Acta Materialia 114 (2016) 80–96

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

Application of a multi-component mean field model to the coarsening behaviour of a nickel-based superalloy

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ARTICLE INFO

Article history:
Received 29 January 2016
Received in revised form
21 April 2016
Accepted 12 May 2016

Keywords:
nickel based superalloy
IN738LC
Particle coarsening
Mean field theory
Multi-components systems

ABSTRACT

A multi-component mean field model has been applied to predict the particle evolution of the γ′ particles in the nickel based superalloy IN738LC, capturing the transition from an initial multimodal particle distribution towards a unimodal distribution. Experiments have been performed to measure the coarsening behaviour during isothermal heat treatments using quantitative analysis of micrographs. The three dimensional size of the γ′ particles has been approximated for use in simulation. A coupled thermodynamic/mean field modelling framework is presented and applied to describe the particle size evolution. A robust numerical implementation of the model is detailed that makes use of surrogate models to capture the thermodynamics. Different descriptions of the particle growth rate of non-dilute particle systems have been explored. A numerical investigation of the influence of scatter in chemical composition upon the particle size distribution evolution has been carried out. It is shown how the tolerance in chemical composition of a given alloy can impact particle coarsening behaviour. Such predictive capability is of interest in understanding variation in component performance and the refinement of chemical composition tolerances. It has been found that the inclusion of misfit strain within the current model formulation does not have a significant affect upon predicted long term particle coarsening behaviour. Model predictions show good agreement with experimental data. In particular, the model predicts a reduced growth rate of the mean particle size during the transition from bimodal to unimodal distributions.

1. Introduction

Nickel based superalloys are commonly used in the energy and aerospace industry for turbine components which operate at elevated temperatures and complex mechanical loading conditions. These alloys are precipitation strengthened through the presence of the γ′ intermetallic phase. The stability of the γ′ particles during thermal exposure has a significant impact upon mechanical properties and thus component performance [1]. The Nickel based superalloys used in turbine applications are often heat treated to obtain a multi-modal distribution of γ′, which are characterised by the mean size of each population. With exposure to elevated temperature, the γ′ particles coarsen towards a unimodal distribution of particles, as observed in the superalloy Nimonic 115 [2]. The ability to predict the evolution of the size and volume fraction of γ′ is needed in the development of location specific property prediction capabilities that explicitly link the particle dispersion to the constitutive response of the material [3].

The evolution of the γ′ particle size distribution is influenced by a number of diffusion related mechanisms, which include growth, coarsening, morphology changes and the coalescence of particles. In the scientific literature a number of theoretical and numerical frameworks have been presented to model such behaviour with varying levels of details. Phase field and sharp interface models are effective in capturing the change in particle morphology, overlapping diffusion fields, and the impact of the elastic misfit of the particles [4]. A challenge of applying such methods to predict the particle kinetics during long thermal exposures is dealing with the change in representative volume size that captures a statistically relevant number of precipitates.

A less computationally expensive method for predicting the transition of a multi-modal particle size distribution towards a unimodal dispersion is a mean field theory description of particle

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http://dx.doi.org/10.1016/j.actamat.2016.05.024
1359-6454/

growth [5]. Greenwood [6], Lifshitz and Slyozov [7] and Wagner [8] (LSW) derived the first complete mean field description of particle coarsening in dilute binary alloy systems. Important findings of these models include the predicted behaviour that any given distribution of particles coarsen towards an asymptotic shape and that the predicted coarsening rate of the mean particle size reaches a value proportionate to $time^{1/3}$.

The theory proposed by LSW describes the coarsening kinetics of a dilute dispersion of particles in a binary alloy and over the last two decades or so, progress has been made in the extension of the approach to model multi-component alloys. The simplest approach is to treat a multi-component alloy as a pseudo-binary system, considering the diffusion of the particle forming species. Such an approach was applied by Coakley et al. [2] to simulate the coarsening kinetics of Nimonic 115. A CALPHAD approach [9] allows for calculation of the chemical composition of the particle phase and the Gibbs free energy of the system. A mobility database can allow for the calculation of the effective diffusivity of the particle interface, considering the local chemical composition. Kuehmann and Voorhees [10] developed a model descriptive of ternary alloys which has been successfully implemented by Mao et al. [11] to a ternary Nickel based superalloy. Jou et al. [12] developed a generic approach to extending the Kuehmann and Voorhees model to multiple alloying elements. Collins and Stone [13] have applied a similar model to optimise the particle dispersion within the Nickel based superalloy RR1000. The derivation of the multi-component particle growth rate has been further refined by Phillipe and Voorhees [14]. Svoboda et al. [15] have also developed a multi-component model, which Radis et al. [16] have applied to the Nickel based superalloy Udimet 720. This model has been implemented in this work and is referred to as the Svoboda-Fischer-Fratzl-Kozeschnik (SFFK) model.

