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Yield strength prediction in Ni-base alloy 718Plus based on thermo-kinetic precipitation simulation

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ABSTRACT

The yield strength of Allvac® 718Plus™ during aging is computed using integrated physical models that take into account intrinsic, grain boundary, solid solution and precipitate strengthening contributions. Precipitation strengthening of γ′ has the main effect on the final yield strength in this alloy during aging, with the coherency and anti-phase boundary effects providing the major strengthening contributions. We utilize transmission electron microscopy to obtain the unknown physical parameters entering the strengthening models and compare precipitate size and distribution with the simulation results.

1. Introduction

The performance of gas turbines and aero-engines can be improved by increasing the operating temperature of these devices. Whereas the Ni-base superalloy Inconel 718 shows superior mechanical properties up to 650 °C [1], the alloy Allvac® 718Plus™ (hereafter 718Plus) developed by ATI Allvac in 2004 can be operated at even 55 K higher service temperature. This advantage is accomplished by alloying with Co and W, and adjusting the Al/Ti ratio, altogether favoring the formation of ordered cubic $L1_2$-type $(Ni,Co)_3(Al,Ti,Cr,Nb,W)$ γ′ over tetragonal $D0_{22}$-type ordered metastable $(Ni)_3(Nb)$ γ″ [2]. To demonstrate the effect of alloying elements on the phase stabilities at high temperatures, in Fig. 1, the computed molar equilibrium phase fraction of γ′ and of metastable γ″ (the equilibrium phase δ suspended) with the thermodynamic database mc_ni_v2.003 [3] at 700 °C is presented as a function of the Al/Ti and Co/Fe ratios at constant weight fractions $w(Nb)=0.055$, $w(Mo)=0.03$, $w(Cr)=0.17$ and $w(Ti)+w(Al)=0.02$, $w(Co)+w(Fe)=0.18$, representing typical sums of γ′-forming alloying elements.

In contrast to the γ″ phase, which has a weakening effect on the material as it transforms to orthorhombic thermodynamic equilibrium Ni_3Nb (δ-phase) under long-term operation, γ′ remains stable and coherent even in over-aged conditions [1,4]. This should be beneficial in terms of precipitation strengthening, which is investigated in the present study by mechanical tensile testing combined with microstructural analysis using transmission electron microscopy (TEM). On comparison of the experimental results with our yield strength modeling and simulation, we were able to determine the prevailing physical strengthening mechanisms. For yield strength modeling, we used an integrated approach considering all types of contributions to the final yield strength (σ_y), which have been implemented in the solid-state transformation kinetics software MatCalc, version 5.60 (rel 0.005) [5–7] by the authors of this paper. In the description of strengthening mechanisms, the main focus is on the shearing of γ′ precipitates with anti-phase boundary (APB) and coherency effects. These are observed to be the dominating mechanisms over the modulus effect, since similar shear moduli of matrix and γ′ precipitates will not produce high resistance forces in front of a moving dislocation [8,9]. The interfacial effect is assumed to play only a minor role, too [9,10].

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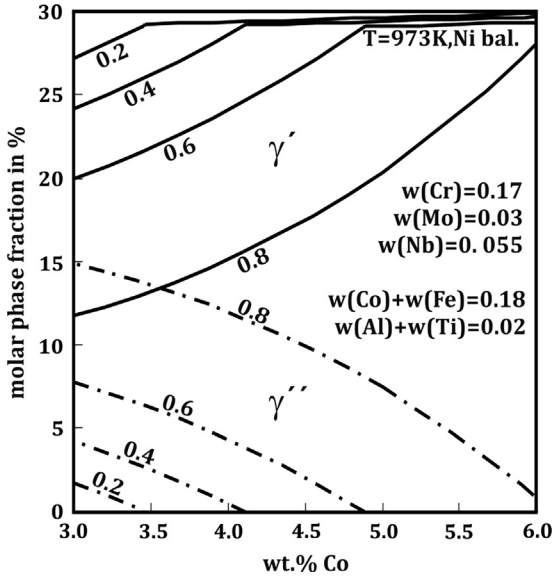

Fig. 1. Computed molar phase fractions of γ′ and γ″ (delta phase suspended in the calculation) at Al/Ti wt. ratios from 0.2 to 0.8 and varying Co-content.

Table 1
Chemical composition of 718Plus.

	Al	Co	Cr	Nb	C	Fe	Mo	Ti	W	Ni
wt. %	1.46	9.13	17.42	5.48	0.028	9.66	2.72	0.71	1.04	Balanced

2. Experimental

Hardness and compression tests of heat-treated 718Plus samples were used to analyze changes of precipitation hardening as a function of aging time. The composition of 718Plus used in this survey is given in Table 1.

