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The compositional dependence of the microstructure and properties of CMSX-4 superalloys

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Novel Aerospace Materials

Introduction

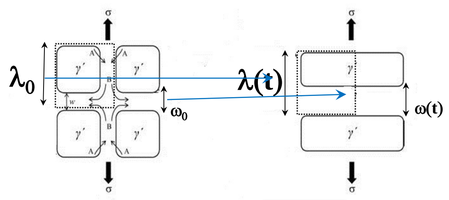
The degradation of creep resistance in Nickel-based single crystal superalloys is essentially ascribed to their microstructure evolution. Yet there is a lack of work that manages to predict (even qualitatively) the effect of alloying element concentrations on the rate of microstructure degradation. In this research, a computational model is presented to connect the rafting kinetics of Ni superalloys to their chemical composition by combining thermodynamics calculation and a modified microstructure model. To simulate the evolution of key microstructural parameters during creep, the isotropic coarsening rate and γ/γ′ misfit stress have been defined as composition related parameters, and the effect of service temperature, time and applied stress are taken into consideration. Two commercial superalloys for which the kinetics of the rafting process are selected as the reference alloys, and the corresponding microstructural parameters are simulated and compared with experimental observations reported in the literature. The results confirm that our physical model not requiring any fitting parameters manages to predict (semi-quantitatively) the microstructure parameters for different service condition, as well as the effects of alloying element concentrations. The model can contribute to the computational design of new Ni-based superalloys.

Model construction

Model background

1. Fedelich's phenomenological model:

*Based on CMSX-4@950°C



$$\lambda(t) = \lambda_0\sqrt{1+\beta t}$$

$$\xi = 1 - \exp(-b\sigma^n t)$$

In which

$$\xi = \frac{\omega(t) - \omega_{cube}(t)}{\omega_{raft}(t) - \omega_{cube}(t)}$$

$$\omega_{cube}(t) = (1 - \sqrt[3]{f})\lambda(t)$$

$$\omega_{raft}(t) = (1-f)\lambda(t)$$

➡ ***ω(t)=Func(time, stress)***

2. Fan's model

*Based on CMSX-4

- **λ increase: Driven by interfacial energy**

$$\lambda(t)^3 - \lambda_0^3 = \frac{BQ}{RT}t$$

- **ω : Driven by strain energy**

$$\dot{\xi} = A(1-\xi)F^n e^{-\frac{Q}{RT}}$$

In which

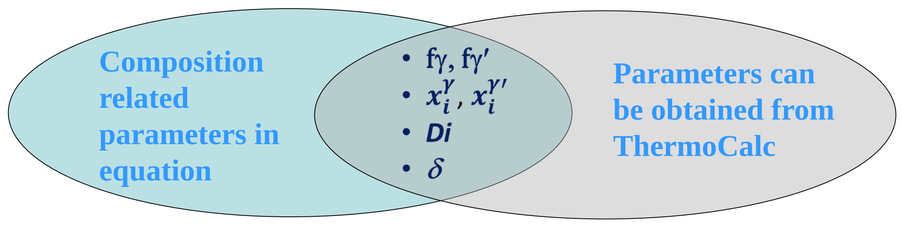
$$F = -\frac{\partial \psi}{\partial \xi};$$

$$\psi = (1 - c\xi)\frac{1+v}{3E}\sigma_s^2$$

***From fitting parameters to physical parameters**

➡ ***ω(t)=Func(time, temperature,stress)***

Model development



- **For isotropic coarsening rate: Oswald ripening**

$$\boldsymbol{\lambda(t)^3 - \lambda_0^3 = Kt}$$

In which

$$\boldsymbol{K = 8\gamma V_m^p / \sum_{i=1}^{n} \frac{9\left(x_i^p - x_i^{mp}\right)^2}{x_i^{mp} D_i / RT}}$$

