International Journal of Plasticity 82 (2016) 112–126

Contents lists available at ScienceDirect

International Journal of Plasticity

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

Precipitate growth in multi-component systems with stress relaxation by diffusion and creep

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ARTICLE INFO

Article history:
Received 16 October 2015
Received in revised form 2 March 2016
Available online 11 March 2016

Keywords:
A. Strengthening mechanisms
A. Phase transformation
A. Creep
A. Stress relaxation
Precipitation kinetics

ABSTRACT

The present paper is devoted to the diffusional growth of spherical precipitates having a volumetric misfit. Thus, the matrix exerts a confining pressure on the growing precipitate retarding its growth. Elastic deformation, creep and diffusion are assumed as mechanisms accommodating the misfit of the precipitate in the matrix. Based on the Thermodynamic Extremal Principle, evolution equations for the state variables (e.g. precipitate radius, chemical composition of the precipitate) are derived. The solution of these evolution equations is compared with a number of limiting cases treated in closed analytic form.

Results are worked out for model parameters similar to those of a steel with 0.5% C and 2% Cr. The most important result is the evolution of the precipitate radius and its dependence on the creep strength of the matrix. If the material creeps readily, the growth rate is controlled by rapid diffusion of interstitial atoms and is, therefore, high. For a creep resistant matrix, the excess volume of the growing precipitate must be accommodated by the slow diffusion of substitutional atoms away from the precipitate. The precipitate grows correspondingly slower, in the present case by four orders of magnitude. Further results are shown for the confining pressure on the precipitate and for chemical variables.

1. Introduction

The precipitate microstructure is decisive for the strength of structural materials both at ambient as well as elevated and high temperatures. Some of the theories relating the strength with precipitate microstructure have been reviewed by Chaboche (2008). Special models have been devoted to polycrystals containing precipitates by Schmitt et al. (1997), to three-dimensional structures of geometrically necessary dislocations in a matrix with inclusions by Ohashi (2004) or to creep behavior of Cr steels by Basirat et al. (2012). The influence of precipitation on plasticity in aluminum alloys has been studied by Glazoff et al. (2004). The role of precipitation on hot working of titanium alloys was investigated by Fan and Yang (2011). A remarkable influence of precipitates on strength of Fe-Al alloys at elevated temperatures has been reported by Morris et al. (2008) and by Muñoz-Morris et al. (2009).

The evolution of the precipitate microstructure in alloys has been studied for many years and is usually described as occurring in three stages, which can, however, considerably overlap (Wagner et al., 2001; Binder and Fratzl, 2001). First,

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http://dx.doi.org/10.1016/j.ijplas.2016.03.001

precipitates nucleate and start to grow, the change in the chemical composition of the supersaturated matrix being still negligible. Then, during the growth stage of the precipitates, the supersaturation of the matrix decreases. Finally, in the coarsening stage, large precipitates grow at the expense of smaller ones and the matrix supersaturation is very low and gradually decreases towards equilibrium. Additionally metastable phases are replaced by stable ones.

There are a number of approaches to model microstructural evolution. The most detailed approach is to describe the alloy at the atomic level (Fratzl et al., 1999; Weinkamer et al., 2004). The usual method, however, is to use a continuum description of the phases separated by interfaces, which are either described as sharp ones (sharp interface models) or by a steep gradient in continuous phase variables, such as order parameters or concentrations of atomic species (phase-field models). Both approaches are able to predict microstructural evolution with good accuracy (for a review see Thornton et al., 2003). Both the phase-field models (Chen, 2002) and the sharp interface models (Akaiwa et al., 2001) have been developed sufficiently far to be applied to many-particle systems. However, since simulations with these methods are time-consuming, they are usually confined to two-phase systems in two dimensions. In principle, there is no restriction to apply these concepts to three-dimensional multiphase configurations as real structural materials. There were also attempts to treat complex precipitation reactions in terms of an extended Johnson-Mehl-Avrami theory, e.g. Refs. Robson and Bhadeshia (1997a,b).