The mean field approach of LSW describes a dilute system of particles where the diffusion field and elastic distortion of neighbouring particles do not interact. Baldan [17] reviewed several mean field approaches to describing the impact of non-zero fraction particle systems and found that the descriptions qualitatively captured the relationship between volume fraction and coarsening kinetics however lacked quantitative accuracy. A recent contribution by Svoboda and Fischer [18] builds upon the work of Voorhees and Glicskmen [19] and Marquesee and Ross [20] that accounts for competitive growth between particles. A complimentary approach to extend LSW mean field theory to include particle coalescence has been derived by Davies et al. [21]. The implication of particle coalescence is to be discussed in a separate paper. The treatment of high volume fraction particle systems using a LSW mean field approach remains an active field of research [22].

The objective of this paper is to further develop the understanding and ability to predict the evolution of multi-modal particle systems, linking chemical composition to particle coarsening behaviour. This paper focuses upon the coarsening kinetics of the intragranular γ' particles in the Inconel 738LC. This builds upon the work of Coakley et al. [2] on Nimonic 115 through the methods used to approximate the 3D size of the particles and the application of a multi-component description of the alloy behaviour. Different approaches to the description of high volume fraction particle systems have been assessed. To support these model developments, isothermal heat treatments have been applied to coupons of the alloy obtained in the as-heat treated condition, capturing behaviour relevant to the operating temperature of turbine engine components. This work is part of an integrated computational materials engineering (ICME) work programme designed to develop location specific property prediction models, allowing for the optimisation of component performance and heat treatment.

The paper is divided in the following sections. Section 2 gives details regarding the experimental conditions, the observed microstructure and the results from quantitative microstructural analysis. Section 3 presents the mean field model and normalised formulation. The model parameters and numerical methods used to perform the calculations are provided in an implementation section. The comparison of predicted and measured behaviour are presented in a results and discussion sections.

2. Experimental

The chemical composition of IN738LC is given in Table 1. Coupons of conventionally cast heat treated IN738LC have been isothermally aged for a maximum of 20,000 h at temperatures of 850 °C and 900 °C. Coarsening of the γ' dispersion was observed after thermal exposure for 1000, 2000, 5000, 10,000 and 20,000 h for both temperatures. The samples were mechanically polished and electrochemically etched in solution of 2% phosphoric acid in water.

The characterisation procedure is similar to that described by Payton et al. [23], capturing the precipitates using FEG-SEM with the back-scattered imaging method. The as-received microstructure is shown in Fig. 1. Upon further magnification (1(b)) the γ' dispersion appears to be tri-modal. The largest population of particles within the grains are cuboidal in morphology. Some of these particles have a serrated surface. These protrusions may be caused by instabilities on interfaces during growth or through coalescence with smaller particles. As the growth of such protrusions would increase interfacial energy significantly, it is likely that these are caused through coalescence. The secondary particles have a globular form, with some particles appearing to be an amalgamation of several smaller particles. The third population are fine spherical particles which quickly dissolve at the high temperatures of interest.

Micrographs of the coarsened structures are shown in Figs. 2 and 3 for the temperatures 850 °C and 900 °C respectively. No secondary particles are observed after aging 10,000 h at 850 °C. At 900 °C a unimodal particle distribution is observed in the sample aged for 5000 h. The morphology of the primary particles can be seen to evolve to a more globular form from the initial cuboidal geometry.

Quantitative image analysis was performed using MATLAB image analysis toolbox. The accurate quantitative measurement of particle size from micrographs is challenging and prone to much error. Sources of error include over-etching and the image processing steps taken to identify individual particles. The total volume fraction of γ' in IN738 has been reported to be approximately 45% [24]. A higher value of 56% has also been measured by Smid et al. [25] with further confirmation from Strunz et al. [26]. The particle volume fraction may be estimated by the area fraction measured from micrographs [26,27]. The measured area fraction of particles for the different conditions examined are presented in Table 2. The mean field modelling method used in this work assumes that the particles remain spherical during growth/dissolution. Measurements of the particle areas were performed from micrographs, and

Table 1
Chemical composition of IN738LC (wt.%).

	Al	B	C	Co	Cr	Mo
Lower	3.2	0.007	0.09	8	15.7	0.6
Nominal	3.4	0.01	0.11	8.5	16	1.75
Upper	3.7	0.012	0.13	9	16.3	2
	Nb	Ni	Ta	Ti	W	Zr
Lower	0.6		1.5	3.2	2.4	0.03
Nominal	0.9	bal	1.75	3.4	2.6	0.05
Upper	1.1		2	3.7	2.8	0.08