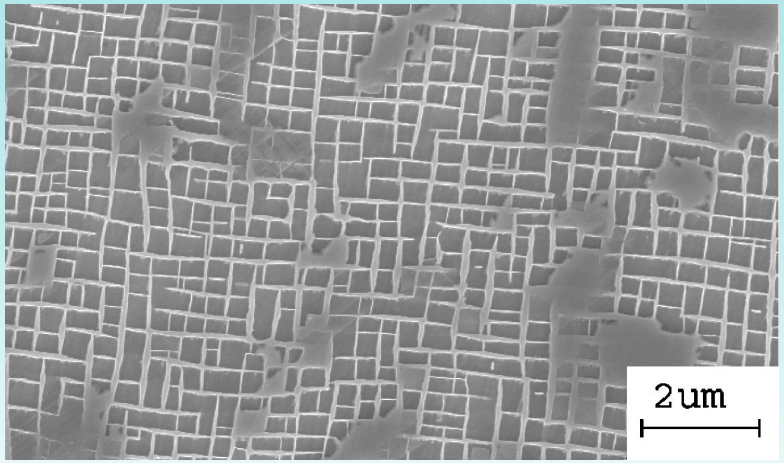
- Ni – base
- Up to 40 wt % of a combination of five to ten other elements
- Primary phases – γ (nickel-based solid solution) and γ' (Ni_3Al)

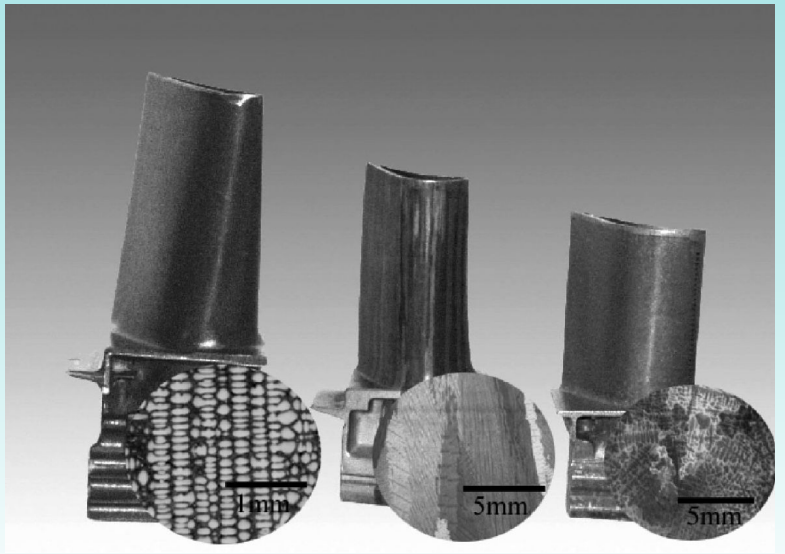
An exceptional combination of high-temperature strength, toughness, and resistance to degradation in corrosive or oxidizing environments

Strengthening mechanisms

- γ-phase solid-solution strengthening by refractory elements
- Precipitation strengthening by γ'-phase
- Grain size (directional solidifying)

