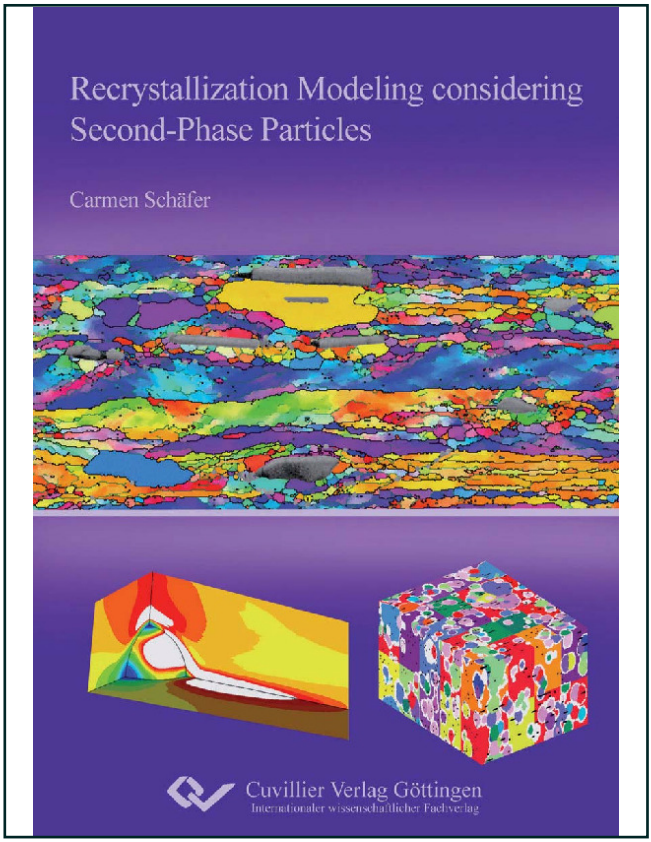
Carmen Schäfer (Autor)

Recrystallization Modeling considering Second-Phase Particles



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Chapter 1

Introduction

The recrystallization of deformed metals has been the subject of research for almost 70 years. Although there is now a reasonable understanding of many aspects of the process, many important areas require further elucidation. Two of these areas, which are addressed in this thesis, are the recrystallization nucleation and the modeling of recrystallization in commercial alloys considering the vast number of possible influences.

During plastic deformation, e.g. rolling, defects are introduced into the material. These defects are removed during a subsequent annealing treatment by recrystallization and recovery. Recrystallization is the complete regeneration of the microstructure by creation and migration of high angle grain boundaries during a heat treatment of deformed materials. The complete change of microstructure is further accompanied by severe texture changes. Texture and microstructure essentially determine the properties of metallic materials. This motivates the interest of industry in this particular process. Since texture and microstructure can be changed within wide margins by respective processing, optimum processing conditions and best materials chemistry have to be found for low cost and high performance products. The ever decreasing product life cycles, and the rising demand for advanced materials and low cost production render empirical practices ineffective. They require reliable models of materials development during processing for prediction of terminal material properties and the optimum processing window. The complication is that materials modeling means microstructure modeling, and microstructure changes during processing. Thus, physical based models are required rather than empirical ones.

From relevant literature on recrystallization it is known that for recrystallization modeling the physical mechanisms of nucleation and their specific growth relationships need to be implemented. This is the consequence of an extensive discussion on the topic of recrystallization being controlled by oriented nucleation and oriented growth during recent years. The common consensus in this respect is that recrystallization is most likely the selected growth (oriented growth) out of a set of nuclei originating at preferred nucleation sites (oriented nucleation). Against this background nucleation is of special importance since it not only influences the orientation, and thus the texture of the material, but also the final grain size. The approaches for nucleation in literature being mostly of empirical nature are not very useful for the application in through-process modeling

since they require very often parameters or experimental data, which is, in general, difficult to access. As a result, a comprehensive description of nucleation is not available. However, the trend in modeling nucleation goes towards models that link the deformation with the recrystallization behavior finding meaningful parameters which allow a more universal application of such models. A model of this type is, for instance, the ReNuc model developed at IMM (Institute of Metal Physics and Physical Metallurgy, RWTH Aachen) for the description of various nucleation mechanisms in Al alloys. However, one of the most important nucleation mechanisms in commercial alloys, the nucleation at second phases or so-called particle stimulated nucleation, was not considered up to know. This nucleation mechanism, if understood, can be used to control texture and microstructure, and thus the final properties by adjusting the number and the distribution of the nucleation stimulating particles.

In the present work, a model was developed, based on experimental observations, to describe the deformation and nucleation around particles. To investigate particle-stimulated nucleation experimentally, high-resolution SEM/EBSD was applied to collect the great amount of statistical data required. With nowadays obtainable high resolutions of the electron microscopes down to the order of 10 nm this provides a good technique to collect statistical data in a reasonable amount of time. The main purpose of this investigation was to understand the development of individual grain orientations in the particle vicinity during deformation and subsequent annealing. This is of special importance since these newly developed grain orientations will significantly determine the final texture. Based on the experimental observations, a model to describe the deformation and nucleation around particles was developed. For the description of the inhomogeneous deformation in the particle vicinity FEM (Finite Element Method) was utilized. This new nucleation model for particles is introduced in Chap. 5, together with the results of the experimental studies. The model for particle-stimulated nucleation was then incorporated in an existing recrystallization model for description of annealing treatments during thermo-mechanical processing (Chaps. 4, 7-9).

