

Modeling of microstructure evolution and properties for Ni-based superalloys

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

Brief overview of Ni-based superalloys

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

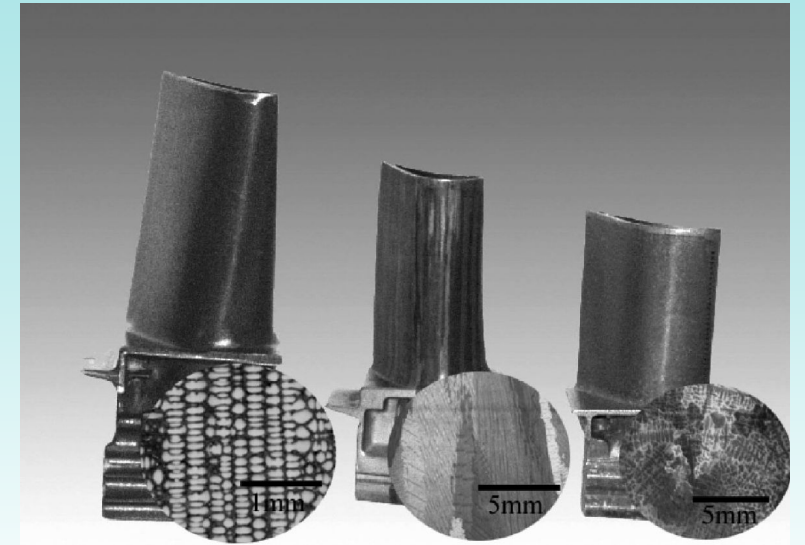
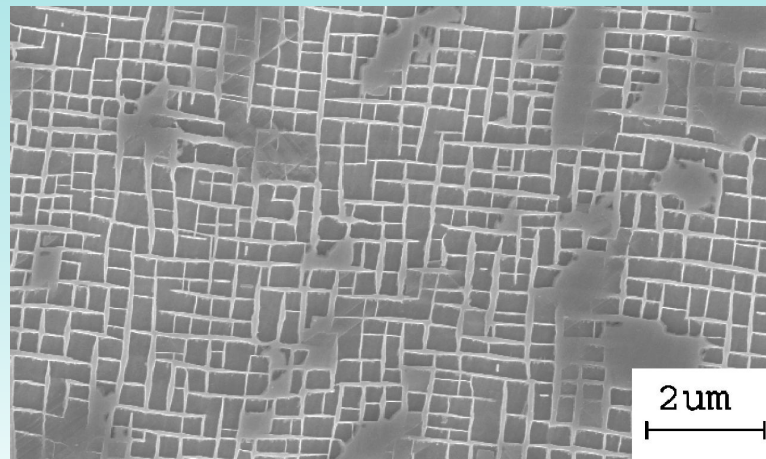
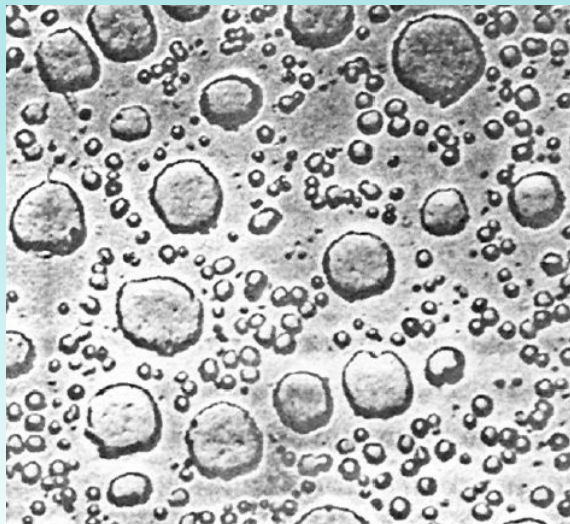
IIA	IIIA	IVB						
	B 0.097	C 0.077						
	Al 0.143		IVA	VA	VIA	VIIA	VIIIA	VIIIA
		Ti 0.147	V 0.132	Cr 0.125		Fe 0.124	Co 0.125	Ni 0.125
	Y 0.181	Zr 0.158	Nb 0.143	Mo 0.136		Ru 0.134		
		Hf 0.159	Ta 0.147	W 0.137	Re 0.138			

γ' former
 Minor alloying additions
 γ former

Element (pointing to C)
 Atomic Radius (nm) (pointing to 0.077)