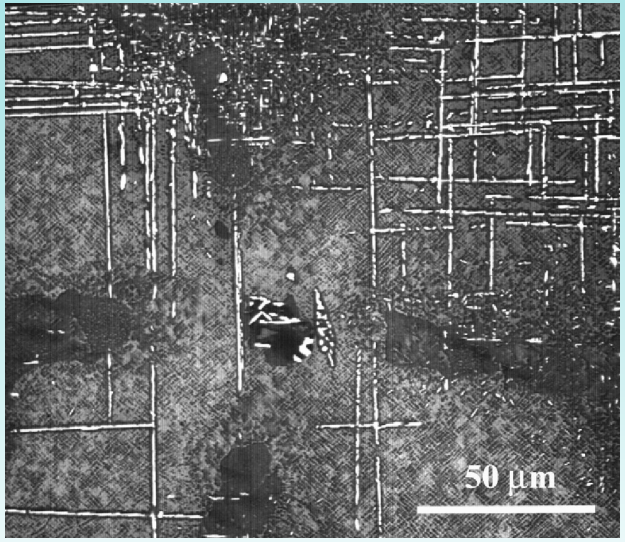


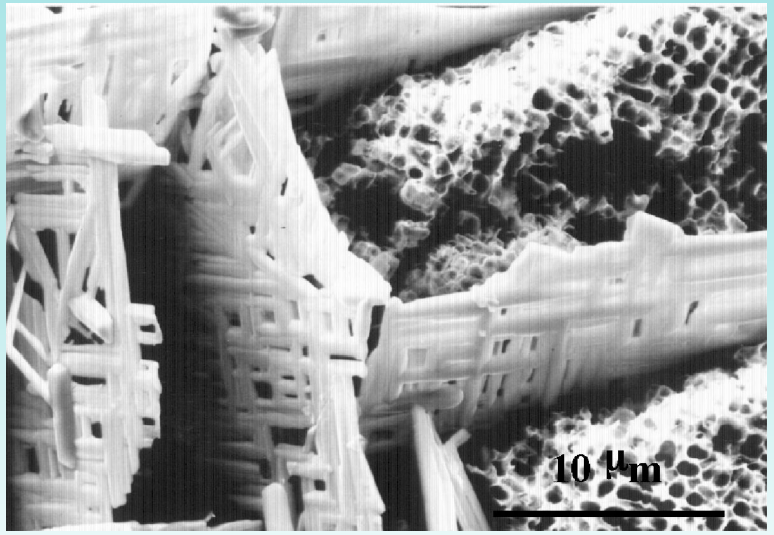




Detrimental phases – topologically closed-packed phases

- Orthorhombic P phase, the tetragonal σ phase, the rhombohedral R, and rhombohedral μ phases
- TCP-phases deplete strengthening elements and/or serve as crack-initiation site



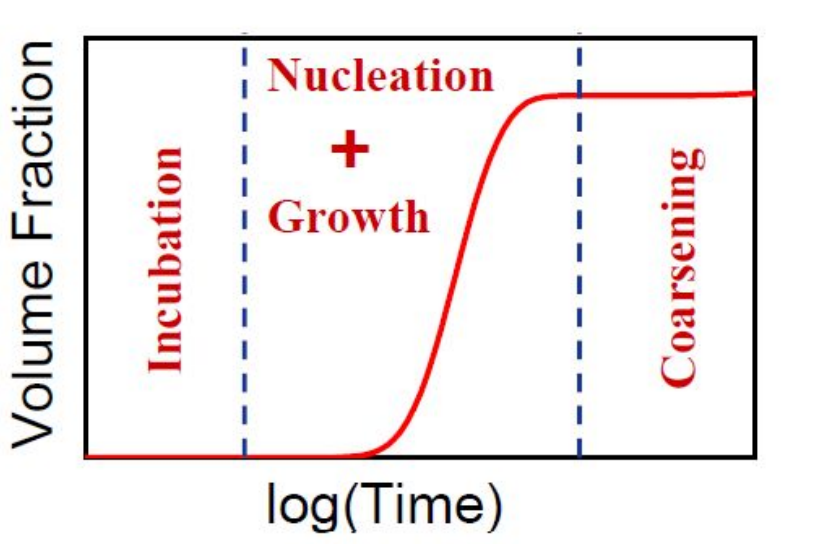


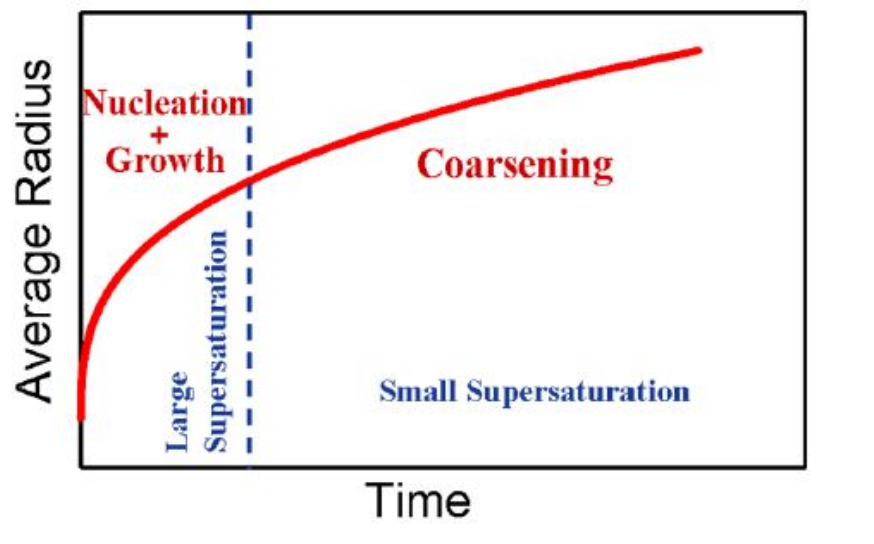
Computational model development

Theoretical models and numerical method

- TC-PRISMA adopts *Kampmann-Wagner* numerical method, based on the theory from *Langer-Schwartz*

