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Coupled crystal plasticity – Probabilistic cellular automata approach to model dynamic recrystallization in magnesium alloys

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ABSTRACT

This study presents a framework to simulate dynamic recrystallization (DRX) in hexagonal closed packed (HCP) metals and alloys using crystal plasticity based finite element model (CPFEM) coupled with a probabilistic cellular automata (CA) approach, as applied to Mg alloys. The CPFEM takes as input the microstructural information from experimental measurements and computes local dislocation density evolution corresponding to active deformation modes. DRX proceeds via nucleation of new grains and their subsequent growth. A new nucleation criterion based on local mismatch in dislocation density is implemented in the model. Nucleation sites are defined solely from the local inhomogeneouty of dislocation density within a grain or across grain boundaries. Cellular automata model with probabilistic state switching rule predicts the growth of viable nucleation sites with high misorientation angle depending on the difference in the stored energy of the nucleus and the stored energy of the surrounding matrix. State switching probability rule is based on the velocity of the grain boundary between the nucleus and the matrix grains. The new approach is validated with recrystallization data on AZ31 sheets. The model captures both the microscopic (texture) and the macroscopic (stress–strain response) properties during DRX.

1. Introduction

Recrystallization (both static and dynamic) plays an important role in thermo-mechanical processing (TMP) of materials. It enhances/restores the ductility of the material and gives a control of the grain structure and to a certain extent of the texture of the final product (Doherty, 1997; Humphreys and Hatherly, 2004a).

Experimentally it is observed that dynamic recrystallization (DRX) accompanying deformation at elevated temperature can enhance formability beyond what can be accomplished due to increased slip activity and grain boundary sliding alone (Doherty et al., 1997). DRX removes new defects continuously and extends the stress–strain curve to high strain values without hardening. Once material is loaded at elevated temperatures deformation is accommodated either by slip or twinning till a critical value is reached, after which the material starts showing some degree of recrystallization, which results in softening instead of hardening in the flow curve. DRX proceeds, similar to static recrystallization (SRX), via (a) nucleation of a new

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grain and (b) growth of the nucleus at the expense of deformed matrix. Unlike SRX, the dislocation content evolves with time in both the matrix and recrystallized region during DRX.

Deformation in magnesium (Mg) alloys is accompanied by high hardening rates and high dislocation content (Sakai and Jonas, 1984). Since Mg alloys exhibit reduced formability at room temperature, hot deformations are routinely resorted to both in the processing of wrought Mg alloys as well as their fabrication to components. Forming operations at elevated temperatures can lead to DRX. The resultant texture and hence, the properties of such deformed material are dependent on the location and crystallographic orientation of the nuclei. Observations have shown that high dislocation content accompanying deformation diminishes further slip with increasing strain as the energy released during deformation is re-distributed to create new subgrains and grains inside the material (Martin and Jonas, 2010). Through grain reconstruction due to DRX, the material can deform further and significantly change the plastic stress–strain response. The resultant texture, and hence, the properties of such a deformed material are dependant on the location and crystallographic orientation of the nuclei of the DRX grains and their subsequent growth. It has been reported that, in Mg alloys, there are no significant changes in the crystallographic texture upon recrystallization as shown for example in AZ31 by Yi et al. (2006). Most of the recrystallized grains preserve the basal texture characteristic of the deformed matrix. The deformed state, from which recrystallization originates, is comprised of matrix grains, in which both slip and twinning (and double twinning) may have been active. It has been reported in literature that not all the regions in the deformed microstructure are likely to nucleate and grow new grains. For example, it has been noted that the primary compression and secondary (double) twins are more likely to nucleate new grain than primary extension twins in magnesium alloys (Martin et al., 2011).

