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MULTISCALE MODEL FOR DYNAMIC RECRYSTALLIZATION INCORPORATING PARTICLE PINNING AND GRAIN SIZE EFFECTS

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Summary. In the present work a finite-strain model for dynamic recrystallization is formulated. The model combines a crystal plasticity formulation, which captures texture evolution as well as grain size strengthening, with a vertex model for the evolution of the grain structure through nucleation and grain growth. The precence of second phase particle in the metal, hindering the grain boundary motions, is included in the vertex formulation. This provides a versatile model capable of simulation dynamic recrystallization in metals containing impurities, and of relating the effect of the particles on the resulting grain size to the macroscopic stress through a relation of Hall-Petch type.

1 INTRODUCTION

During thermomechanical processing of metals, the microstructure of the material will undergo a number of transformations which affect the macroscopic properties. For example, the grain size affects the strength of the material through the classical Hall-Petch relation, which states the yield stress to be inversely proportional to the square root of the grain size. An accurate constitutive model is therefore needed to be able to describe the evolution of the microstructure and relate it to macroscopic material properties such as strength and hardness. In the present work, a multiscale model is formulated, where a crystal plasticity model, combined with a vertex model of grain structure evolution, is employed in a finite element formulation. A grain size dependent hardening is added to the crystal plasticity formulation, allowing simulation of materials processing including grain size strengthening, whereas the vertex model handles not only grain boundary migration due to differences in stored energy between grains, but also the interaction between grain boundaries and second-phase particles.

2 CONSTITUTIVE MODEL

The crystal plasticity model describes plastic deformation in the material due to slip in the crystal structure, resulting in an increased dislocation density. This makes the material harder and increases the stored energy. The slip rate $\dot{\gamma}^\alpha$ is given by the power law

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left(\frac{|\tau^\alpha|}{G_r^\alpha} \right)^m \operatorname{sign}(\tau^\alpha) \tag{1}$$

where the slip resistance G_r^α is given by

$$G_r^\alpha = G_0 + Q \sum_{\beta=1}^{n} h_{\alpha\beta} g^\beta \tag{2}$$

with g^α evolving according to

$$\dot{g}^\alpha = (1 - Bg^\alpha) \frac{|\tau^\alpha|}{G_r^\alpha} |\dot{\gamma}^\alpha| \tag{3}$$

To incorporate grain size strengthening into the model Q is given the form

$$Q = Q_\infty \left(1 + \frac{k}{\sqrt{d}} \right) \tag{4}$$

where k controls the influence on hardening of the average grain diameter, denoted by d. The increase in stored energy due to plastic deformation can be evaluated from

$$\dot{E} = \dot{W}^p - \mathcal{D} = \sum_{\alpha=1}^{n} \tau^\alpha \left(1 - Bg^\alpha\right) \frac{G^\alpha}{G_r^\alpha} \dot{\gamma}^\alpha \tag{5}$$

2.1 Vertex model

For the topological evolution of the grain structure, a vertex model is used where the grain structure is represented by vertices connected by grain boundaries. Each grain boundary has individual properties in terms of the boundary energy and mobility, depending on the crystallographic misorientation across the boundary. The forces acting on the vertices, driving the grain structure evolution, stem both from the topology of the grain structure and from the difference in stored energy between neighboring grains.

During evolution of the grain structure a number of topological changes or transformations will take place, for example when two triple junctions meet and recombine, and when a small triangular grain gradually shrinks and disappears. Introducing stored energy as a driving force for grain boundary migration, and with particle pinning impeding the movement of the grain boundaries, also more complex transformations may occur, for example the splitting of a grain or one grain growing to encircle another. Another type of topological change in the grain structure is nucleation. In the present work nuclei are introduced at triple junctions where one of the surrounding grains has reached a stored energy above a certain threshold.

