OTTO VON GUERICKE UNIVERSITÄT MAGDEBURG

Micromechanical simulation of deformation and fatigue of polycrystalline materials

Oleksandr Prygorniev[1]. Supervisors: Prof. Konstantin Naumenko[1] and Prof. Holm Altenbach[1]
[1]Institute for Mechanics, Faculty of Mechanical Engineering, Otto-von-Guericke-University Magdeburg

As it well-known life time of structures can be evaluated through numerical simulations. An accurate and efficient material model is the most important step in such simulations. Accuracy can be achieved by taking into account all significant effects which are observed during testing of specimens. However, testing of a specimen is very expensive. Whereas, numerical simulation of material microstructure can produce similar effects and limited by computational costs. An additional advantage is the possibility to perform experiments like tension of a specimen for different directions but with the same initial microstructure, which is impossible in reality. Finally, analysis of stresses and strains at microscale is useful for explanation and description of macro material behavior.

Problem Definition

Usually, for identification of macro material behavior and material model parameters simulations of a representative volume element (RVE) are used. Inside the RVE microstructure is generated as close as possible to reality. Representativeness of a RVE is based on periodic geometry and periodic boundary conditions. Therefore, good accuracy can be achieved in bulk region of structures, while on free surfaces the use of classical RVE-methods is questionable. Existence of a high deformation gradients makes application of RVE-technique difficult. For this reason, it is necessary to check applicability of RVE in an arbitrary point of a structure. This can be done through simulation of a specimen with discrete microstructure and without kinematic boundary conditions on free surfaces.

Objectives

- Modeling of polycrystalline microstructure for the example of pure copper
- Development of an automated tool to perform the full cycle of simulation: From generating grains to postprocessing
- Analyses for different loads and boundary conditions
- Statistical assessment of stresses, strains and displacements at micro- and macroscale
- Implementation of mapping and interpolation algorithms to perform point-wise averaging of fields
- Implementation of damage mechanisms
- Comparison with gradient type macro-material model

Cooperation

Development of the software framework for modeling and simulation of polycrystalline microstructure was done in cooperation with the following students of the GRK-school: O. Ozhoga-Maslovskaja, M. Ievdokymov, I. Lvov, A. Kutschke, A. Girchenko. The exchange of experience in discussions with other members of the GRK-school was also very beneficial especially on workshops. Recommendations of M. Weber, S. Roy, etc. significantly improved functionality and performance of the developed tool. For example, Voronoi algorithm was implemented in collaboration with Y. Wang. Additional motivation and experience were achieved during participation in conferences with financial support of the GRK-school.

Modeling

Polycrystalline microstructure is represented as Voronoi diagram with randomly distributed grains. Due to anisotropy of single grains and random crystal lattice orientation high heterogeneity in the polycrystal is observed. Therefore, stresses, strains, etc. in a polycrystalline and a homogeneous model are not comparable. However, smooth fields can be achieved through point-wise averaging of fields from multiple statistically randomized realizations of the same domain and load.

