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Level Set Modeling of Microstructure Evolution

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Mesoscale models of microstructure evolution, for example due to recrystallization, have historically been established using a number of different methodologies such as Monte Carlo Potts formulations, cellular automata, phase fields and front tracking algorithms [1]. Since introduced in [2], the level set method has gained increasing interest as one of the more promising approaches when it comes to trace the evolution of interfaces in a wide range of physical systems. These beneficial traits can also be utilized in mesoscale simulations of microstructure evolution due to the ability of the level set method to represent, for example, grain boundaries in polycrystal microstructures with high spatial and temporal accuracy. In addition, employed in a finite element setting, the use of level set-based RVE models provides new possibilities in multiscale modeling of crystalline materials.

Recognizing that the level set method has not yet reached its full potential when it comes to microstructure modeling, a number of developments of the method were recently proposed in [3], where also simulations of dynamic discontinuous recrystallization (DDRX) were performed, see Figure 1. The suggested developments include an "interface reconstruction" method which has a number of useful implications. One example is the clear geometrical definition of grain boundary triple junction points, in contrast to standard level set implementations where triple junctions lead to artificial voids between the level sets. Another benefit is the possibility to prescribe boundary conditions along grain boundaries. A third gain is the observation of the possibilities by which gradient effects within the individual grains can be included, based on the distance information held in the level sets.

The present contribution discusses the level set formulation, proposed in [3], and its application to modeling of aspects of microstructure evolution in polycrystal solids. Possibilities related to mesoscale modeling of recrystallization and grain growth, formation of stored energy gradients due to dislocation pile-ups at grain boundaries and the evolution of

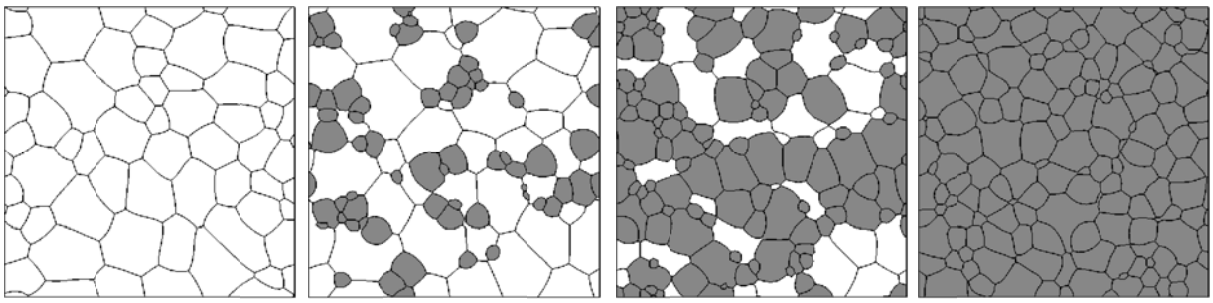

Figure 1: Evolution (from left to right) of a polycrystal grain structure due to DDRX. Recrystallized material is shaded gray. The images show simulation results based on the level set model proposed in [3].

grain boundary texture will be highlighted. The latter is based on the incorporation of anisotropic grain boundary properties in terms of grain boundary energy and mobility, which is an elaboration of the model in [3].

REFERENCES

[1] H. Hallberg, Approaches to modeling of recrystallization, *Metals*, Vol. **1**, pp. 16-48, 2011.

[2] S. Osher and J.A. Sethian, Fronts propagating with curvature dependent speed: algorithms based on Hamilton-Jacobi formulations, *J. Comput. Phys*., Vol. **79**, pp. 12-49, 1988.

[3] H. Hallberg, A modified level set approach to 2D modeling of dynamic recrystallization, *Modelling Simul. Mater. Sci. Eng.*, vol. **21**, pp. 085012, 2013.