A simple tool for an approximate – but for the practice still sufficiently accurate – prediction of the evolution of a complex precipitate structure, which also rigorously takes into account multi-component multi-phase thermodynamics, has been developed recently (Svoboda et al., 2004; Kozeschnik et al., 2004a, 2004b) employing the Thermodynamic Extremal Principle (TEP), see (Fischer et al., 2014). This concept has become the basis for the software package MATCALC http://matcalc.tuwien.ac.at/. The model was developed by combining the TEP with a mean field approach. It simultaneously retains the complexity and the most important features of the real microstructure. In the current form the model is restricted to microstructures with a low volume fraction of different kinds of nearly spherical precipitates, as it is the case, e.g., in low alloy steels. The model delivers evolution equations for all relevant variables such as size distributions or chemical compositions of all precipitating phases in all stages. The classical theories of nucleation, growth and coarsening can be considered as limiting cases of the model.

Still missing is the mechanical precipitate/matrix interaction beyond the elastic interaction, which is included in the present form of the model. Usually the formation of a precipitate is associated with a substantial volumetric misfit. The excess volume can be accommodated elastically and also by creep and diffusion driven by the stresses caused by the volumetric misfit. Special cases have been treated previously by Riedel (1987), namely accommodation of the excess volume by either elastic deformation or creep deformation or grain boundary diffusion alone. The analysis was focused on the precipitation of cementite in iron/carbon alloys. The stress/strain accommodation by combination of elasticity and diffusion in iron/carbon alloys has been treated by Svoboda et al. (2005a, 2006a).

The goal of the present paper is to develop a much more general model, which couples the multi-component thermodynamics with the mechanical aspects of precipitate growth. A straightforward path to the evolution equations can be offered to the community for this rather sophisticated problem.

2. System description

Let a spherical matrix with radius Z and a spherical precipitate with radius R ($R << Z$) in its center be considered as a system. The precipitate/matrix interface is supposed to act as a non-ideal source and sink for vacancies; in other words, the deposition to or the removal of atoms from the interface is associated with a nonzero dissipation rate. Precipitate growth is accompanied by an excess volume, and hence the matrix exerts a pressure on the precipitate. The pressure is calculated depending on the mechanisms by which the excess volume is accommodated in the matrix. We assume s substitutional components and l interstitial components in the system, $n = s + l$, and the numbers s and l are fixed. Let $\tilde{N}_i$, $[\tilde{N}_i] = \mathrm{mol}$, ($i = 1,...,n$) be the fixed total number of moles of component i in the system. The mean site fraction of component i in the precipitate is u_i, ($i = 1,...,n$), and U is the fixed stoichiometry parameter of the precipitate, e.g., $U = 6/23$ in the case of $M_{23}X_6$. Note that in this case the fixed stoichiometry refers only to the ratio between metal atoms M and interstitial atoms X, while within the sets M and X the atom fractions may vary. Then the following constraints hold as

$$\sum_{i=1}^{s} u_i = 1, \quad \sum_{i=s+1}^{n} u_i = U. \tag{1}$$

In the matrix, being a solid solution, we introduce the site fractions $\overline{u}_i$, ($i = 1,...,n$).

The volumes of the precipitate, Ω, and of the matrix, $\overline{\Omega}$, corresponding to one mole of substitutional atoms, are given by the partial molar volumes of the components, Ω_i, in the precipitate and in the matrix (considered for simplicity to be the same) by

$$\Omega = \sum_{i=1}^{n} u_i \Omega_i, \quad \overline{\Omega} = \sum_{i=1}^{n} \overline{u}_i \Omega_i. \tag{2}$$

The number of moles $\overline{N}_i$ of the component i, $[\overline{N}_i] = \mathrm{mol}$, in the matrix is given by