Available online at www.sciencedirect.com
ScienceDirect
Computational Materials Science 40 (2007) 234–245
COMPUTATIONAL MATERIALS SCIENCE
www.elsevier.com/locate/commatsci

Modeling recrystallization in a material containing fine and coarse particles

Xiaoyan Song [a,*], Markus Rettenmayr [b]

[a] College of Materials Science and Engineering, Key Laboratory of Advanced Functional Materials, Ministry of Education, Beijing University of Technology, Beijing 100022, PR China
[b] Materials Science and Technology Institute, Friedrich-Schiller-University, 07743 Jena, Germany

Received 17 August 2006; received in revised form 30 November 2006; accepted 5 December 2006
Available online 19 December 2006

Abstract

Recrystallization is simulated for a material containing both fine and coarse particles. A deterministic expression is developed for describing the heterogeneous distribution of the stored energy density that arises due to the presence of coarse particles. The effect of recovery reducing the stored energy density, and the different effects of coarse and fine particles on recrystallization are quantified. The criteria for nucleation and growth of the recrystallizing grains are given in energy balances. With 3D Monte-Carlo simulations, various stable recrystallized microstructures are generated by applying different combinations of parameters of the two size classes of particles. In a quantitative study, the effects of recovery and varying volume fractions of the two particle types on the recrystallization kinetics are investigated. The simulation calculations are compared with experimental results obtained with Al–Zr alloys. The model is verified concerning microstructural morphology and recrystallized volume fraction.

PACS: 07.05.Tp; 05.10.Ln; 81.05.Bx; 81.40.Ef

Keywords: Recrystallization; Recovery; Particle stimulated nucleation (PSN); Monte-Carlo simulation; Aluminium alloys

1. Introduction

Recrystallization is a phenomenon that is observed in different forms in metallic materials during annealing after plastic deformation. Even though the basic features of recrystallization are understood at least qualitatively, there remain open questions, mainly concerning the nucleation of recrystallizing grains, but also the recrystallization kinetics of materials with complex (heterogeneous) microstructures. As the annealing heat treatment leading to the recrystallization process will also stimulate other thermally activated processes, particularly recovery, modeling the kinetics of recrystallization is rather complex and dependent on the interaction of different materials' parameters.

In single phase alloys, nucleation and grain growth during recrystallization were extensively studied theoretically and experimentally (see e.g. [1–5]). Expertise has been accumulated on recrystallization kinetics under a variety of experimental conditions, as shown in recent monographs (e.g. [3]) and overviews (e.g. [4]). For alloys whose microstructure consists of at least two phases, the recrystallization process is substantially more complex, concerning both nucleation and recrystallization kinetics. First, the interaction of the second phase with dislocations can reduce or entirely suppress nucleation and/or recovery. Second, the migration of the grain boundaries of recrystallizing grains may be pinned by dispersed fine particles, yielding a tendency toward slower recrystallization kinetics. On the other hand, non-deforming particles of a size

* Corresponding author. Tel.: +86 10 67392311; fax: +86 10 67391756.
E-mail address: xysong@bjut.edu.cn (X. Song).

0927-0256/$ - see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.commatsci.2006.12.002

of 1 μm or above additionally exert an accelerating influence on recrystallization by providing a higher nucleation site density. This effect, termed particle stimulated nucleation (PSN), is based on a local accumulation of stored energy at specified locations in the vicinity of the particles. PSN was identified first by Humphreys [6] and has been observed in several alloy systems [7–10].

In technical alloys, particles usually exhibit wide size distributions that may extend over the length scale of fine as well as coarse particles. Also, particles of identical type can be present as primary and secondary precipitates with different mean sizes. Examples are the precipitation of primary and secondary carbides in high speed steels, or the different types of particles in high-strength Al alloys. In those cases, the prediction of a recrystallized grain structure requires careful modeling of the interaction of a grain boundary with particles, as well as a thorough consideration of the physical mechanisms that stimulate nucleation. A few experimental studies have been carried out on recrystallization in materials containing particles with a bimodal size distribution [7,8,10–13]. However, most of these works focus on an empirical determination of the effects of the particles without attempting to correlate the interaction mechanisms of particles and recrystallization kinetics quantitatively with observed microstructures.