- **For lattice misfit stress:**

$$\boldsymbol{\sigma_s = |\sigma_p + \sigma_\delta|}$$

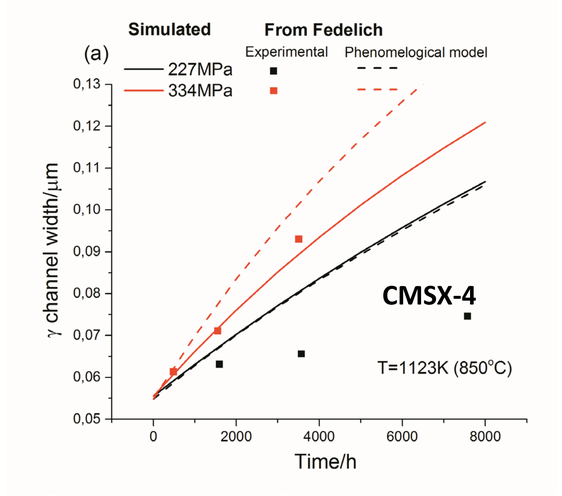
In which

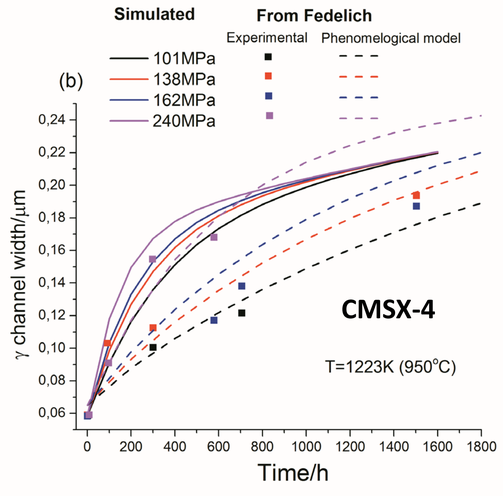
$$\boldsymbol{\sigma_\delta = |E\delta|}$$

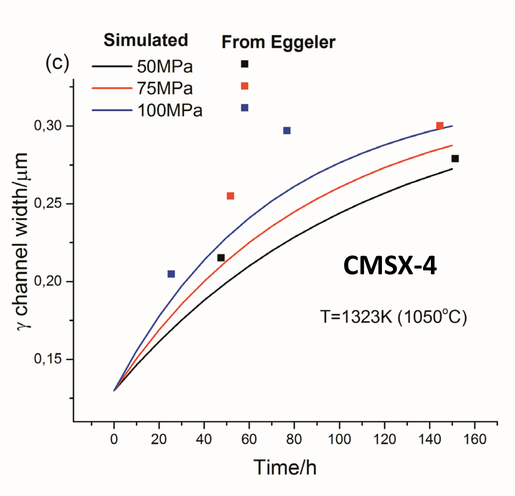
$$\omega(t) = \omega_{cube}(t) + [\omega_{raft}(t) - \omega_{cube}(t)]\left\{1 - \exp[-A'' \exp(-\frac{Q}{RT})t]\right\}$$

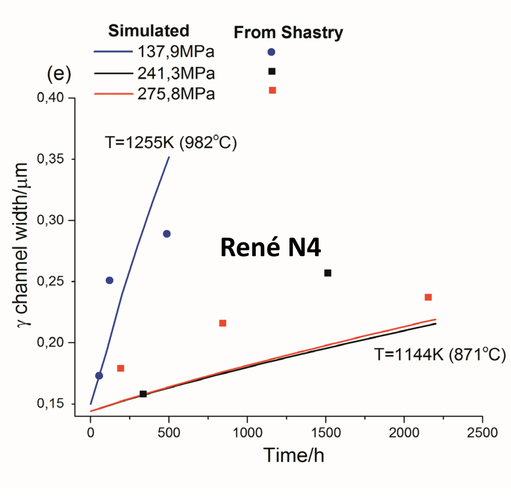
➡ ***ω(t)=Func(time, stress, temperature, chemical composition)***