For the modeling and simulation of recrystallization various models are available from the literature (Chap. 2), such as phenomenological models, geometric microstructure models, vertex models, statistical models and discrete models, such as Monte Carlo and cellular automata methods [Raabe 1998]. For the present work, a cellular automaton approach was chosen due to the possibility to resolve microstructure inhomogeneities in sufficient detail. With respect to the recrystallization modeling on different time and length scales cellular automata are a promising modeling technique (able to bridge a large scale 10^{-10} to 100 m, for comparison MC only 10^{-9}-10^{-5} m) [Raabe 1998]. The first who applied cellular automata to model the recrystallization phenomenon were Hesselbarth and Göbel in 1991 [Hesselbarth 1991].

Whereas the recrystallization models available in the literature are mostly restricted to the validated range, to single-phase materials or to the prediction of only kinetics, microstructures or textures; this work was dedicated to create a recrystallization model which is able to capture the full set of physical micro-scale mechanisms occurring during a heat treatment in commercial alloys as well as to reach reasonable predictions of kinetics, grain size and texture in equal measure. The recrystallization modeling is therefore focused on sub-structural quantities, e.g. orientation-resolved dislocation densities, which are traced along the process chain. The cellular automaton for recrystallization (CORe) as used in the present work is outlined in detail in Chap. 3. In contrast to an earlier version of the CORe model developed at the IMM [Mukhopadhyay 2007], the present model was extended for the application to commercial alloys including the required micro-scale mechanisms. In commercial alloys, such micro-scale mechanisms are recovery (Chap. 6), which reduces the driving force for recrystallization, and all effects connected to second-phases (Chaps. 7, 8). Those can be the development, coarsening or dissolving of particles, which hinder or even suppress recrystallization. These processes can occur prior to recrystallization, concurrent to it or even after it is completed. Chap. 4 presents a validation of the recrystallization model limiting the number of simultaneous influence factors.

Beside the growth, the correct description of nucleation is essential for the quantitative texture and grain size prediction. A further transfer to industrial problems proves itself even more complicated due to the use of non-isothermal heat treatments as well as more complicated alloying systems. Therefore, extensive validations for the recrystallization model were carried out for two commercial aluminum alloys AA3103 (Chap. 7) and AA8079L, applying, e.g. non-isothermal heat treatments (Chap. 8). The required experimental data was provided using X-ray diffraction, metallographic, optical - and electron microscopic techniques.

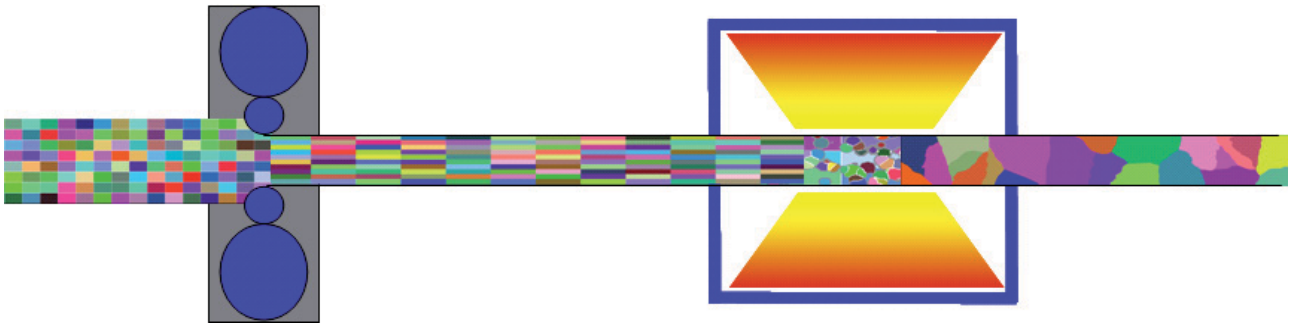

Fig. 1.1: Scheme of the modeling setup for predicting recrystallization. Prior to recrystallization a deformation simulation (rolling) is required to provide the major inputs for CORe. Microchemistry simulations are accompanying the process.

The main interest in the above introduced recrystallization model was its implementation into an existing through-process modeling setup displayed in Fig. 1.1. After deformation (rolling) the material, displaying elongated grains, is subjected to annealing treatment after which the microstructure is completely renewed. Here, the interaction of different models used for describing different parts of the system is the crucial problem to solve. The different incorporated phenomena do not necessarily take place on the same time-scale and it is not ensured that the parameters obtained from one model can be directly transferred to the subsequent model. This was particularly important in Chaps. 7-9 where alternating cycles of deformation and annealing are modeled on grain scale. The thesis is concluded by addressing a through-process modeling exercise for the application to a commercial Al-alloy AA3103 alloy (Chap. 9), considering simultaneously all introduced effects, i.e. recovery, recrystallization and precipitation.