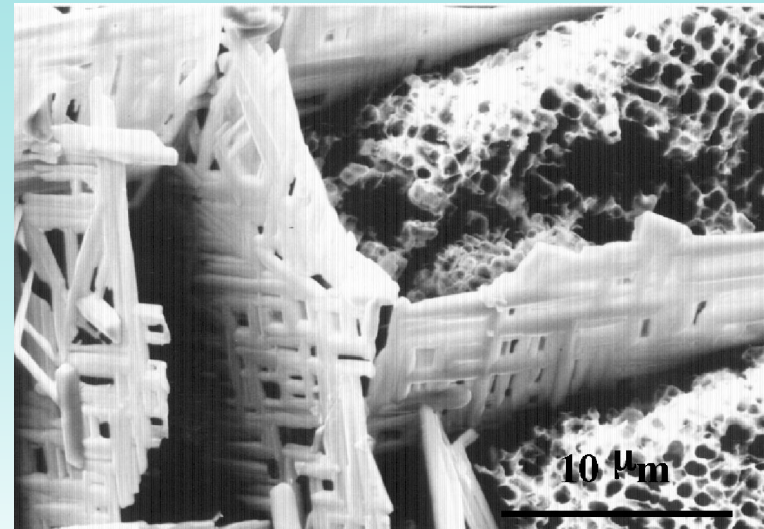
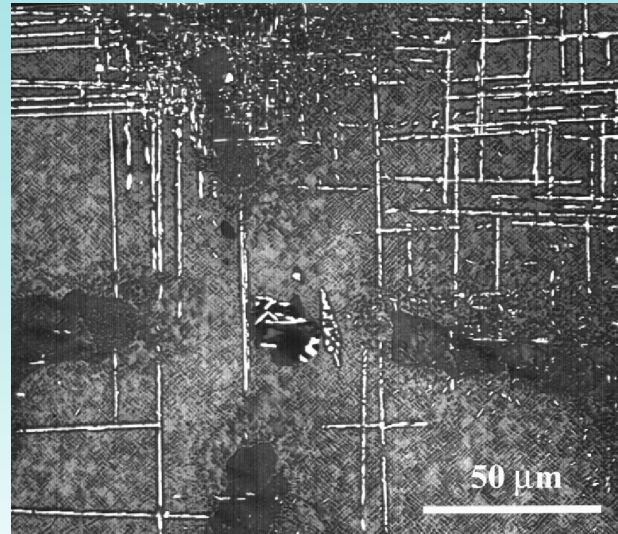
Strengthening mechanisms

- 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

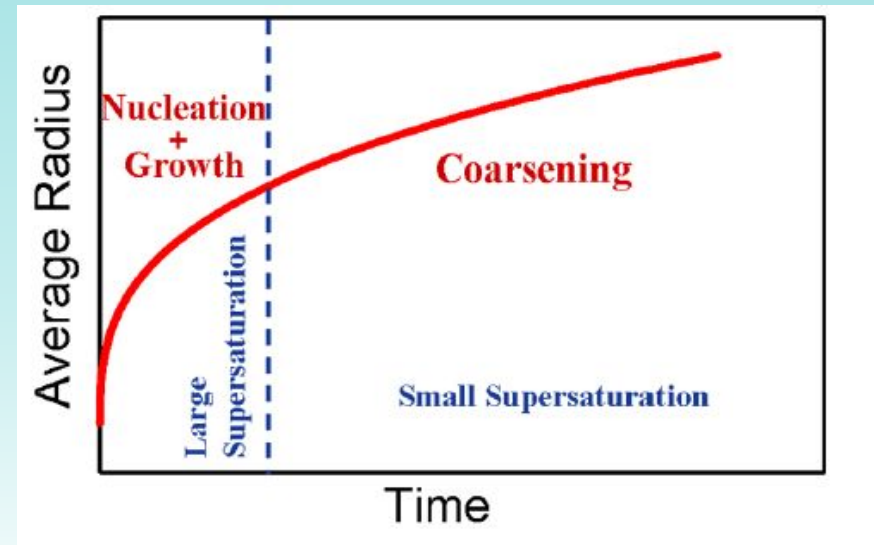
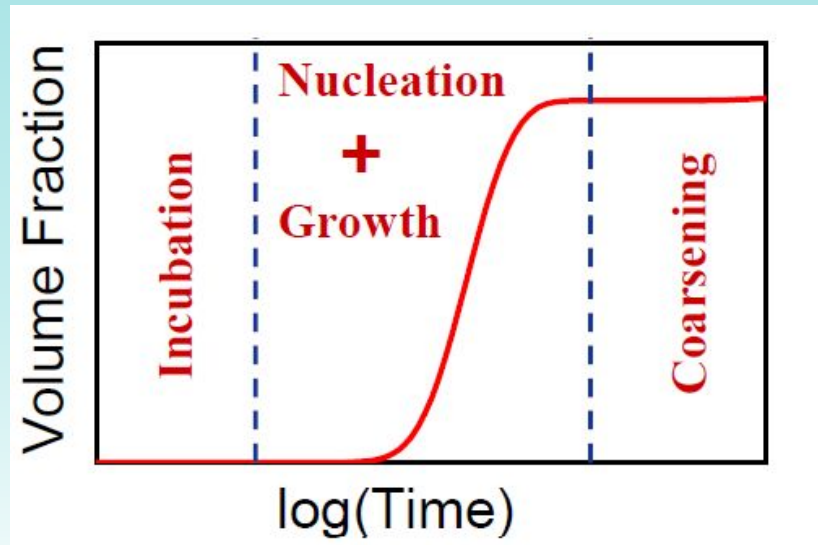