Nucleation ⇨ Growth/dissolution ⇨ Coarsening





Nucleation rate

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

where

N_v - 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

$$\Delta G^* = \frac{16\pi\sigma^3}{3\left(\Delta G_m^{\alpha\to\beta} / V_m^{\beta}\right)^2}$$

where

σ - interfacial energy of the matrix/particle interface
$\Delta G_m^{\alpha\to\beta}$ - molar chemical driving force for nucleation
V_m^{β} - molar volume of the precipitate phase

Growth rate

$$v = \frac{dr}{dt} = \frac{K}{r}\left(\Delta G_m - \frac{2\sigma V_m^{\beta}}{r}\right)$$

where

r – particle radius
K – coefficient of precipitate morphology
ΔG_m- driving force

Simplified model - calculates the velocity of a moving phase interface in multicomponent systems using simply the tie-line across the bulk composition

$$v' = v\left(1 + r\sqrt{4\pi N_V \langle r \rangle}\right)$$

where

v' - corrected velocity
$\langle r \rangle$ - mean radius
N_V - number density

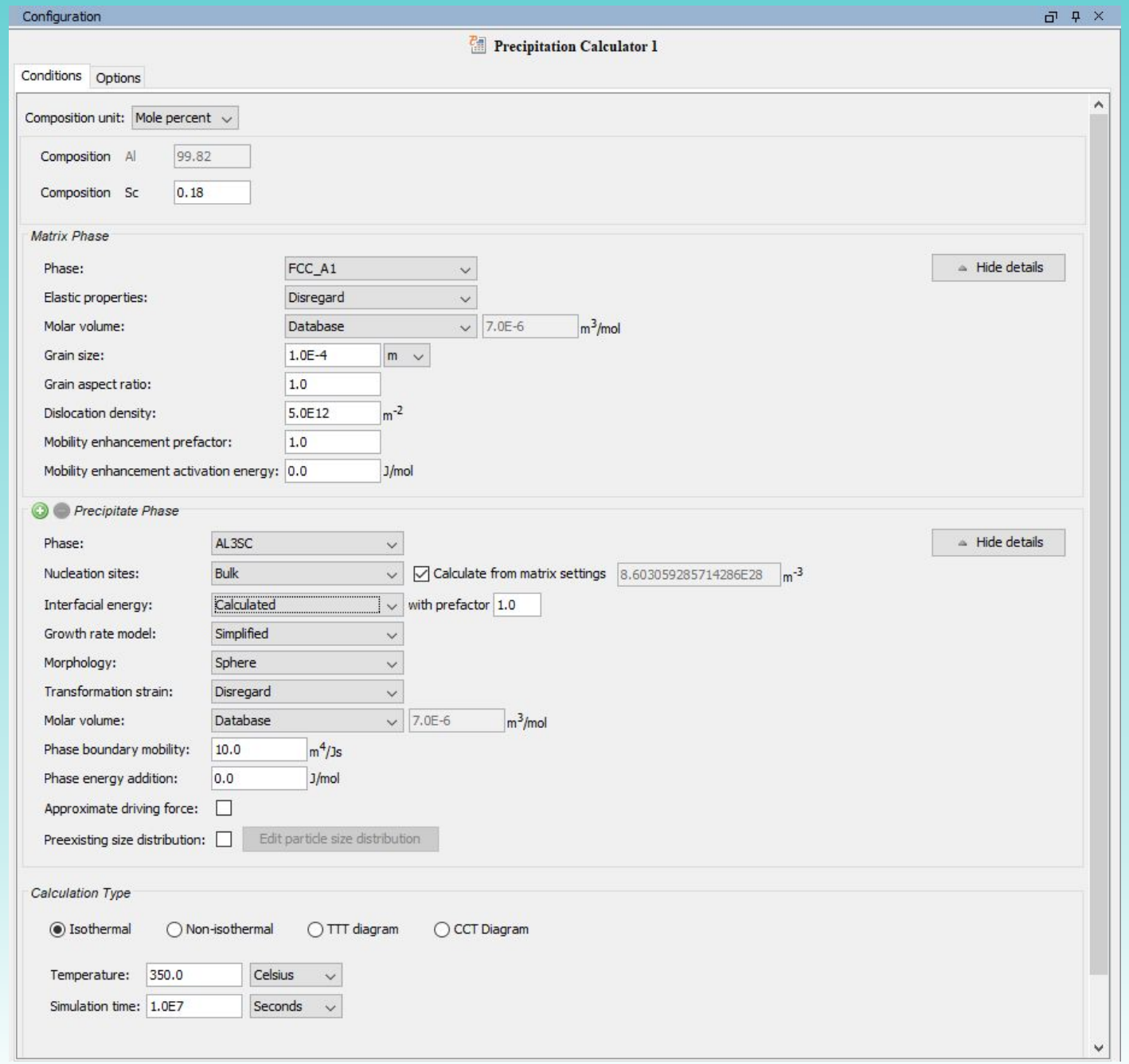
Advanced model - identifies the operating tie-line

For *coarsening* the growth equation is applied

Input

Nucleation

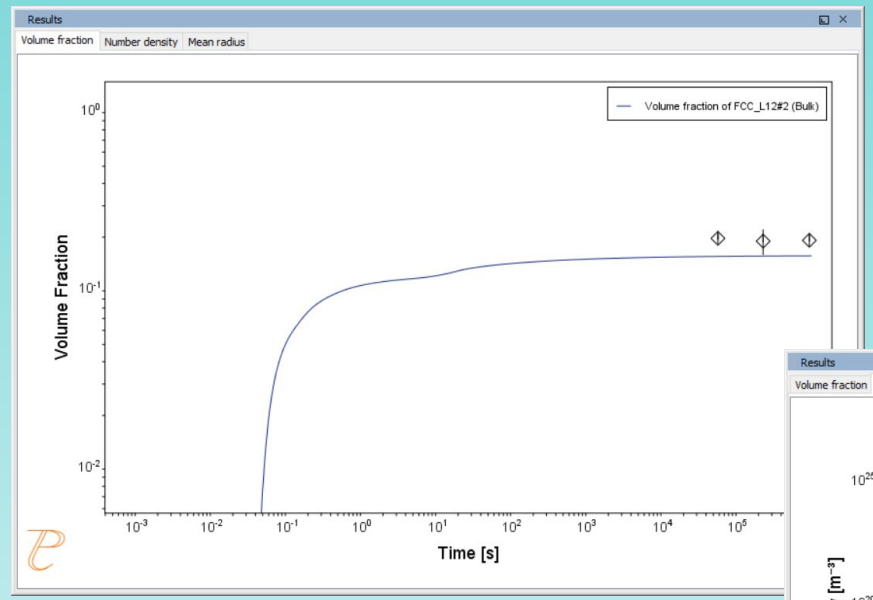
Growth



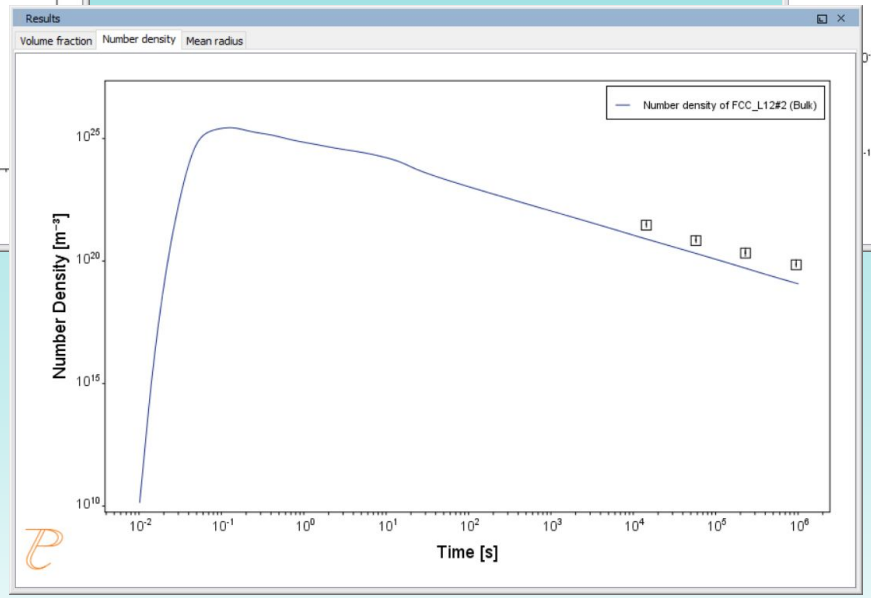
Output

Also:

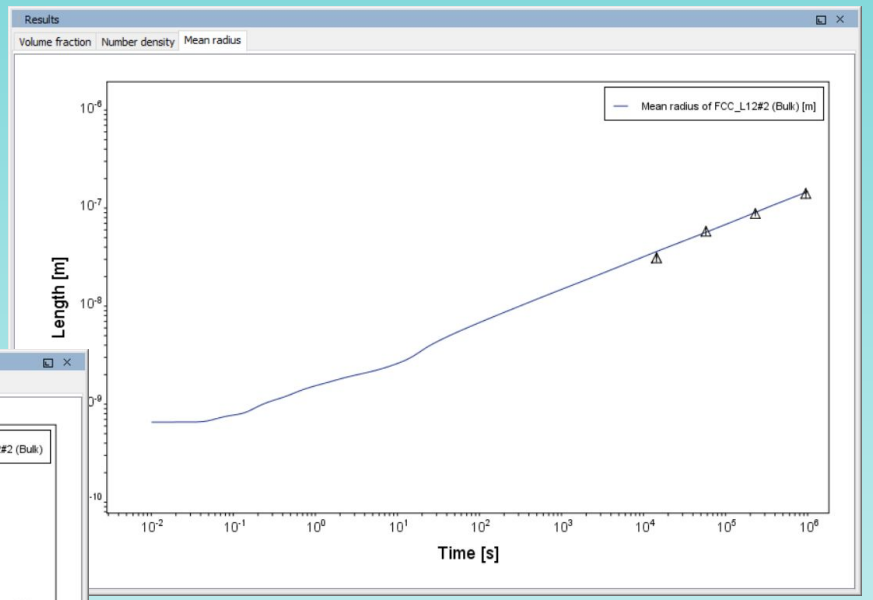
- Particle size distribution
- Matrix composition
- Nucleation rate
- Critical radius
- Driving force
- TTP/CCP diagrams



