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Effect of magnetic fields on microstructure evolution

Philip E. Goins*, Heather A. Murdoch, Efraín Hernández-Rivera, Mark A. Tschopp

U.S. Army Research Laboratory, Weapons and Materials Research Directorate, Aberdeen Proving Ground, MD 21005, United States

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ABSTRACT

Tailoring microstructure evolution with the use of external forces (magnetic, electric, mechanical, etc.) can expand the ability to control material properties and performance through microstructure engineering. In particular, crystalline materials are comprised of a distribution of grains of differing sizes, crystallographic orientations (texture), and topologies, which may evolve differently under the influence of various fields and lead to changes in material properties, bounded by movable grain boundaries. In this work, simulations are used to demonstrate the effect of an applied field, in this case a magnetic field, on the evolution of microstructure at the grain scale. The simulation results show that fields can be used to control microstructure geometry and texture. They also show that a dynamic field application of the field, through a changing field direction over time, can create new microstructure features even in a system that does not seem as sensitive to as static field, and that temperature can play a key role in this evolution as well. This work overall demonstrates how unconventional processing techniques on polycrystalline microstructures can be impacted by applying fields, and ultimately be used to improve properties and performance through engineered microstructures.

1. Introduction

Microstructure plays a profound role in the bulk properties and performance in materials. Perhaps the most famous example of a structure–property relationship at the grain scale is the Hall-Petch relationship, which characterizes the widely-observed inverse relationship between average grain size and the yield strength/hardness of polycrystalline materials [1–3]. This grain size can also impact a material's wear resistance [3–5], toughness [5,6], corrosion resistance [7–10], electrical conductivity [11–14], and magnetic [15–17] properties. Hence, material grain size should be an important consideration for materials in engineering applications. Microstructure texture—the overall distribution of crystallographic orientations of individual grains within the system—also significantly affects material properties [18–20], enhancing or detracting from material properties, and often resulting in anisotropic responses in bulk material properties. For example, Goss steel is a famous example of how texture can be used to tune magnetic properties, widely used in electrical transformers; by aligning grain orientations, the magnetic flux density can be increased by over 30% [21]. An example relating to catalysis is that certain film surface orientations, which depend on film texture, offer improved catalytic performance in the same material [22,23].

Of particular relevance for the current study, magnesium is a hexagonal close-packed (HCP) metal known for having the lowest density of structural metal. Despite its low density and high specific strength, magnesium maintains a low market share due to challenges in forming the material. One of the primary technical challenges of forming magnesium is its anisotropic texturing during processing and forming, contributing to a sharp basal texture that leads to highly anisotropic mechanical properties [23–26]. At present, popular approaches to limit this texture formation use costly strategies employing rare earth alloying elements in magnesium alloys [26].

One strategy for controlling microstructure evolution in polycrystalline materials is the use of external fields, thereby using the anisotropy for different grain orientations to engineer the underlying microstructure. The first known use of magnetic fields to manipulate microstructure in weakly magnetic materials is generally attributed to Mullins [27], who demonstrated that applying a magnetic field to a bismuth bicrystal created a free energy difference and enabled measurement of the boundary property. Magnetic fields used under annealing conditions have also been shown to alter texture in a number of non-ferromagnetic metals, as well as accelerate microstructure evolution to an extent in some cases, including copper [28], aluminum [29], titanium [30,31], zinc [32], among other systems. Common to many of the texture formations observed in this is an argument on a preference for the lowest magnetic susceptibility to become increasingly dominant in the new texture. In these cases, grains with an orientation that offers a lower susceptibility in the direction of the magnetic field is energetically favorable, and expand into higher energy grains. Overall, this creates a net texture in the material and new driving force for

* Corresponding author.
E-mail address: philip.goins.ctr@mail.mil (P.E. Goins).

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microstructure evolution. Also, grain growth appears to be affected by the application of the field itself. For example, above the paramagnetism transition temperature in nickel, changes in abnormal grain growth conditions have been observed between the AC and DC magnetic field application [33].

This microstructure evolution process has seen some preliminary modeling efforts, generally in two dimensions for weakly magnetic materials. Barrales-Mora et al. published a study on simulating titanium in two dimensions under a magnetic field using a vertex model [34], which was followed up in a Monte Carlo study of titanium [30]. Lei et al. and Allen reported results from two-dimensional Monte Carlo model simulations on weakly magnetic systems as well [35–36]. Lei and colleagues report no change in the grain growth exponent, but both Lei and Allen report increased mean grain size under applied magnetic fields. Barrales-Mora and colleagues reported little increase in mean grain size in their vertex model [34], though their subsequent work showed more significant increases in grain growth using their Monte Carlo model [30].

