
Sub-project: Scale bridging techniques from atomic scale to continuum level for plasticity - Plastic Deformation of Metal Matrix Composites and Multiphase Steels under External Loading

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Summary

The scope of the project is the prediction of plastic deformation by coupled simulations at different length scales present in materials. The model material systems are (Al-)MMCs and dual-phase steels. Both systems exhibit the presence of coarse (μm) and fine (nm) second phase particles. The former result in the need for gradient-plasticity in the FEM simulations of the microstructure, the latter necessitate the application of dislocation dynamics simulations to determine the strengthening caused by them. The combined multiscale approach then allows considering the macroscopic behaviour of the materials. The mechanism-based strain-gradient plasticity theory (MSG) [1, 2] provides the theoretical background for the size effect present around the coarse second-phase particles. Its implementation into the FEM simulations is provided using an ABAQUS-USER element, which allows calculating strain gradients and the resulting hardening depending on the magnitude of the gradient.

State of Current Work

The general implementation of the multiscale scheme for the nanoscale has been employed to different material systems and provides a workable solution to the calculation of precipitation-induced strengthening. The strengthening caused by the presence of coarse second-phase particles can be calculated using a simple FEM model for large particles, where the size effect does not play a role. The MSG theory based USER element currently is only applicable to 2D elements, meaning that real microstructures with particle sizes around $1 \mu\text{m}$, where the size effect is very pronounced currently cannot be modelled with satisfying accuracy. Therefore, the development of an accurate 3D element is an important next step.

Interim Results and Collaboration

For the system of Al-MMCs a simplified model for the deformation and fracture was developed without considering the influence of gradient plasticity on the material behaviour. This limited approach already employs the element deletion technique, but is quite inaccurate, as the gradient effects that arise from the presence of so-called geometrically necessary dislocations (GNDs) has high influence on the matrix material in the vicinity of the coarse particles which are the preferred sites for failure in MMCs. There, it is essential to include these effects to predict the failure correctly.

Nanoscopic second-phase particles

The influence of small precipitates on the dislocation motion has been investigated for different material systems in this project. Interesting results have been observed for the binary Ag/Cu system which – due to its simplicity – serves as a model system for the lower scales of the multiscale approach. This is especially important for the transition from 2D dislocation dynamics used in the previous project to the 3D formulation which is more representative of real mesoscopic volumes.

Collaboration with Université Paris XIII

As Prof. S. Queyreau at UP13 is a renowned expert on dislocations and the simulations thereof, the chance to collaborate in the framework of the DAAD program PROCOPE was used. The project entailed the investigation of dislocation/precipitate interaction in the iron system on an atomistic level, especially with respect to improving the accuracy of the simulation of the influence of nanoscopic precipitates on the propagation of dislocations. As the strengthening of the matrix material has a significant influence on the overall material behaviour, this subproject provided valuable insights for the multiscale approach.

References

- [1] Gao, H., Huang, Y., Nix, W. D., & Hutchinson, J. W. (1999). Mechanism-based strain gradient plasticity - I Theory. *Journal of the Mechanics and Physics of Solids*, 47, 1239 – 1263.
- [2] Gao, H., Huang, Y., Nix, W. D., & Hutchinson, J. W. (2000). Mechanism-based strain gradient plasticity - II Analysis. *Journal of the Mechanics and Physics of Solids*, 48, 99 – 128.
- [3] Ghassemi-Armaki, H, Maaß, R., Bhat, S.P., Sriram, S., Greer, J.R., and Kumar, K.S. (2014). Deformation response of ferrite and martensite in a dual-phase steel. *Acta Materialia*, 62, 197 – 211.

Future Work

One of the future aims is the extension of the multiscale approach to the fracture of materials with both, coarse and fine second phase particles, especially considering fracture at the interfaces for the case of MMCs. The main access to the simulation of fracture will be the element deletion method, which removes severely plastically deformed elements from the simulation. The other big focus is the application of the multiscale approach to dual-phase steels in which martensite takes over the role of the strength-increasing ceramic inclusions. This necessitates an adaption of the model, as the metallic inclusions are susceptible to plastic deformation [3], whereas the brittle ceramic inclusions can be assumed to behave perfectly elastic.

Important Publications

- [1] Molnar, D., Weber, U., Binkele, P., Rapp, D., and Schmauder, S. (2015). Prediction of macroscopic damage behaviour of precipitation strengthened steels via multiscale simulations. *GAMM-Mitteilungen*, 38, 228 – 2478. doi: 10.1002/gamm.201510013
- [2] Schmauder, S., Rapp, D., Molnar, D., and Binkele, P. (accepted). Multiscale Materials Modelling: Procedures – Examples – Challenges. *Proceedings of the Sixth International Conference on Structural Engineering, Mechanics and Computation*, Paper No. 293.