Volume Fraction



Number Density



Mean Radius

Microstructure modeling during specified heat treatments

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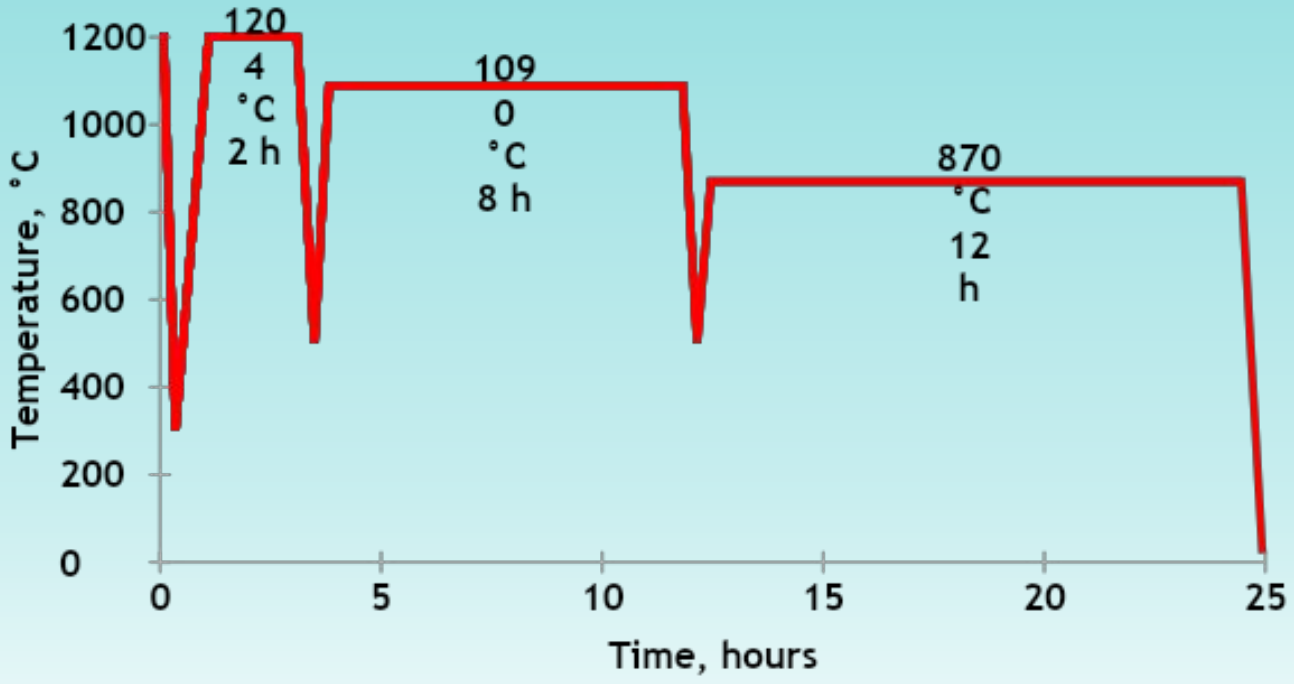
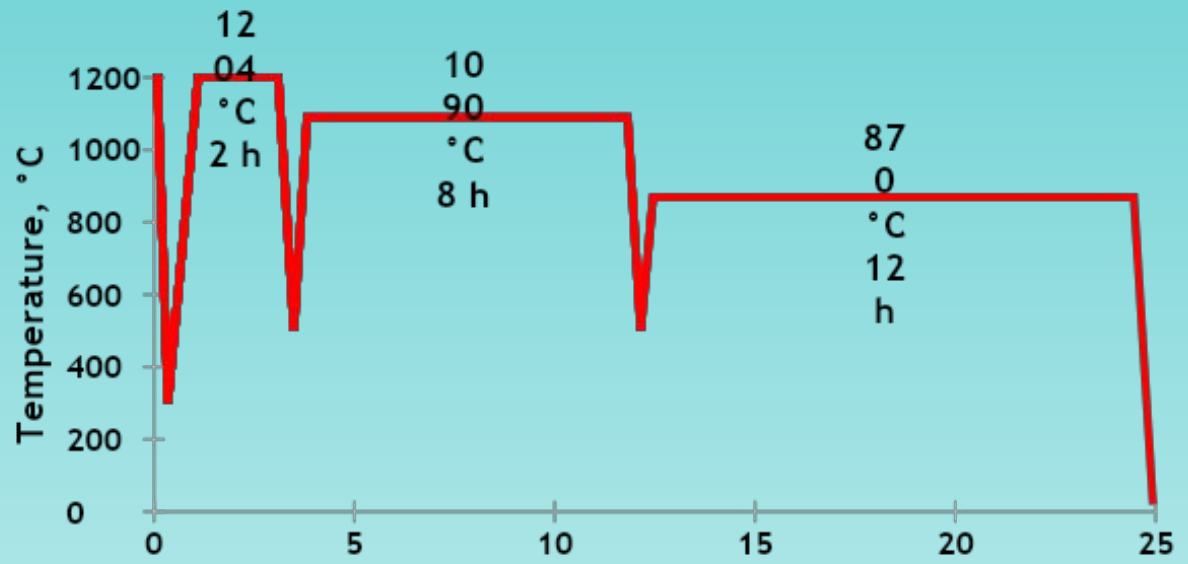
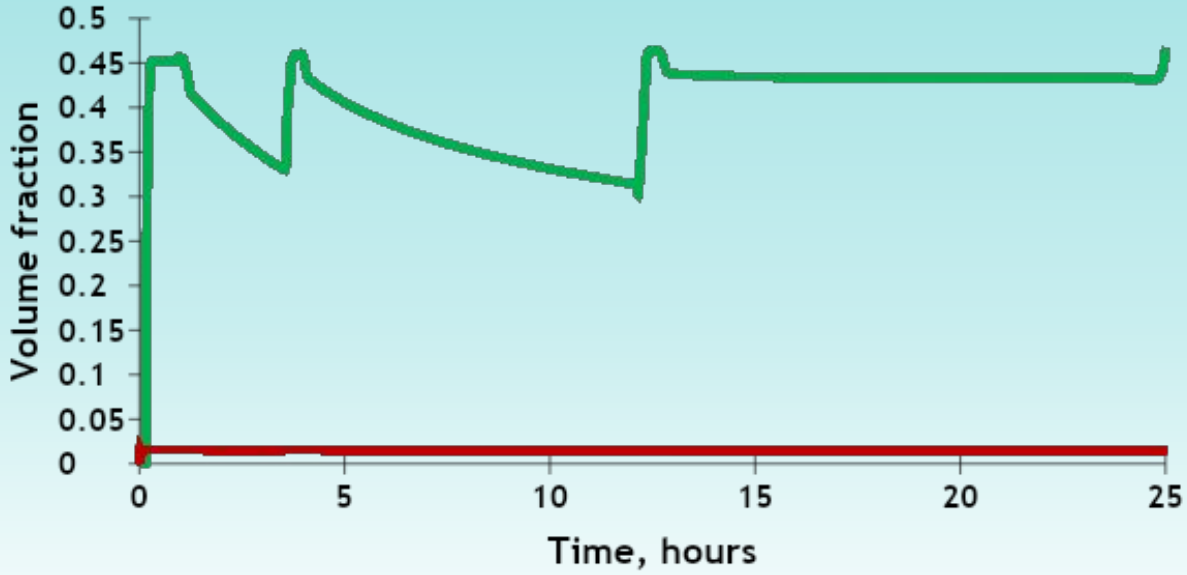
Composition, %											
Ni	C	Cr	Co	W	Ti	Al	B	Zr	Nb	Ta	Mo
base	0.17	14	9.5	4	5	3	0.015	0.052	0.1	0.1	4

