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Modeling of non-isothermal annealing: Interaction of recrystallization, recovery, and precipitation

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Abstract

A procedure for modeling recrystallization in the course of non-isothermal heat treatments is introduced. For this purpose a three-dimensional cellular automaton is utilized. The model is capable of predicting the microstructure, texture, and kinetics. A special focus is laid in this study on the complex interactions of recrystallization with recovery and precipitation. The model is applied to a commercial Al–1 wt.% Mn alloy cold rolled and annealed using heat treatments with different temperature–time profiles. The resulting microstructures and recrystallization kinetics are compared with experimental data.

Keywords: Recrystallization kinetics; Non-isothermal; Precipitation; Simulation; Cellular automata

1. Introduction

Non-isothermal heat treatments, especially the use of low heating rates, are frequently encountered during thermo-mechanical processing cycles, and hence are of importance for industrial purposes. During non-isothermal heat treatment recovery and precipitation are likely to occur, generating complex interactions with recrystallization. Recrystallization is a softening mechanism which significantly changes the microstructure and texture, and thereby the material properties. Static recovery, another softening mechanism, occurs particularly in high stacking fault materials, such as aluminum and its alloys. It has an influence on recrystallization by reducing the driving force. Recovery, in contrast to recrystallization, hardly changes the microstructure and essentially conserves the deformation texture.

Precipitation can also strongly influence the recrystallization behavior. The precipitation of dispersoids in the course of an annealing treatment can hinder or even suppress recrystallization [1–7]. When precipitation occurs concurrently recrystallization is accompanied by the occurrence of specific texture components, as well as larger grain sizes [2,4,8]. Furrer and Warlimont [2] found that at low heating rates an inhomogeneous and predominantly coarse grain size was observed in an Al–1% Mn alloy, in contrast to fast heating, where the time–temperature region of segregation and precipitation was bypassed. This results in a finer, more homogeneous grain size. Tangen [7] observed that the electrical conductivity and, consequently, the degree of precipitation of AA3103 alloys with various solute contents increased considerably for lower heating rates. Liu et al. [8] attributed the occurrence of larger, inhomogeneous grain sizes in AA3105 to the occurrence of concurrent precipitation. These authors also reported the presence of a strong P-texture component in the recrystallization texture in the case of concurrent precipitation, as confirmed by Bampton et al. [4]. The latter authors attribute the occurrence of large grains to the earlier activation of highly favored nucleation sites which become activated at relatively low temperatures. Thus they have a growth advantage and consume neighboring, less favored nucleation sites before the latter are activated. The extent of recovery and precipitation also influence the recrystallization temperature [9].

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In principle dispersoids that initially hinder or suppress recrystallization can coarsen or dissolve during further annealing, such that recrystallization can proceed at later times [10–16].

In contrast to the effect of dispersoids, primary phases, the so-called constituents, usually enhance recrystallization by particle-stimulated nucleation (PSN) [17–19]. In combination with precipitation, specific texture components such as the P- and 22°ND-rotated cube component can evolve during recrystallization [20–23].

Hence, by varying the heating rate the relative extent of various physical mechanisms (recrystallization, recovery, precipitation) can be strongly influenced. The complexity of the phenomena involved renders experimental investigations laborious and difficult. An understanding of the processes involved is important for microstructure control during annealing, and computer simulations seem to be a suitable and powerful tool to study and probe the complex interactions during non-isothermal annealing treatments.

The modeling approach presented by Dunlop et al. [24] considered the influence of recovery on recrystallization, but precipitation reactions were not considered, since a single phase material was studied. The modeling of recrystallization with concurrent precipitation was treated by Martin [25] by means of non-isothermal Johnson–Mehl–Avrami–Kologoromov (JMAK) kinetics in steel.

Despite much modeling activity of recrystallization, approaches to model kinetics, microstructure, and texture during non-isothermal heat treatment [24,26–28] are sparse.

In the current study a spatially and temporally resolved model based on cellular automata (CORe, cellular operator for recrystallization) was used to model the recrystallization microstructure, texture, and grain size distribution (GSD) [29,30]. The model uses physical descriptions of the phenomena involved and can account for heterogeneous microstructural features. For consideration of non-isothermal heat treatment the model was extended to include the effects of recovery, precipitation, and particle-stimulated nucleation. In the following we will focus on the modeling of recrystallization kinetics and microstructure evolution for AA3103. The corresponding macrotexture predictions have been presented elsewhere [31].

2. Recrystallization model CORe

CORe is a three-dimensional (3-D) cellular automata model which simulates the growth of recrystallization nuclei in an array of equally sized grains with a deformed microstructure. The grain structure of a polycrystal is discretized by subdivision into small volume elements which can change their state from "deformed" to "recrystallized" during annealing. The nuclei are implanted into this microstructure as described by separate nucleation models. The model allows the inclusion of a variety of substructural information, such as orientation-dependent dislocation densities and local orientation gradients, as well as inhomogeneous nucleation at different nucleation sites [29,30,32].

2.1. Nucleus growth

Recrystallization nuclei grow by displacement of their grain boundaries owing to the action of driving forces. In this study nucleus growth was also affected by effects such as recovery and precipitation. The radial growth velocity v is determined by the driving force p and the grain boundary mobility m.

$$v(t,T,\theta,\rho,g) = m(T,\theta)\cdot(p(\rho,t,T,g) - p_Z(t,T)) \quad (1)$$

Here ρ is the dislocation density, θ the misorientation, T the temperature, g the orientation of the grain being consumed, and p_Z the Zener drag. Besides recrystallization, recovery and precipitation are also affected by temperature changes imposed by the chosen time–temperature profile.

Coupling this with the dislocation density-based work hardening model 3IVM+ [30] the prediction of recovery rates is carried out grain by grain and for different time–temperature profiles [31]. The effective driving force is reduced by both recovery and precipitation. The resulting back-driving force from precipitates [33] is

$$p_Z = \frac{3}{2}\gamma\frac{f}{r} \quad (2)$$

Here γ is the grain boundary energy, f the volume fraction of dispersoids and r the mean dispersoid radius. The mobility in the model depends on misorientation, temperature and solute content. In the presence of solute atoms, i.e. Mn atoms in the current study, the mobilities for special, high angle and low angle grain boundaries are reduced in comparison with the pure metal by a factor of $1/(1 + c\cdot D_m/D_{Im})$, where c is the solute content of manganese and D_m and D_{Im} are the self-diffusion coefficient of aluminum and the diffusion coefficient of manganese in aluminum, respectively, due to solute drag. For a more detailed description of the recrystallization model CORe the reader is referred to Mukhopadhyay et al. [29] and Schäfer et al. [30]. CORe is a pure growth model. Nucleation is implemented separately, as outlined below.

2.2. Recrystallization nucleation

The activation of nucleation at grain boundaries, transition bands and/or shear bands in a deformed microstructure can be derived from the ReNuc model [34–36]. The ReNuc model is a compilation of various sub-models which represent the various nucleation mechanisms and their promotion during deformation. The introduction of particle-stimulated nucleation was recently enabled by the GIA-DZ model [32]. This is a sub-model to describe the evolution of deformation zones (DZ) in the particle vicinity in the interior of individual crystals. However, these sub-models only predict nucleation probabilities, not absolute nucleus densities.