

Master's Thesis Proposal

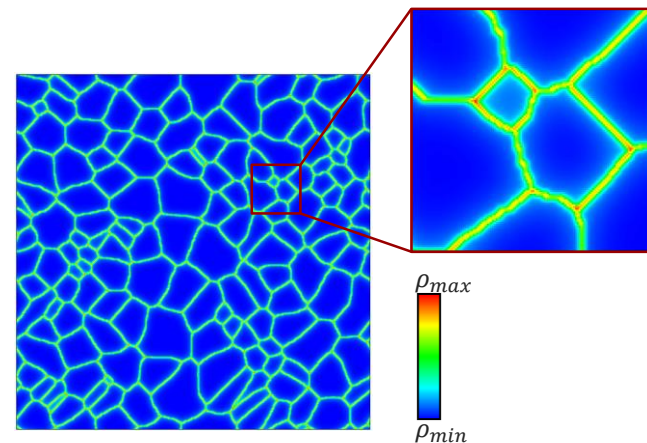
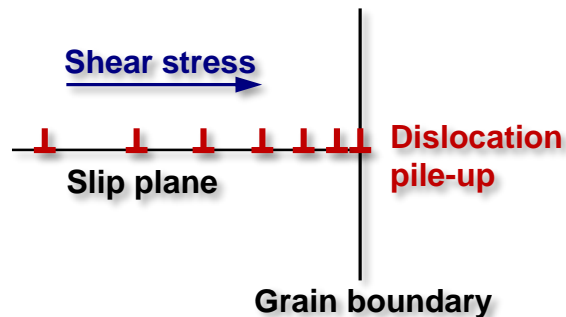
Reaction-Diffusion Modeling of Dislocations

Background

In metals, *dislocations* (imperfections in the crystal lattice) are central to plastic deformation of the material. The distribution of the dislocations in the material microstructure and the formation of dislocation patterns have a major impact on the material properties. One effect is the classical Hall-Petch relation, whereby smaller crystals give a harder material. This is related to dislocation pile-ups at the grain boundaries.

Project

This project will use a so-called *reaction-diffusion* approach to model the stability of the dislocation distribution in metal microstructures and the formation of dislocation patterns. The modeling will be performed using finite difference and/or finite element methods. The project is directly linked to ongoing research



References

- H. Hallberg and M. Ristinmaa (2013), *Microstructure evolution influenced by dislocation density gradients modeled in a reaction-diffusion system*, Computational Materials Science, 67:373-383



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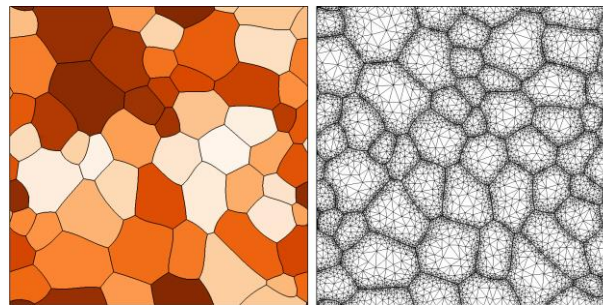
Physics-Based Mesh Adaption

Background

Microstructure changes in metals is mainly due to the movement of interfaces, such as grain boundaries. To trace the interface evolution a very fine mesh is required. However, using a very fine mesh everywhere will be too computationally expensive. The solution is an *adaptive mesh* which is continuously adapted to the moving interfaces.

Project

This project will consider microstructure physics such as interface curvature and gradients in the fields which move the interfaces to control the mesh size in critical regions. The interfaces will be modeled by so-called *level sets*. A Fortran-based finite element implementation of level sets exists and the project will focus on improving the meshing algorithm. The project is directly linked to ongoing research



References

- H. Hallberg (2014), *Influence of anisotropic grain boundary properties on the evolution of grain boundary character distribution during grain growth - A 2D level set study*, Modelling and Simulation in Materials Science and Engineering, 22(8):085005
- H. Hallberg (2013), *A modified level set approach to 2D modeling of dynamic recrystallization*, Modelling and Simulation in Materials Science and Engineering, 21(8):085012

