

Modeling of microstructure evolution and properties for Ni-based superalloys

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- Computational model development
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- 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 ' (Ni₃Al)

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

IIA	IIIA	IVB	_ /	Elemen	nt			
	B 0.097	C 0.077		-Atom	ic Radiu	ıs (nm)		
	Al 0.143	IVA	VA	VIA	VIIA	VIIIA	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								

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 \implies Growth/dissolution \implies Coarsening



Nucleation rate

$$J = N_{v} Z \beta^{*} e^{-\frac{\Delta G^{2}}{kT}} e^{-\frac{\tau}{t}}$$

where

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

 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

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

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

where

 \boldsymbol{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

	Configuration 과 무 ×					
	Precipitation Calculator 1					
	Conditions Options					
Innut	Composition unit: Mole percent 🗸					
INPUL	Composition Al 99.82					
	Composition Sc 0.18					
	Matrix Phase					
	Phase: FCC_A1 ~					
	Elastic properties: Disregard V					
	Molar volume: 7.0E-6 m ³ /mol					
Nucleation	Grain size: 1.0E-4 m v					
Nucleation	Grain aspect ratio: 1.0					
	Dislocation density: 5.0E12 m ⁻²					
	Mobility enhancement prefactor: 1.0					
	Mobility enhancement activation energy: 0.0 J/mol					
	O Precipitate Phase					
	Phase: AL3SC 🗸					
	Nucleation sites: Bulk V Calculate from matrix settings 8.603059285714286E28 m ⁻³					
	Interfacial energy: Calculated v with prefactor 1.0					
	Growth rate model: Simplified V					
Crowth	Morphology: Sphere V					
Growin — — —	Transformation strain: Disregard 🗸					
	Molar volume: V 7.0E-6 m ³ /mol					
	Phase boundary mobility: 10.0 m ⁴ /Js					
	Phase energy addition: 0.0 J/mol					
	Approximate driving force:					
	Preexisting size distribution: Edit particle size distribution					
	Calculation Type					
	Isothermal Non-isothermal OTTT diagram OCCT Diagram					
	Temperature: 350.0 Celsius					
	Simulation time: 1.0E7 Seconds					
	· ·					

Output



Also:

Number Density

Microstructure modeling during specified heat treatments

Rene 80

Composition, %											
Ni	С	Cr	Со	W	Ti	Al	В	Zr	Nb	Та	Мо
base	0.17	14	9.5	4	5	3	0.015	0.052	0.1	0.1	4



Matrix Y Growth rate model Simplified Nucleation sites Dislocations, grain boundaries Interfacial energy Molar volume Dislocations Nucleation sites Interfacial energy Molar volume Nucleation sites Dislocations Interfacial energy Molar volume Nucleation sites Dislocations Interfacial energy Molar volume 14