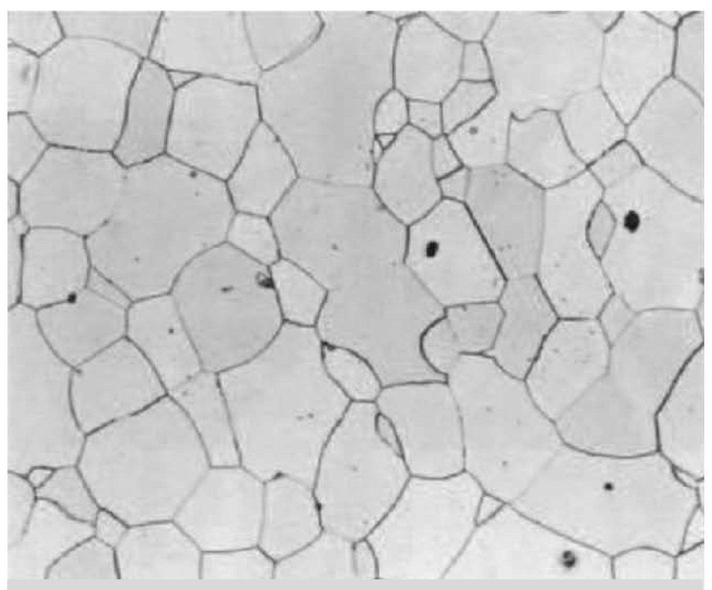

Figure 1. Example of microstructure

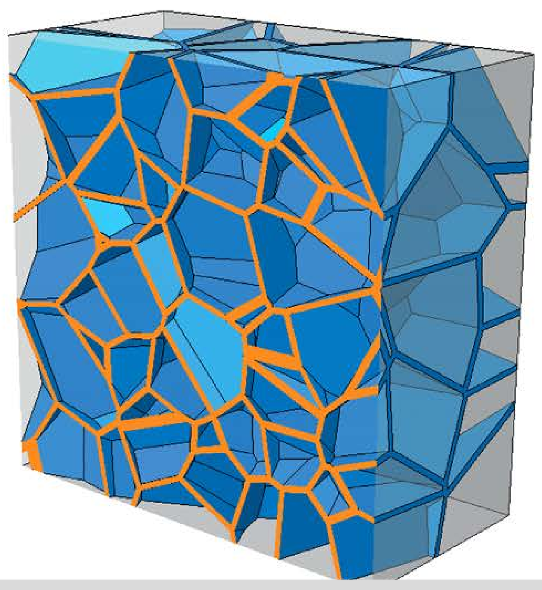

Figure 2. Unit cell with grain boundaries

Figure 3. Polycrystal

Comparison of stresses, strains, etc.

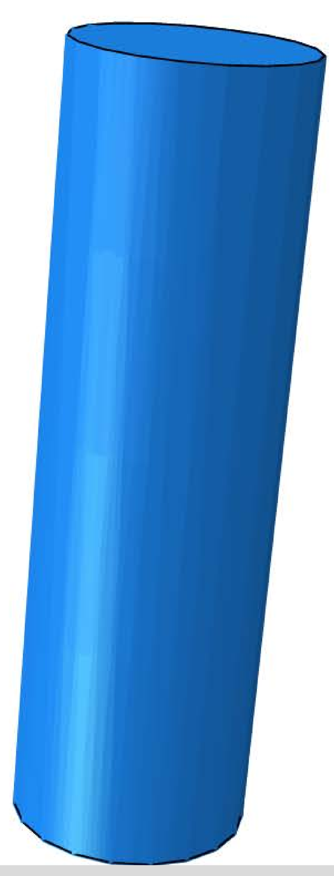

Figure 4. Homogeneous model

Simulation

In the first example 200 realizations of a rectangular plate with 1000 grains are generated and computed for cyclic creep test conditions with a predefined strain amplitude (Fig. 7). Example of one realization is shown in Fig. 5. Averaged distribution of stresses in x direction is presented in Fig. 6 for time point 50 h. The stress-strain hysteresis loops in the bulk and the surface regions are plotted in Fig.8 by blue and red line respectively. Figure 8 shows the stress distribution along the path given in Fig. 6.