A conventional heat treatment process is applied in this work. The specimens are solution annealed at 975 °C for 60 min, continued by water quenching and aging at 788 °C temperatures for different aging times (1, 5, 10, 25 and 50 h). Vickers hardness is determined using a Reichert-Jung Micro Duromat 4000 hardness tester equipped with a Vickers diamond pyramid indenter. The compression tests are reproduced twice for each point using a Bähr-Thermoanalyse DIL805A/D quenching and deformation dilatometer. The dimensions of the cylindrical specimens are 4 mm diameter and 8 mm length.

The specimens for TEM investigation are ground with silicon carbide paper to approximately 0.1 mm and electro-polished in a solution containing 5% perchloric acid and 95% ethanol at 32 V and −10 °C. They are cleaned in He plasma to remove all the oxides and impurities of the surface. An FEI Tecnai F20 FEGTEM is utilized at 200 kV acceleration voltage for microstructure analysis.

Transmission electron microscopy (TEM) was used to determine the mean radius, number density and phase fraction of the γ′ precipitates. Dark-field imaging was used to resolve the individual precipitates, combining the diffracted beams arising from the unique chemical ordering of the γ′ phase. Approximately 1000 precipitates were measured in Digital Micrograph for each heat treatment to determine the mean radius. Number density and phase fraction were calculated by measuring the number of precipitates in a known volume of the specimen. The volume was determined by area measurement from TEM images and thickness measurement using electron energy-loss spectroscopy (EELS) and the standard log-ratio method described in [4]. Only regions less than 100 nm thickness were used for this analysis to avoid inaccuracy due to overlap of precipitates. A correction factor was applied, according to the procedure described in [4], to correct for the fact that a proportion of precipitates intersect the foil surface.

3. Modeling of precipitation

To calculate the nucleation rate J of γ′ precipitates per unit volume and time, the classical nucleation theory [11] is used:

$$J = N_0 Z \beta^* \exp\left(\frac{-G^*}{k_B T_k}\right) \exp\left(\frac{\tau_{incub}}{t}\right), \quad (1)$$

where N_0 is the number of potential nucleation sites, Z is the Zeldovich factor, β^* is the condensation rate of solute atoms at a cluster of critical size, k_B is the Boltzmann constant, T_k is temperature, G^* is the energy required to form a nucleus of critical radius, τ_{incub} is the incubation time and t is time. G^* depends on the chemical driving force evaluated by CALPHAD-type thermodynamic parameters stored in mc_ni_v2.003, and the interfacial energy between matrix and precipitate. The interfacial energy is evaluated with the generalized broken bond (GBB) approach as described in Ref. [12] and taking into account interfacial curvature size effects [13].

The precipitate growth kinetics is simulated with the SFFK mean-field model for multi-component multi-phase systems [5,6]. In a precipitation environment of an arbitrary number of spherical particles nucleating and growing in a unit volume of matrix phase, the total Gibbs energy of the system is described by

$$G = \sum_{i=1}^{n} N_{0i}\mu_{0i} + \sum_{k=1}^{m} \frac{4\pi\rho_k^3}{3}\left(\lambda + \sum_{i=1}^{n} c_{ki}\mu_{ki}\right) + \sum_{k=1}^{m} 4\pi\rho_k^2\gamma, \quad (2)$$

where N_{0i} is the number of moles of component i in the matrix phase and λ is the contribution from elastic energy. μ, ρ and c denote chemical potential, radius and concentration, respectively. The index k refers to the index of individual precipitate size classes [6].

During isothermal heat treatment, the total free energy of the system decreases and the precipitate microstructure evolves. The difference in free energy between the initial and the evolved state is dissipated. The free energy dissipation takes place by interface movement, diffusion of atoms inside of the precipitates and diffusion of atoms in the matrix. The total rate of dissipation is given as the sum of these individual contributions. The rate of total free energy change is connected with the free energy dissipation rate using the thermodynamic extremum principle [14–16], and the system evolution is given by a set of linear equations, in which the rate of radius and chemical composition change of each precipitate is evaluated. To determine the evolution of the entire precipitate population, the rate equations are integrated numerically under the constraint of mass conservation. The integration is carried out based on the numerical Kampmann–Wagner approach [6,17]. For every time increment in the precipitation simulation and for each precipitating phase, the growth kinetics and the change in composition are evaluated based on the evolution equations [5] and the nucleation rate expression Eq. (1). Further details about the models and the numerical treatment of the evolution equations are given by Svoboda et al. [5] and Kozeschnik [18]. In MatCalc, the evolving precipitate properties under user-defined heat treatments are directly used for the simulation of yield strength.

4. Yield strength modeling

The final yield strength (σ_y) in annealed crystalline materials is constituted by grain boundary strengthening ($\sigma_{y,g}$), solid solution