It has also been shown in the works of Barnett (2001) and Dudamell et al. (2012) that the initial texture of magnesium AZ31 alloy has significant effect on the recrystallization behaviour. Basal slip is known to have the lowest critical resolved shear stress (CRSS) value, however, at elevated temperatures, non-basal slip systems are activated as their CRSS is lowered shown for example by Srinivasarao et al. (2012). At low values of Zener–Hollomon parameter $Z = \dot{\epsilon} exp(Q/RT)$ (Zener and Hollomon, 1944), twins are suppressed, and $\langle c + a \rangle$ pyramidal slip systems are activated. These processes influence DRX of Mg alloys and ultimately affect the mechanical properties, and thus, any modelling of DRX in Mg alloys must take the microstructure and deformation mechanisms into consideration.

Enhancements in the experimental abilities and numerical techniques have led to increase in the theoretical and experimental knowledge of the DRX phenomenon in recent years. However, modelling of DRX phenomenon is still a challenging problem. This is mainly due to the multi-scale nature of DRX phenomenon, which involves the effects of impurities, precipitation, dislocation motion, movement of the grain boundaries, etc. Moreover, DRX is widely accepted as a problem, which is not completely deterministic due to the concurrency of the grain boundary motion and the complexity of the solutions from dislocation based mechanics (such effects as interactions between boundaries during recrystallization can have more than one stable state solutions (Pond and Casey, 1992)).

There are numerous of works to model recrystallization problem, and one of the widely used models are Monte-Carlo Potts and Cellular Automata models. DRX has been modelled in the past using cellular automata (CA) (Hesselbarth and Göbel, 1991; Raabe, 2002, 1999), Monte-Carlo Potts model (Anderson et al., 1984a,b; Rollett and Raabe, 2001) and other techniques. The CA method is based on the discretized cells with state variables, which characterize the cell. An initial state is assigned to represent microstructure. The kinetics of CA are defined on the switching the state of the cell depending on its previous state as well as the state of the neighbouring cell (Miodownik, 2002). The state of the entire aggregate is updated simultaneously, unlike in Monte Carlo models, for which the update of each site occurs randomly. Therefore, coupling of these two approaches is widely used and seem to provide good match with experimental results (Raabe and Becker, 2000; Rollett and Raabe, 2001; Goetz and Seetharaman, 1998; Ding and Guo, 2001; Hallberg et al., 2010; Hesselbarth and Göbel, 1991).

The CA method is capable of capturing local effects and is computationally efficient (Hallberg, 2011). However, the CA models alone lack the ability to predict microstructure evolution during deformation Hallberg et al. (2010). Therefore, when coupled with other techniques, including finite element, CA has been shown to be an effective tool for modelling recrystallization (Raabe, 2002; Gawad and Pietrzyk, 2007; Roters et al., 2010b; Seyed Salehi and Serajzadeh, 2012; Madej et al., 2013).

The Monte Carlo probability technique with application to recrystallization was used in the Potts model, which is a modified Ising model (Potts, 1952). Extensive studies were performed to model recrystallization and grain growth using the Monte Carlo method by Anderson et al. (1984a, 1989), Srolovitz et al. (1986, 1988), Grest et al. (1985) and others.

In the Monte Carlo models, the domain is divided into lattice sites by a grid. An index s_i is assigned to each site, and this index is the same within one grain. Every lattice site is assigned its state variables. The switching parameter for the Monte Carlo step, ω_{switch}, depends on the energy change ΔE. According to the Monte Carlo method, a random number $\xi \in [0, 1]$ is generated, and the switch is accepted if $\xi \leqslant \omega_{switch}(\Delta E)$; when the switch is accepted, the current site s_i takes an orientation of the neighbouring site s_j.

Monte Carlo models are attractive with their simplicity as a numerical model, and they are relatively easy to implement. Furthermore, the computational costs of the model are minimal. However, since the update of the microstructure in Monte Carlo models happens randomly, the process of defining correctly the nucleation sites becomes extremely important, since the final texture is highly dependent on the initial determination of the nuclei. Various nucleation models for Monte Carlo simulations were examined in Peczak and Luton (1993, 1994). Another disadvantage of the model is a non-trivial correlation of the simulation time and length with physical time and length. Therefore, there is a need for scaling or matching with experimental data. Possible solutions of this problem were discussed for example in Raabe (2000) and Glazier et al.