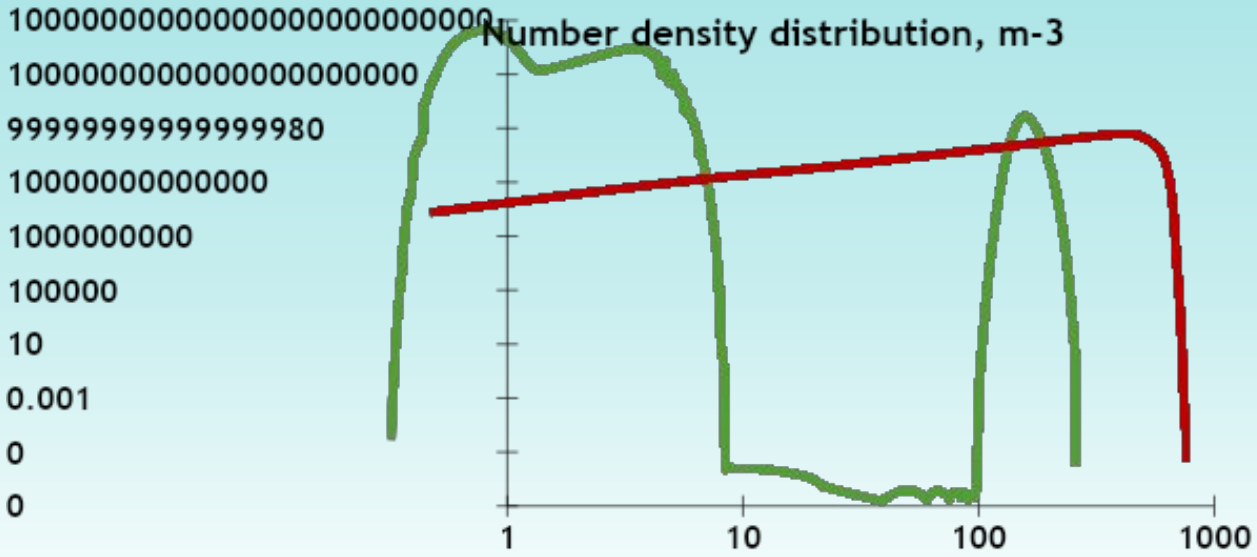


Settings	
Matrix	γ
Growth rate model	Simplified
Nucleation sites	Dislocations, grain boundaries
Interfacial energy	
Molar volume	
Nucleation sites	Dislocations
Interfacial energy	
Molar volume	
Nucleation sites	Dislocations
Interfacial energy	
Molar volume	
Nucleation sites	Dislocations
Interfacial energy	
Molar volume	