Due to the large number of parameters that exert an influence on recrystallization, a quantitative understanding of the recrystallization process is more readily achieved in combination of experiments with computer modeling. Different calculation techniques have been adopted so far, including the Monte-Carlo technique [14–17], numerical JMAK models [18–20], cellular automata [21–24] and vertex models [25,26]. All of these models have been applied for a description of recrystallization in single-phase materials (see e.g. [14,15,17–26]). Recrystallization in a two-phase material was originally simulated by Rollett et al. [16] with a two-dimensional (2D) Monte-Carlo method. In the model, only the pinning effect of particles (of a uniform size distribution) on the growth of nuclei was considered. Also, in some recently presented Monte-Carlo simulations of two-phase materials [27,28], only fine particle pinning and its effect on microstructure evolution were studied.

The question of the twofold effects of different size classes of particles has so far not been addressed systematically. In the present work, a model is elaborated for describing these effects on the recrystallization kinetics. Deterministic expressions are presented that describe distribution of the stored energy density and the conditions for nucleation and growth of recrystallizing grains. These are incorporated in a 3D Monte-Carlo model, and the recrystallization behavior is predicted for a variety of initial microstructures and conditions. For verification of the model, experiments have been carried out with a series of Al–Zr alloys. Discussions about PSN efficiency, the possible characterization of the recrystallization kinetics in particle-containing materials with a modified JMAK model are given in the end.

2. Development of the model

2.1. Heterogeneous distribution of the stored energy

We consider that dispersed fine particles of sub-micron size do not affect the deformed grain structure nor the distribution of stored energy within the grains. In contrast to this, coarse particles that are non-deforming are assumed to lead to a strain incompatibility [3,4,29] between matrix and particle. As a consequence, the local matrix deformation in the vicinity of the particle is different from the mean deformation in the bulk. Depending on the type of deformation, several geometries of the particle-affected deformation zone have been introduced so far [30–32]. For the present case, i.e. cold-rolling, a particle-affected zone consisting of a distorted region and a rotated zone [30] is applied. As depicted in Fig. 1, for rolling in horizontal direction we assume that the distorted regions above and below the particle (denoted 'A') are subject to a larger deformation, whereas the zones on the left and right side of the particle (denoted 'B') are 'shielded' from deformation. Following the approach of Ashby [33], the density of additional 'geometrically necessary' dislocations ρ_a can be written as

$$\rho_a = \frac{6\varepsilon}{b}\cdot\frac{f_c}{d_c} \tag{1}$$

where ε is the true strain, b is the Burgers vector, and f_c is the volume fraction of coarse particles with diameter d_c. The extra deformation leads locally to a higher amount of stored energy density, expressed by

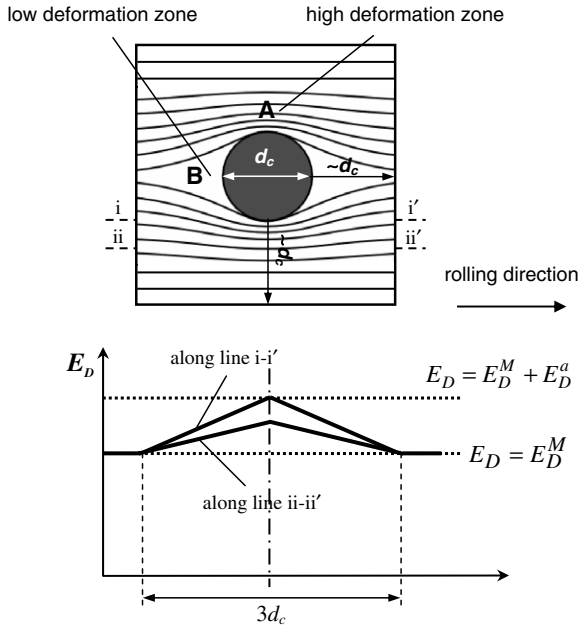

Fig. 1. Variations of the deformation (after [27]) and the stored energy E_D in the vicinity of a coarse non-deforming particle; the solid black circle represents the particle with diameter d_c; the square region with a dimension approximately equal to $3d_c$ is the particle-affected region.