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Luc Rougier, Alain Jacot, Charles-André Gandin, Paolo Di Napoli, Pierre-Yvan Théry, et al.. Numerical Modeling of Microstructure Formation during Solidification and Heat Treatments of Ni-base superalloys. Journées Annuelles de la SF2M 2012 - SF2M Annual Meeting 2012, Oct 2012, Paris, France. 2 p. hal-00759486

HAL Id: hal-00759486

<https://hal-mines-paristech.archives-ouvertes.fr/hal-00759486>

Submitted on 30 Nov 2012

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Numerical Modeling of Microstructure Formation during Solidification and Heat Treatments of Ni-base superalloys

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Abstract

Numerical models have been developed for the simulation of microstructure formation in Ni-base alloys. The first step consists of a calculation of the segregation of solutal species in the primary solidified γ -phase and formation/dissolution of the interdendritic γ' -phase. Finally, local compositions of solutal species are used to calculate the nucleation, growth and coarsening of γ' -precipitates with a precipitation model.

Introduction

Single crystal Ni-base superalloys exhibit outstanding mechanical properties at elevated temperatures, in particular creep resistance. This feature is closely related with the microstructure, which consists of finely dispersed γ' -precipitates embedded in a γ -matrix. The volume fraction and size distribution of the γ' -precipitates are directly influenced by the initial microstructure prior starting the ageing process. Among the existing numerical models for precipitation [1-3], only a few of them can address the influence of solidification [2, 4]. The present work is an extension of the approach of [2] to Ni-base superalloys, which present additional difficulties associated with non-diagonal terms in diffusion matrices and high volume fractions of precipitates.

Two models were used to simulate the formation and evolution of the microstructure during solidification and heat-treatment. The microsegregation of solutal species was calculated with the Pseudo Front-Tracking (PFT) technique, which is based on the resolution of mass conservation equations over a multiphase domain with a finite volume method [5]. This model can also calculate the formation and dissolution of interdendritic secondary phases during dissolution/homogenization heat treatments performed after the solidification of the alloy [6]. The second model addresses precipitation of γ' in primary γ , which is simulated using a particle size distribution (PSD) model based on the calculation of the evolution of individual precipitate classes [1]. Nucleation is described using the classical nucleation theory (CNT) and an analytical law for the calculation of the growth rate of each class of precipitate size. Curvature effects are taken into account by adding a contribution to the free Gibbs energy of the γ' -phase, which has for effect to modify the equilibrium concentrations at the interface.

In a previous contribution [4], the PSD model alone was applied to the case of γ' precipitation in a Ni-7.56at%Al-8.56at%Cr alloy at 600°C. The simulation results were successfully compared with the experimental results obtained on the same alloy at the same temperature [7, 8].

The present work is focused on chaining the PFT and PSD models. The local concentrations calculated at various locations within the PFT domain are used as inputs to the PSD model, which enables to estimate the potential variations of the precipitation response in terms of γ' fractions and size distribution due to residual microsegregation.

Results

The PFT model was first applied to a Ni-17at%Al-2at%Cr ternary alloy. Figure 1 shows the evolution of temperature and γ' -phase fraction. γ' starts to form at $t=265.09s$, which corresponds to a temperature of 1357.7°C, 195.4°C above the solvus of the nominal composition.

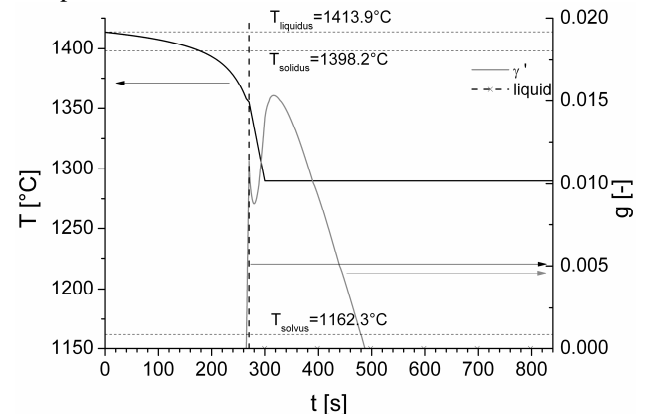


Figure 1: Evolution of temperature and phase fractions during the PFT microsegregation simulations.

After 300s, γ' is temporarily growing in the interdendritic space due to non-equilibrium solidification of γ , which results in solute accumulation in the liquid. After this temporary growth stage, the interdendritic γ' phase dissolves before completely disappearing during the holding stage at an intermediate temperature between the solidus and the solvus of the alloy. Figure 2 shows the evolution of concentration profiles calculated with the PFT model during the solidification and the homogenization heat treatment. The higher Al and Cr concentrations in the liquid phase can be explained by a

preferential partitioning of these elements in the liquid phase. As T decreases, γ' starts to form in the interdendritic area. The distribution of solute elements is changed by the formation of γ' : as compared with γ , γ' contains more Al and less Cr, as shown by the corresponding concentration profiles. The final concentration profiles exhibit concentration differences reaching 2.20% for Al and 0.42% for Cr across the calculation domain. Three local concentrations predicted with the PFT model (A, B and C) were then used as inputs for the PSD model, where, A and C correspond to the extremities of the PFT simulation domain, ($x=0$ and $x = 100 \mu\text{m}$), and B is the nominal alloy composition. A constant temperature of 800°C was used for the PSD calculations. Figure 3 shows the evolution of the average radius R , the total number density N , and the volume fraction of γ' -precipitates. The initial concentration influences the kinetics of the phase transformation and the equilibrium volume fractions, due to the different supersaturations. For all the concentrations considered here, the three main precipitation stages, i.e. nucleation, growth and coarsening are observed.