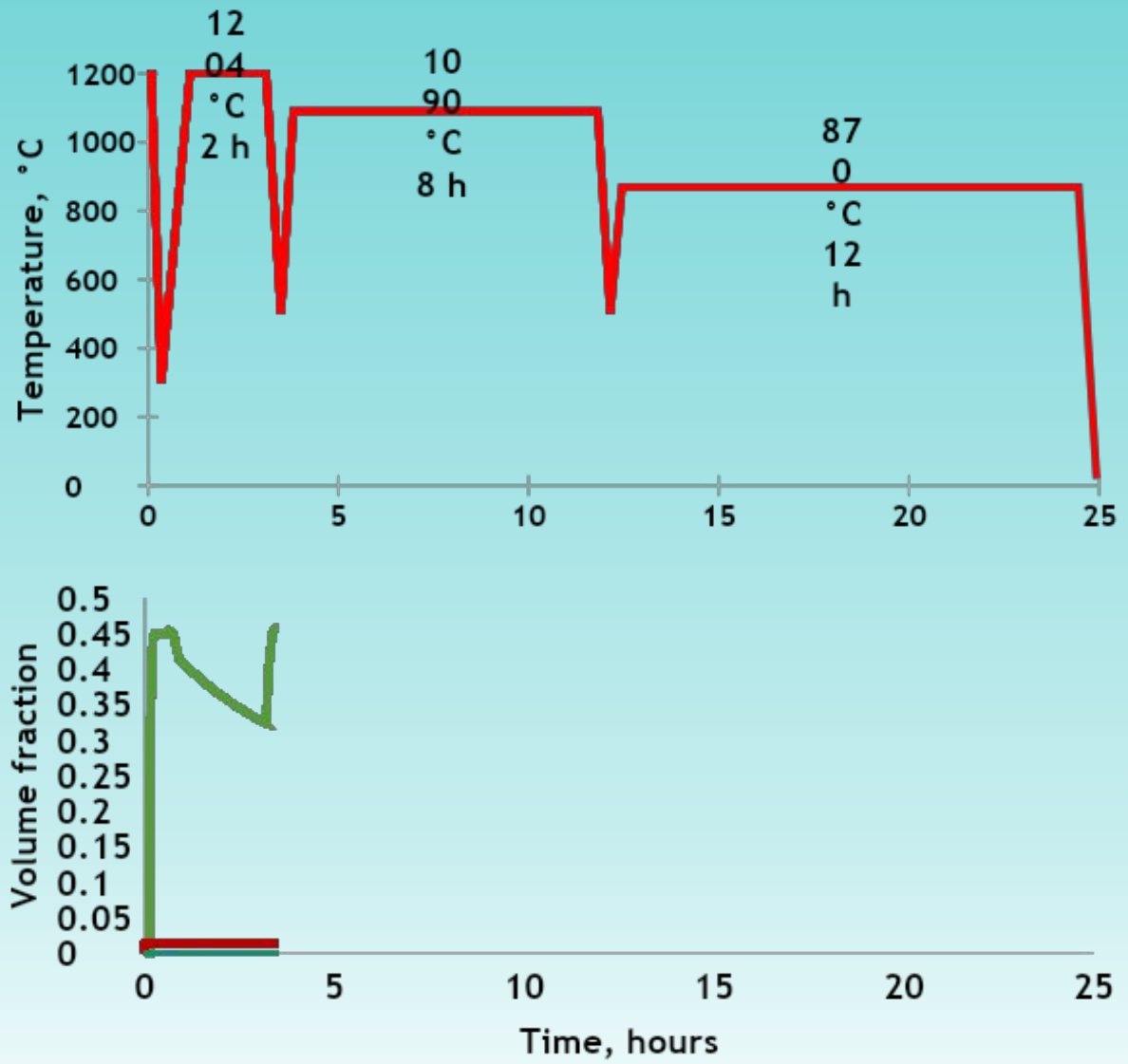
Results #1


12
04
°C
2 h
10
90
°C
8 h
87
0
°C
12
h
Temperature, °C
1200
1000
800
600
400
200
0
0
5
10
15
20
25


Volume fraction
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0
5
10
15
20
25
Time, hours


Number density distribution, m-3
1000000000000000000000000000
100000000000000000000
99999999999999980
10000000000000
1000000000
100000
10
0.001
0
0
1
10
100
1000

Results #2


12
04
°C
2 h
10
90
°C
8 h
87
0
°C
12
h
Temperature, °C
1200
1000
800
600
400
200
0
0
5
10
15
20
25
Volume fraction
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0
5
10
15
20
25
Time, hours