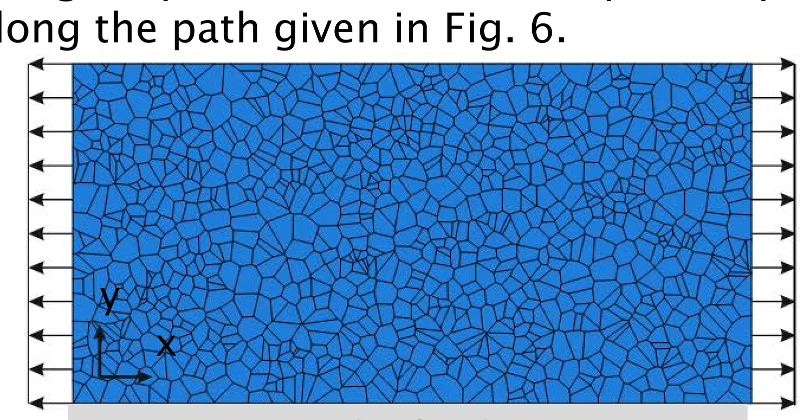

Figure 5. Example of realization

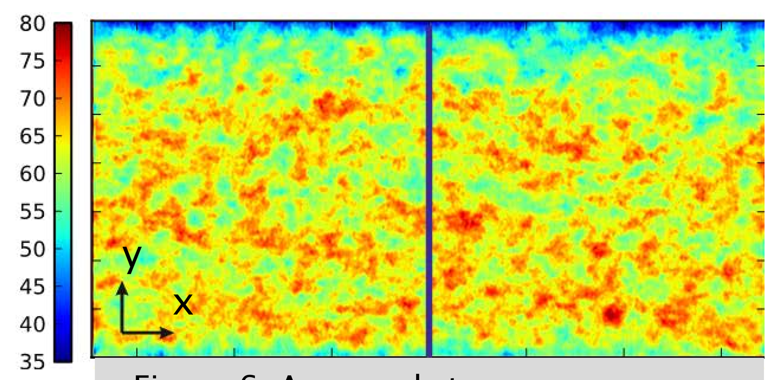

Figure 6. Averaged stresses

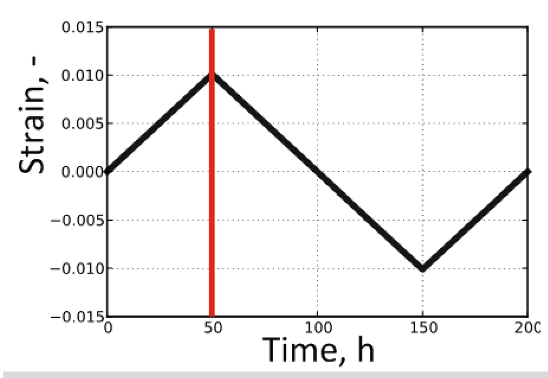

Figure 7. Loading amplitude

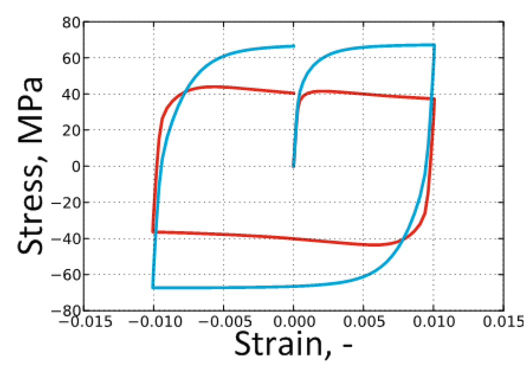

Figure 8. Hysteresis loops

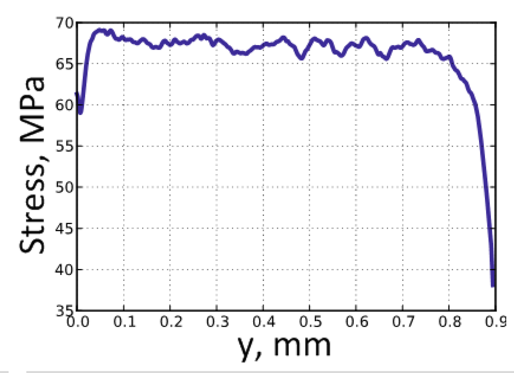

Figure 9. Stresses vs y

As a second example (Fig. 10) 200 realizations of a cylindrical bar with 1500 grains are analyzed.

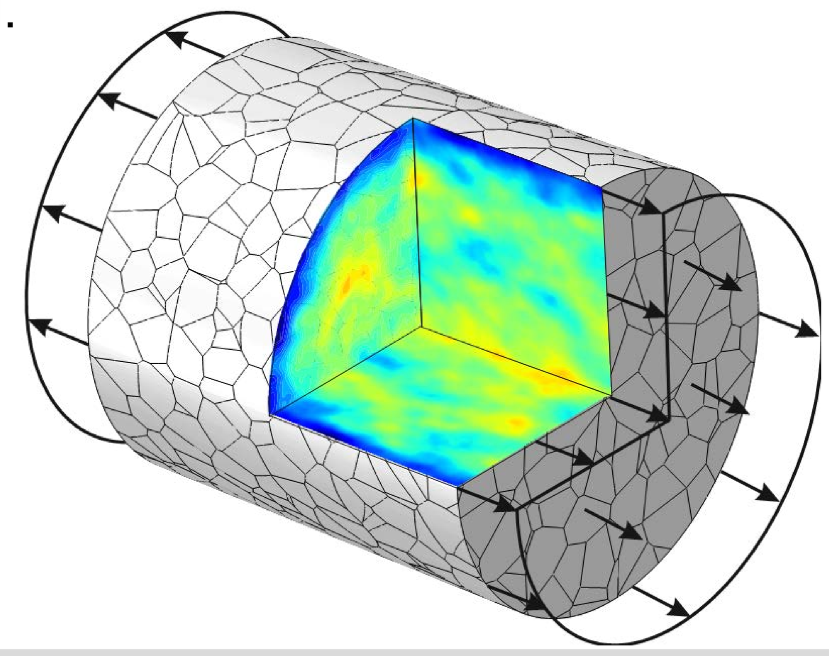

Figure 10. Averaged stresses in three orthogonal cross sections

Results and Discussion

By point-wise averaging of stresses from 200 realizations of a rectangular plate (Fig.5) averaged distribution is calculated and presented in Fig.6 for time equal to 50 h. Top surface of the model is free of constraints while on bottom symmetric boundary conditions are applied. In Fig. 6 one can clearly see appearance of surface layer effect as decreasing of stresses. The same behavior is confirmed in a similar analysis of a cylindrical bar under tension shown in Fig. 10. Stresses in a homogeneous model (Fig. 4) computed within classical continuum theory are uniform. Therefore, in the bulk region RVE-methods can be applied without restrictions while close to the surface of structures additional analyses are required.

Conclusions

The framework for simulation of polycrystalline microstructure is implemented and used for examples of a cylindrical bar and a rectangular plate. Averaged distributions of stresses in both cases clearly illustrate appearance of surface layer effects. To capture surface layer effects classical continuum models should be extended.

DFG-Graduate School 1554 “Micro-Macro-Interactions in Structured Media and Particle Systems”