Computational model development

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

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

where

σ - interfacial energy of the matrix/particle interface

$\Delta G_m^{\alpha \rightarrow \beta}$ - 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

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

where

v' - corrected velocity

$\langle r \rangle$ - mean radius

N_V - number density

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

Advanced model - identifies the operating tie-line

For *coarsening* the growth equation is applied

Input

Nucleation

Growth

Configuration

Precipitation Calculator 1

Conditions Options

Composition unit: Mole percent

Composition Al 99.82

Composition Sc 0.18

Matrix Phase

Phase: FCC_A1

Elastic properties: Disregard

Molar volume: Database 7.0E-6 m³/mol

Grain size: 1.0E-4 m

Grain aspect ratio: 1.0

Dislocation density: 5.0E12 m⁻²

Mobility enhancement prefactor: 1.0

Mobility enhancement activation energy: 0.0 J/mol

Precipitate Phase

Phase: AL3SC

Nucleation sites: Bulk ☒ Calculate from matrix settings 8.603059285714286E28 m⁻³

Interfacial energy: Calculated with prefactor 1.0

Growth rate model: Simplified

Morphology: Sphere

Transformation strain: Disregard

Molar volume: Database 7.0E-6 m³/mol

Phase boundary mobility: 10.0 m⁴/Js

Phase energy addition: 0.0 J/mol

Approximate driving force: ☐

Preexisting size distribution: ☐ Edit particle size distribution

Calculation Type

☒ Isothermal ☐ Non-isothermal ☐ TTT diagram ☐ CCT Diagram

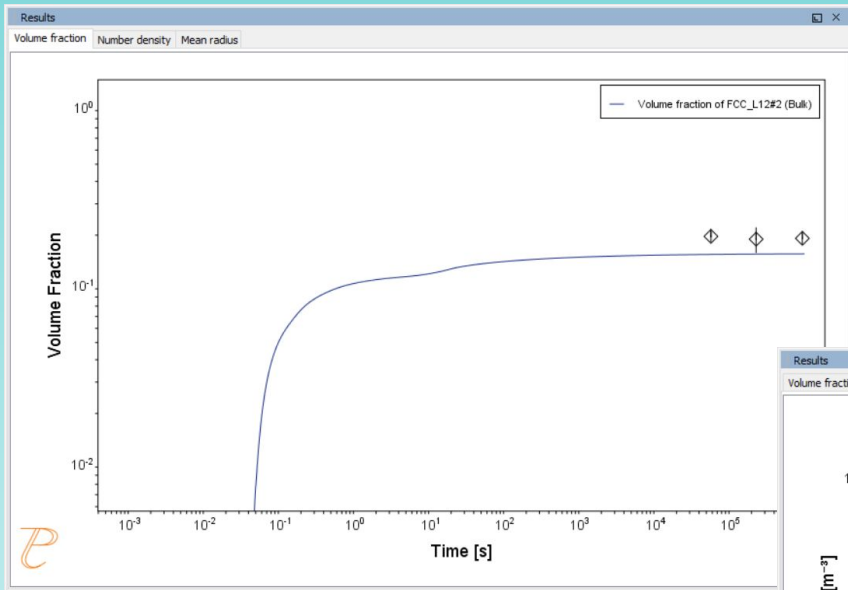
Temperature: 350.0 Celsius

Simulation time: 1.0E7 Seconds

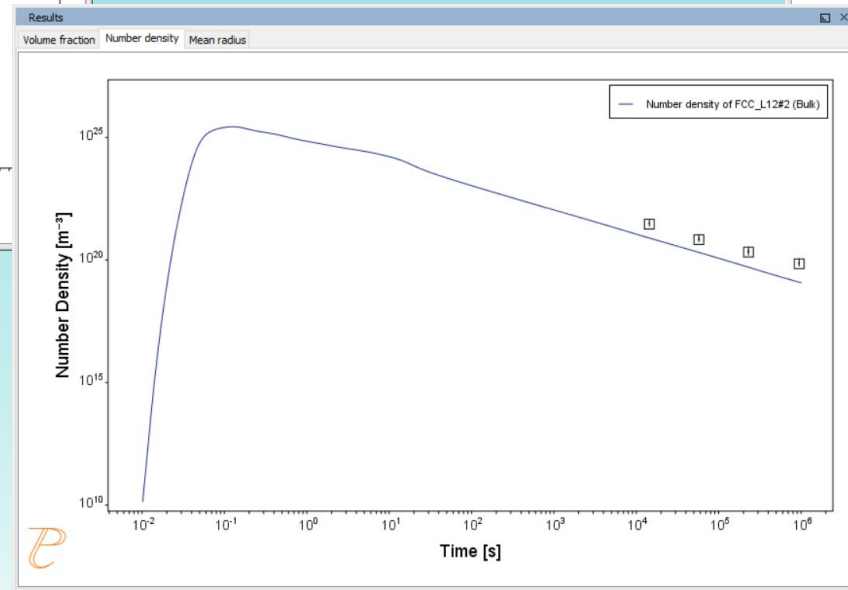
Output

Also:

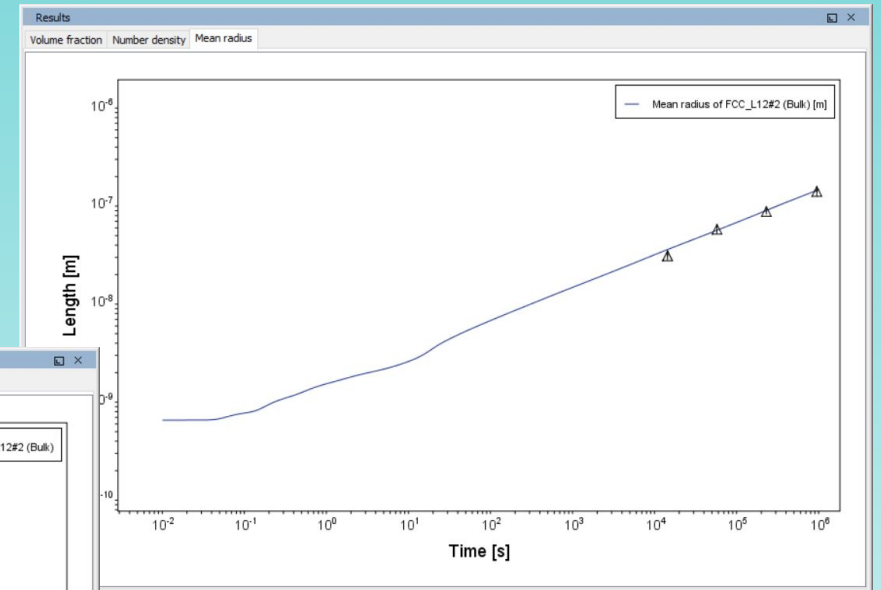
- Particle size distribution
- Matrix composition
- Nucleation rate
- Critical radius
- Driving force
- TTP/CCP diagrams