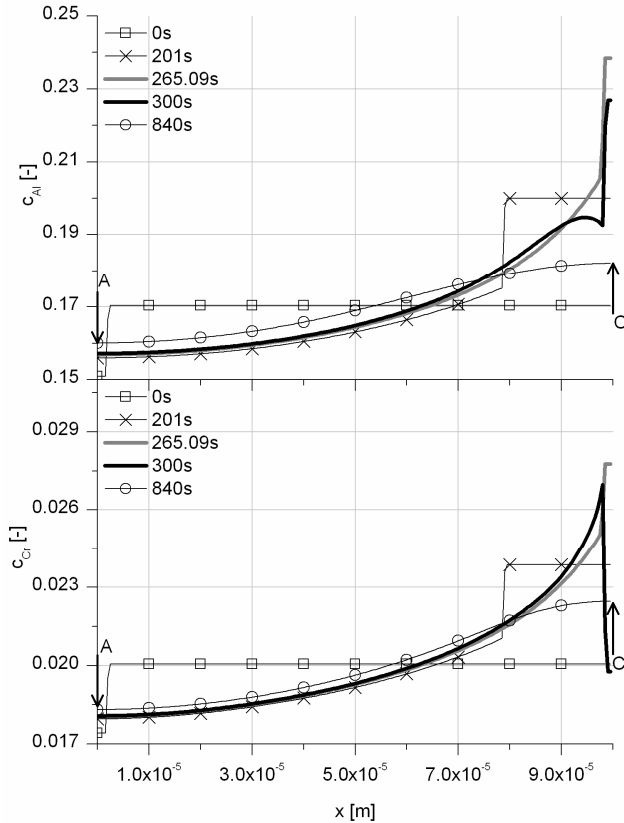


Figure 2: Concentration profiles during the solidification and dissolution/homogenization heat treatments.

Nucleation translates into a quick increase of the precipitate density, while the γ' -fraction evolves slowly. Growth occurs simultaneously, which has the effect of increasing the γ' -fraction and reducing the supersaturation. A growth controlled regime is then reached, characterized by constant precipitates density and increasing average radii and γ' -fractions. The last step is a coarsening regime, which is characterized by a decreasing precipitate density, $N \sim t^{-1}$, and an increasing average precipitate radius $R \sim t^{1/3}$ [3].

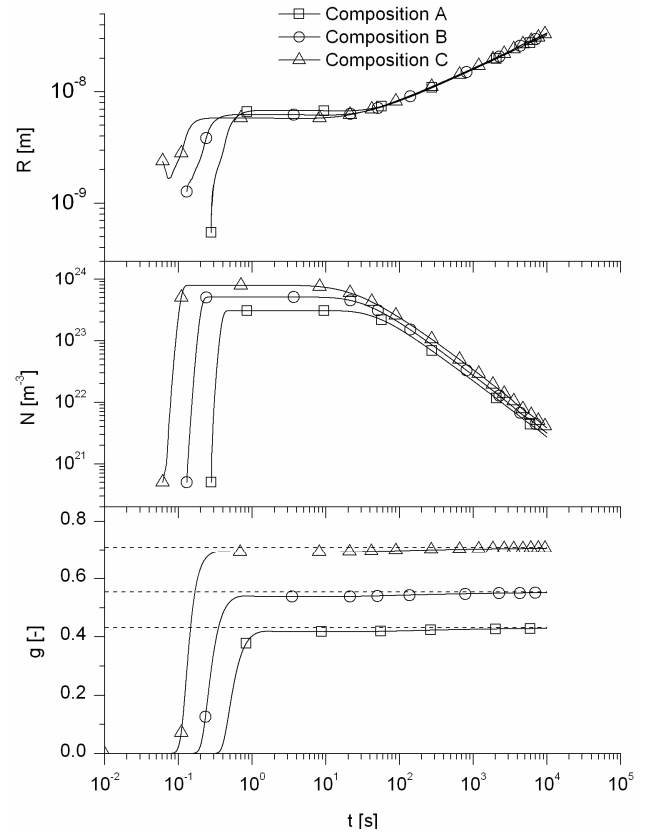


Figure 3: Evolution of γ precipitates size, $R[\text{m}]$, density $N[\text{m}^{-3}]$ and fraction $g[-]$ of the precipitates versus time, for the compositions A, B and C.

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