Model validation



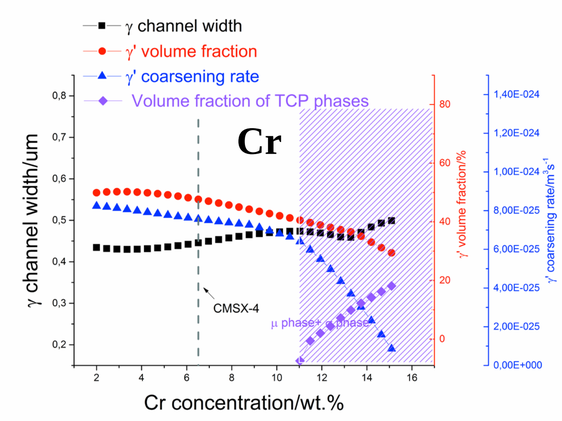


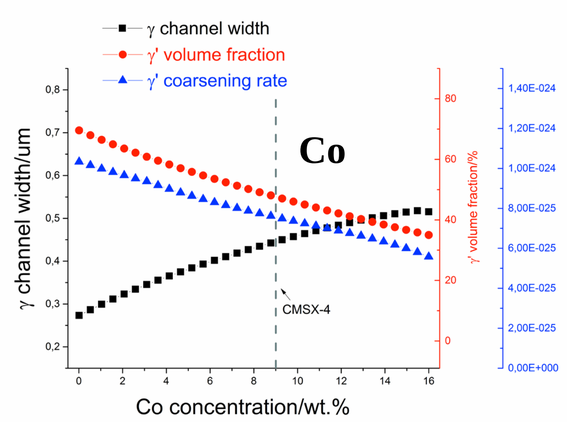


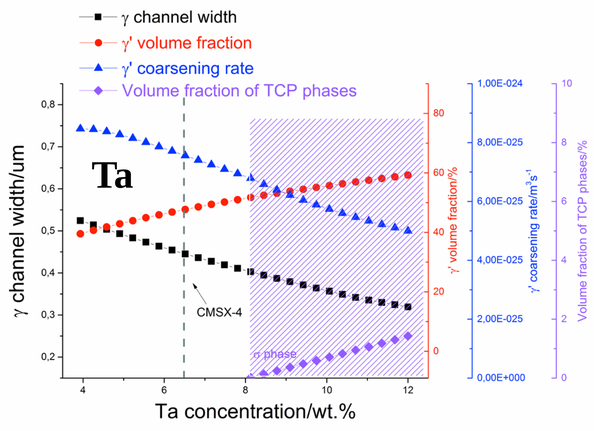


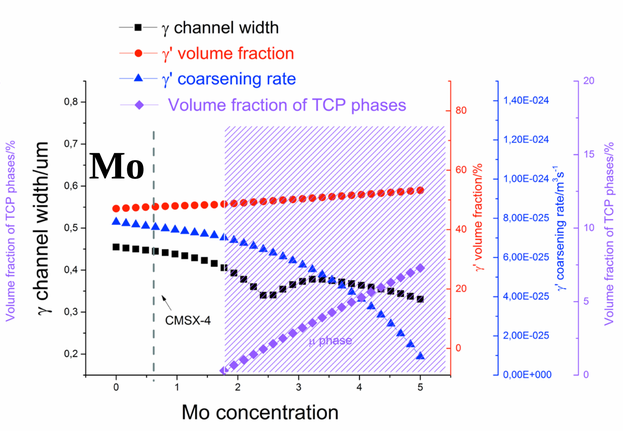
Model prediction

***CMSX-4**









Conclusion

- **A computational model: the microstructural stability of Ni-SX superalloys as a function of temperature and applied tensile stress**
- **The microstructure characteristics of rafting process: γ channel widening of Ni commercial grades can be well simulated by the model**
- **The effects of alloying elements on the microstructures: chemical composition in Cr, Co, Ta, Mo can be improved in CMSX-4**

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