Volume Fraction



Number Density

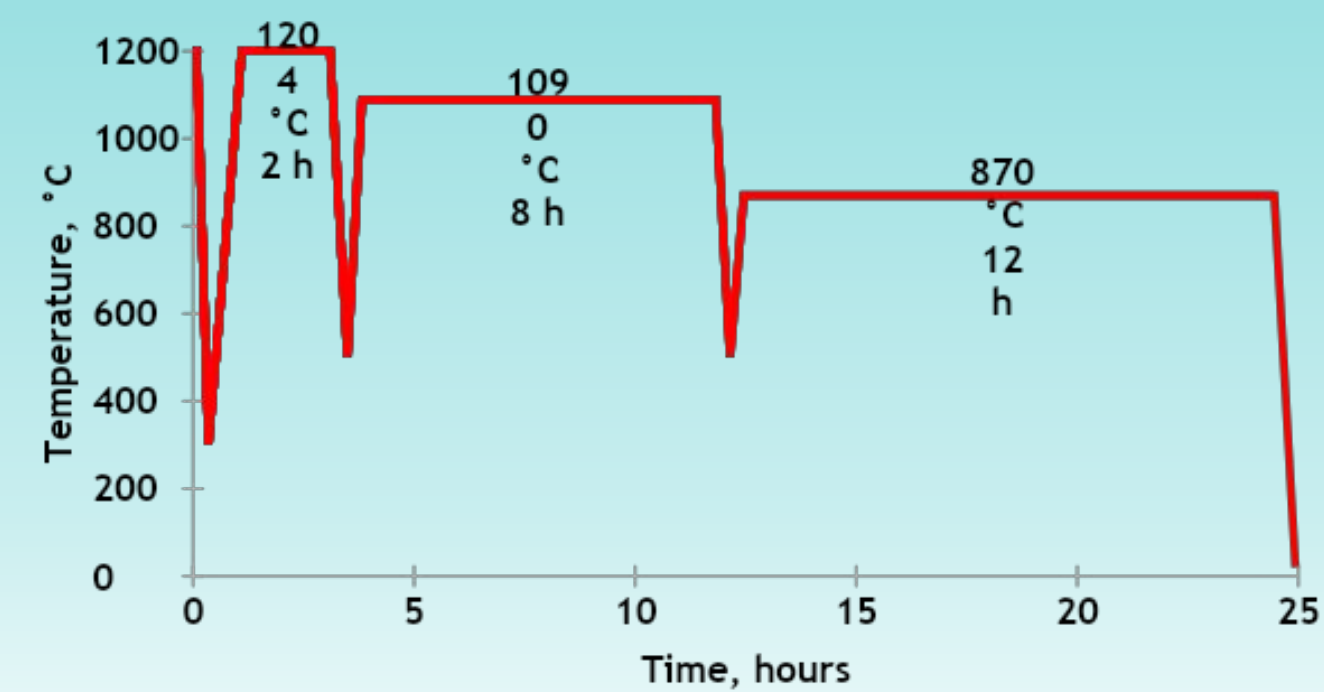


Mean Radius

Microstructure modeling during specified heat treatments