In the present work, the research objective is to develop a model that advances recent simulation methods, extending the consideration of magnetic fields from two-dimensional (2-D) to three-dimensional (3-D) materials, which may offer improved predictions of microstructure and properties in polycrystalline materials. Furthermore, modeling the microstructure in 3 dimensions will enable the exploration of variations in applied field directions – e.g. rotating or switching magnetic fields – that are not practical if applied to a 2-D plane microstructure. By studying microstructure evolution in model materials under a wide set of conditions, including dynamic field direction and temperature gradients, the results may offer insight into the most effectual processing approaches. Desired texture and grain growth effects may be unachievable with static magnetic fields at reasonable field strengths, but attainable through a dynamic field approach. We explore static, switching, and rotating magnetic fields in a variety of strengths and temperatures as applied to a magnetically anisotropic material.

2. Simulation methodology

In this work, a three-dimensional hexagonal close-packed material is simulated under various field conditions. The recently-developed Material Point Monte Carlo model (MPMC) is used for this work [37]. The MPMC, which is an off-lattice extension from the Monte Carlo Potts model [38] used in previous magnetic annealing reports by Molodov [30], Lei [35], and Allen [36], the material volume is represented by a set of randomly-placed, time-evolving set of material points. The MPMC offers computationally-affordable three-dimensional simulations over longer time scales, without the lattice artifacts that are present in the Potts model approach. A material point is placed randomly within the volume, and the new material point's data, such as phase and grain state, are assigned probabilistically based on the statistical mechanics relationship:

$$p_i = \frac{e^{-E_i/kT}}{Z} \tag{1}$$

where p_i is the probability of the material point adopting state i, E_i is the state's configurational energy, kT is a simulation thermal energy value, and Z is a partition function that describes the sum of all Boltzmann factors of all n possible states the site could adopt which normalizes the probabilities to one.

$$Z = \sum_{j=1}^{n} e^{-Ej/kT} \tag{2}$$

Here, the partition function is defined as the sum of the Boltzmann factor of the energy that a material point would adopt by picking state j, over all possible n configurations. The simulation temperature does not necessarily need to reflect the physical temperature for other processes.

The MPMC simulation method operates as follows. First, material points are introduced randomly within the space of the volume. In contrast to other off-lattice Monte Carlo models, there is no acceptance or rejection step in material point placement depending on the system energy. Instead, the energy only affects which state the newly-placed material point adopts. However, there is a probability that controls whether a newly-placed material point is rejected based on kinetics, since the local flux of material points is controlled by the interfacial mobility. For each Monte Carlo time step, N material point movement steps are proposed, where N is the number of material points in the system. The choice of using N points per time step ensures that the rate of system evolution is not dependent on simulation size. For each material point added, another material point must be removed to ensure a conserved number of material points. This point removal step is not physical process, but does ensure that the computational expense (and resolution) does not increase as a function of simulated time. The probability of removing a material point from a specific spatial region must match the probability that a material point may be placed there, ensuring that the density of material points remains uniform throughout the simulation volume.

The material thermodynamic and kinetic descriptor functions for the MPMC method are responsible for the microstructure evolution process of the material system. Here, we use a crystallographically-anisotropic polycrystalline material with hexagonal symmetry in three dimensions under an applied field. The energy of a state, E_i, is divided into two components: the bulk energy η and the interfacial energies γ.

$$E_i = \eta_i + \frac{1}{n_s}\sum_{j=1}^{n_s} \gamma_{ij} \tag{3}$$

Here, E_i is the energy of state i, η_i is the bulk energy term associated with state i, n_s is the number of material points found in the neighborhood of the material point, and γ_{ij} is the interfacial energy between grains i and j.

The relationship between grain boundary misorientation and the interfacial energy/mobility terms must be defined for the energy function E_i in the MPMC method. Grain boundary interfacial energies and mobilities in a pure material at 0 K are material-specific and depend on the five grain boundary degrees of freedom: three degrees of freedom that define the misorientation between two grains, and two degrees of freedom that define the inclination of the plane that bisects the grains [39–42]. Nonzero temperature can lead to multiple energetically-degenerate structures or changes in faceting behavior, as well as boundary-specific changes in mobility [43]. Impurities can substantially alter grain boundary properties further, and often dominate the late stages of grain growth even in fairly pure, single-component materials [44–49]. Nonetheless, many general behaviors of polycrystals are captured well with a more simplified model, given that the exact functional forms and parameterizations that capture these characteristics are still not known for many systems. Hence, the grain boundary energy and mobility values herein are described by the Read-Shockley model for grain boundaries [50], in which grain boundaries are described as arrays of dislocations and energy depends on the misorientation angle between grains, i.e.,

$$\gamma_{ij} = \begin{cases} \gamma_{max}\left(\frac{\theta}{\theta_{max}}\right)\left(1-\ln\frac{\theta}{\theta_{max}}\right), & \theta < \theta_{max} \\ \gamma_{max}, & \theta \geqslant \theta_{max} \end{cases} \tag{4}$$

Here, γ_{max} is the energy associated with a high-angle grain boundary, θ is the minimum misorientation between grains i and j, and θ_{max} is the cutoff for high-angle boundaries (typically 15°). While the Read-Shockley equation describes the relationship between misorientation angle and grain boundary energy well for many materials, there is far less agreement on a function relating misorientation angle and grain boundary mobility. Here, a model developed by Shvindlerman and colleagues [51,52] has been adopted: