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Multiscale modelling of the morphology and spatial distribution of θ′ precipitates in Al-Cu alloys

H. Liu [a], B. Bellón [a], J. LLorca [a, b, *]

[a] IMDEA Materials Institute, C/Eric Kandel 2, Getafe 28906, Madrid, Spain
[b] Department of Materials Science, Polytechnic University of Madrid, E. T. S. de Ingenieros de Caminos, 28040, Madrid, Spain

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ABSTRACT

A multiscale approach based on the phase-field model is developed to simulate homogeneous and heterogeneous formation of θ′ precipitates during high temperature ageing in Al-Cu alloys. The model parameters that determine the different energy contributions (chemical free energy, interfacial energy, lattice parameters, elastic constants) were obtained from either computational thermodynamics databases or from first-principles density functional theory and molecular statics simulations. From this information, the evolution and equilibrium morphology of the θ′ precipitates is simulated in 3D using the phase-field model. The model was able to reproduce the evolution of the different orientation variants of plate-like shaped θ′ precipitates with orientation relationship $(001)_{\theta'}//(001)_{\alpha}$ and $[100]_{\theta'}//[100]_{\alpha}$ during homogeneous nucleation as well as the heterogeneous nucleation on dislocations, leading to the formation of precipitate arrays. Heterogeneous nucleation on pre-existing dislocation(s) was triggered by the interaction energy between the dislocation stress field and the stress-free transformation strain associated to the nucleation of the θ′ precipitates. Moreover, the mechanisms controlling the evolution of the morphology and the equilibrium aspect ratio of the precipitates were ascertained. All the predictions of the multiscale model were in good agreement with experimental data.

1. Introduction

Precipitation hardening is well-established as one of the most efficient strategies to increase the yield strength of metallic alloys [1–3]. Precipitates are normally intermetallic particles with sizes in the range from a few to a few hundred nm which appear during ageing. They hinder the glide of dislocations that have to by-pass or shear the precipitates, increasing the critical resolved shear stress to move the dislocation in the slip plane. The strengthening effect of the precipitates depends on a number of factors, which include their size, shape [4–7] and spatial distribution [8–11]. Precipitation hardened alloys are usually subjected after casting to a homogenization treatment above the *solvus* temperature followed by quenching, which leads to a supersatured solid solution of the solute atoms. Afterwards, precipitation is promoted by ageing the alloy at intermediate temperatures (sometimes in combination with mechanical deformation) and the final precipitate structure can be controlled up to some extent from the ageing temperature and time [2,3,12]. In general, it is accepted that the highest hardening is provided by uniform distributions of precipitates with large aspect ratio but the optimum combination of precipitate size, shape and spatial distribution depends on many factors, including the actual number of slip systems, the critical resolved shear stress of each system, the presence of other deformation mechanisms (such as twinning), etc. Thus, the design of novel precipitation hardened alloys and the optimization of the current ones is based on the ability to determine the precipitate features as a function of the alloy composition and of the precipitation process. However, this task has been carried out so far by means of costly experimental trial and error approaches [13].

Modelling of precipitation in engineering is, thus, a very important and complex issue because precipitation is controlled by a number of phenomena that include the chemical free energies and elastic strain energies of the different phases, the interfacial energies between the precipitates and the matrix, the nucleation sites, etc. The classical nucleation and growth theories [14,15] stated the basic mechanisms controlling the formation and growth of precipitates, and remain unchallenged in most aspects, but they could only

* Corresponding author. IMDEA Materials Institute, C/Eric Kandel 2, Getafe 28906, Madrid, Spain.
E-mail address: javier.llorca@imdea.org (J. LLorca).

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provide rough qualitative estimations. The phase-field methods built upon these theories and the diffuse interface treatment and gradient thermodynamics of Cahn and Hilliard [16] have emerged as a powerful tool to provide quantitative information about the evolution of precipitates during ageing [17,18] and the interaction between precipitates and lattice defects, such as dislocations [19].

From the predictive viewpoint, one of the main challenges of the phase-field modelling strategy is that the input parameters are often empirical or difficult to establish. This includes, for instance, the quantitative thermodynamic description of metastable precipitates, the anisotropic interfacial energy between the matrix and the precipitate, the elastic constants of the precipitate, etc. In order to overcome these limitations, a multiscale modelling strategy based on the phase-field modelling of precipitation [20,21] is presented in this paper and applied to predict the shape and spatial distribution of θ′ precipitates in an Al-Cu alloy. This alloy was selected to demonstrate the capabilities of the multiscale approach because it is the one of the alloy systems in which precipitation hardening is more effective [1,2] and often used as an example of precipitation hardened alloys in text books [22]. The parameters of the phase field model were obtained from atomistic simulations performed by means of first-principles Density Functional Theory (DFT) or Molecular Statics (MS) or from well-established thermodynamic descriptions of the system, leading to parameter-free predictions of the precipitate shape and spatial distribution, which were compared with experimental data.

The characteristics of θ′ precipitates in Al-Cu alloys and the construction of the multi-scale model are introduced in sections 2 and 3, respectively. The processing and characterization of the Al-Cu alloys are briefly presented in section 4 and the simulation results are shown and discussed in combination with the experimental observations in section 5. Final conclusions are summarized in section 6.

2. Characteristics of θ′ precipitates in Al-Cu alloys

The precipitation of binary Al-Cu alloys has been extensively studied from both the experimental and theoretical viewpoints [3,12,21,23,24]. The precipitation sequence in the Al-Cu alloys follows the path [3]:

SSSS (super saturated solid solution) → Guinier Preston zones → θ^″ → θ′ → θ.

The θ′ phase is suggested to be the key strengthening phase of this alloy, and its structure is well known [1,21,24,25,26]. θ′ is a stoichiometric phase with chemical composition Al_2Cu and tetragonal structure (space group *I4/mmm*, a = 0.404 nm, c = 0580 nm). The unit cells of α-Al ($Fm\overline{3}m$, a = 0.404 nm) matrix and θ′ are shown in Fig. 1a and b respectively. The arrangement of the atoms in the $(001)_{\theta'}$ plane is similar to $\{001\}_{\alpha}$ except for the absence of an atom in the face centre, whereas the $(100)_{\theta'}$ and $(010)_{\theta'}$ planes are quite different from those of α-Al matrix [3]. The orientation relationship between θ′ and α-Al is $(001)_{\theta'}//(001)_{\alpha}$ and $[100]_{\theta'}//[100]_{\alpha}$, and the θ′ precipitates have three orientation variants. Previous studies [3,27,28] revealed the presence of a shear strain when the α-Al lattice transforms to that of θ′, and a detailed analysis of the transformation was shown by Nie et al. [3,28]. It is composed of three successive steps (Fig. 1c–f). The first one is the shift of the Al atoms in layers 2 and 3 in opposite directions by a distance $a/6$ (from Fig. 1c to d). This is followed by a homogeneous shear of the whole cell by an angle *arctan*(1/3) (from Fig. 1d to e) and finally by the shuffle of one Cu atom to the centre of the cell and diffusion of the other Cu atom away to the matrix (Fig. 1f).

According to this phase transformation mechanism, the lattice correspondence between α-Al and θ′ is: $[013]_{\alpha} \rightarrow [001]_{\theta'}$ and $[010]_{\alpha} \rightarrow [010]_{\theta'}$ [3,28]. The θ′ precipitates were reported to have a plate shape with $\{001\}_{\alpha}$ habit planes. The broad faces of the θ′ plates are nearly fully coherent with the α-Al matrix while the edges of the plates are semi-coherent. It is known that the nucleation of θ′ is favoured by the presence of dislocations or pre-existing particles [3] and it has also been reported that θ′ precipitates are often randomly distributed in the matrix, but aligned precipitate

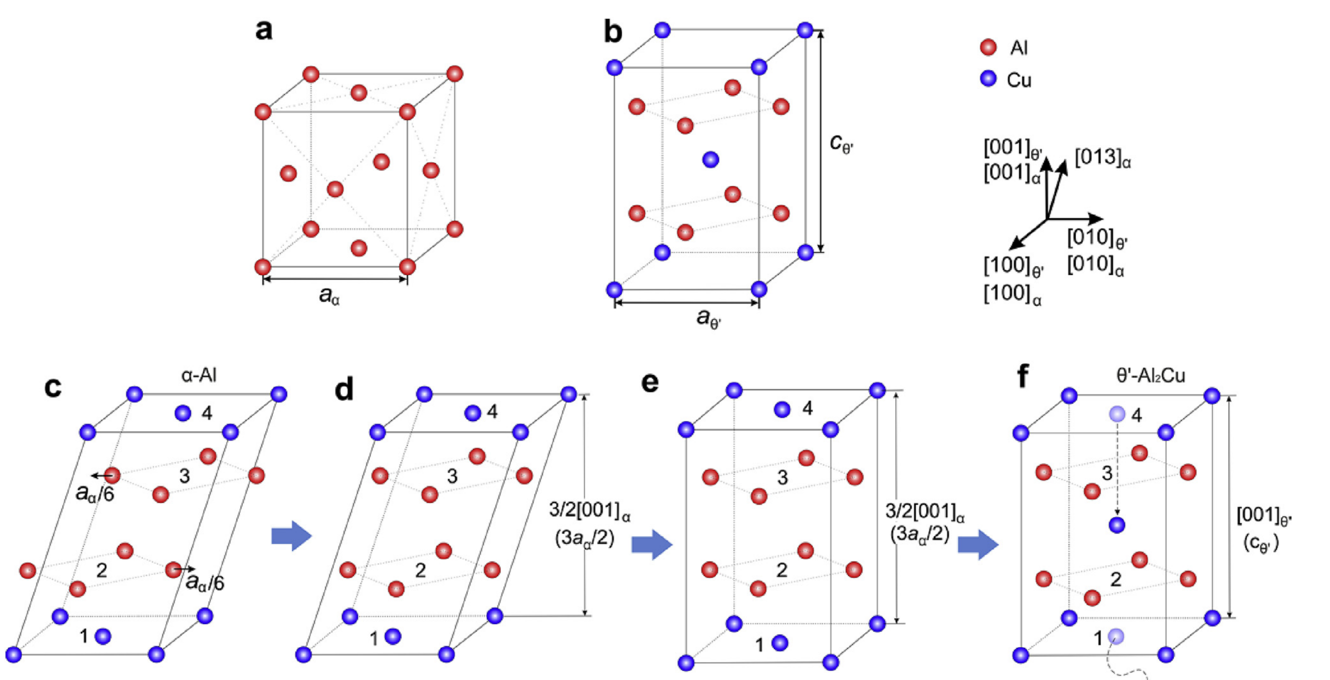

Fig. 1. Unit cells of (a) α-Al and (b) θ′. (c–f) shown the transformation pathway from the lattice of α-Al to that of θ′ [3]. Red and blue spheres represent Al and Cu atoms, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)