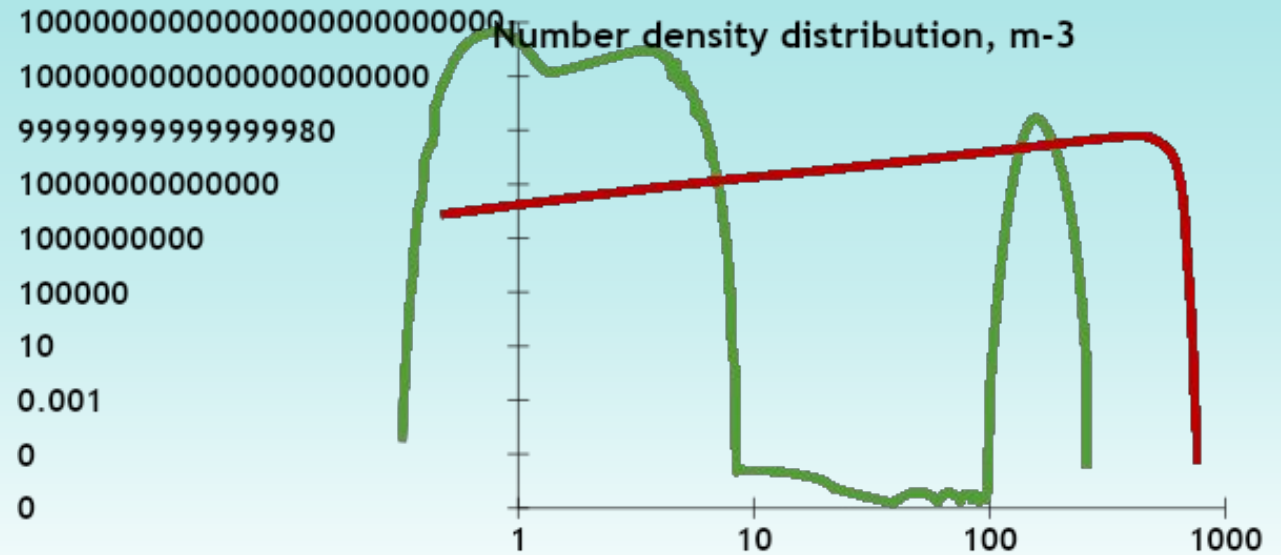
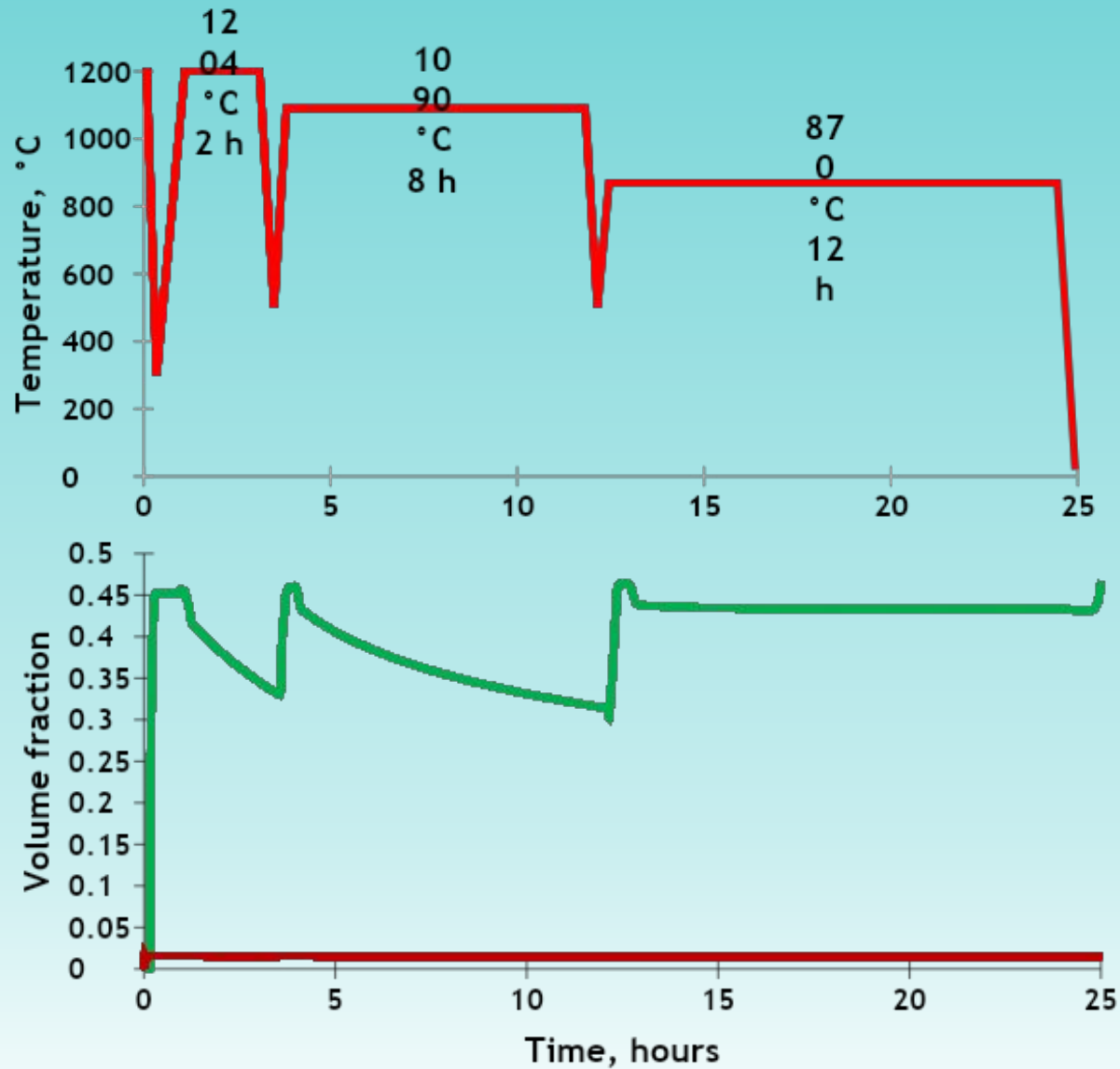
Rene 80

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	
14	

Results #1



Results #2