In addition to the ordinary vertices, immobile second phase particles are added to the grain structure. If, during evolution of the grain structure, a grain boundary reaches a particle, the boundary will become pinned to the particle. Unpinning of a grain boundary, as illustrated in Figure 1, will occur once the angle ϕ becomes larger than the critical unpinning angle ϕ_{cr}. A slightly more complex situation arises when a triple junction should become unpinned. When this occurs, two of the grain boundaries will become unpinned, and form a free triple junction together with a new grain boundary segment, see Figure 1b.

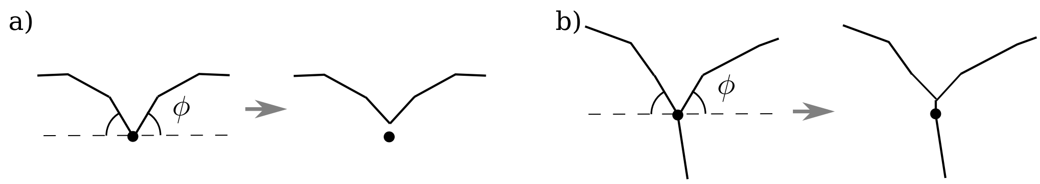

Figure 1: Illustration of different unpinning transformations: a) illustrates how a pinned grain boundary segment becomes unpinned and break away from the pinning particle b) illustrates how a pinned triple junction becomes unpinned, followed by the creation of a new triple junction and an additional grain boundary segment.

2.2 Multiscale coupling

The crystal plasticity model is used for modeling of the deformation and texture evolution of the grain structure and the vertex model is used to represent the evolving topology of the grain structure during recrystallization. For the solution procedure, a staggered approach is used. In each time step, the crystal plasticity model is first used for finding equilibrium, after which the evolution of the grain structure during that time step is calculated using the vertex model. The stored energy in each grain, calculated using crystal plasticity, is used to provide the driving forces in the vertex model, and for determining viable nucleation sites. In order to calculate the stress at a particular point, an area-weighted average over all grains at that point is calculated, using the grain areas from the vertex model. The grain sizes from the vertex model are also used for the grain size hardening in (4).

3 RESULTS

Calibration has been performed against experimental results related to compression of pure copper at different temperatures, showing that the present model captures the transition from single peak flow stress behavior at lower temperatures to a serrated flow stress curve at higher temperatures. Also some simulations at room temperature has been performed to allow comparison with experimental data for the Hall-Petch effect, showing good agreement. Comparison to experimental results for different initial grain sizes has also been performed at elevated temperatures. It is concluded that the initial grain size affects the initial response, where a large initial grain size yields a higher initial peak. However, after a few recrystallization cycles the initial difference vanishes.

With the addition of second-phase particles in the material, the recrystallization process is delayed. It becomes evident that, unlike the case with different initial grain sizes, the final result, even after several recrystallization cycles, is affected by the presence of pinning particles. Simulations with different numbers of particles do not converge towards the same stress level. It is clear that with a large number of particles grain boundary migration is affected. The particles hinder the grain boundary movement, and the resulting delay of the recrystallization process yields a smaller grain size, which in turn results in a harder material.

In addition to the difference in grain sizes, the particles affects the shapes of the grains, yielding irregular grain boundaries. The uneven grain boundaries which stem from particle interaction result in longer perimeters of grains having the same area. As the nucleation rate is given by unit grain boundary length, this will increase the nucleation, resulting in an effect similar to particle stimulated nucleation. Thus the presence of second phase particles will both act to increase the recrystallization rate through increased nucleation and decrease it through impeding the grain boundary migration.

4 CONCLUSIONS

The combined model is able to capture the process of dynamic recrystallization, where the hardening of the material due to dislocation density buildup is competing with the nucleation and growth of new grains, resulting in an oscillating flow stress behavior. With an efficient implementation, including GPU parallelization of the crystal plasticity calculations, the model can be applied to full scale simulations of thermomechanical materials processing. The model makes it possible to study how different factors, for example process temperature, strain rate and particle concentration, affects the grain structure and capture the effects on the macroscopic properties of the material.