Project Network 2: Data-enhanced scale-bridging from particles to continuum

Sub-project Machine-learning approach towards complex dislocation/precipitate interactions in Discrete Dislocation Dynamics

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Summary

Aim of the project is to improve the consideration of nano-scale precipitates in Discrete Dislocation Dynamics (DDD) codes, in order to provide a physically based treatment of the dislocation/precipitate (d/p) interaction at small (i.e., atomistic) scales which is responsible for precipitation strengthening in metals and alloys. Currently these precipitates are frequently treated as Eshelby-type inclusions (perfectly elastic ellipsoids embedded in a perfectly elastic matrix) that are impenetrable for dislocations, and interact with dislocations via the stress fields from the Eshelby solution. This continuum solution is no longer accurate at nanoscopic length scales. To include the experimentally observed cutting of precipitates by dislocations this approach is usually combined with a single critical resolved shear stress (CRSS) value at which a dislocation starts to cut through the precipitate. Data from Molecular Dynamics (MD) simulations of these d/p-interactions in dependence on glide plane (*p*), precipitate radius (*R*), dislocation type (*t*) and plane intersection height (*h*) will be used to train an Artificial Neural Network (ANN) to provide the CRSS for different geometrical d/p-arrangements. This is required, as the direct calculation of the d/p-interaction from MD is computationally far too expensive to be applied within DDD.

State of Current Work

Researchers have provided some analytical solutions to the problem of the discrete nature of the d/p-interaction at the nanoscale [1], which, however, do not account for effects that arise from interface misfit dislocations found in our prior work [2] and assume coherent precipitate/matrix-interfaces, which is correct only for very small precipitate sizes (usually a few nm).

Previous Work of the Principal Investigator

A detailed investigation of possible d/d-interactions was provided in [2]. Additionally, in [3] a complete multiscale approach for precipitation strengthening was presented. Therein the simple interaction model from current DDD codes was employed for assessing the strengthening due to precipitation, leaving potential for improving the accuracy using the new d/p-interactions.

Literature

[1] N. G. Kioussis and N. M. Ghoniem: Modeling of Dislocation Interaction with Solutes, Nano-Precipitates and Interfaces: A Multiscale Challenge. *Journal of Computational and Theoretical Nanoscience* **7** (2010), 1 – 30.

[2] S. Hocker, D. Rapp, S. Schmauder: Molecular dynamics simulations of strengthening due to silver precipitates in copper matrix. *Physica Status Solidi B* **254** (2017),1600479.

[3] D. Molnar, U. Weber, P. Binkele, D. Rapp, S. Schmauder: Prediction of macroscopic damage behaviour of precipitation strengthened steels via multiscale simulations. *GAMM-Mitteilungen* **38** (2015), 228 – 247.

Project Goals

The main goal is to integrate ANN results into an existing DDD code (microMegas) and to provide sufficient data from MD simulations to accurately train the ANN to provide reliable predictions for the d/p-interactions in subsequent DDD simulations by querying the correct behaviour (circumvention mechanism, CRSS) for each d/p-interaction from the ANN.

Work Schedule (November 2017 – December 2018, 14 months)

In order to reach the goal of improving the DDD model for small particles with regard to their strengthening ability, the following steps are needed during the 14-months period of the project:

- MD calculations of shear tests to provide reference data (CRSS) for the ANN
- Training of the ANN with the CRSS as a function of radius *R*, height *h*, glide plane *p*, d-type *t*
- Providing the ANN data to the code for d/p-interactions in the DDD software
- Parameter study on the influence of particle distributions on strengthening with the old and new approach in order to determine the effect of including details (residual stresses, d/d-reactions, possible change in circumvention mechanism, i.e. cutting or Orowan bypassing)
- Authoring reports and papers

Cooperation with Scientific Partners

This project is related to the work on DDD from our prior cooperation partner S. Queyreau at “Université Paris XIII” working on the implementation of atomistic, i.e. non-Eshelby influences of small precipitates in DDD codes, such as microMegas (mM) and ParaDiS (both free software).

Perspective Work Schedule

Another feature missing from current DDD implementations is the simulation of polycrystalline samples. This is due to many parts of solving the contributions of the elastic stress fields originating at the individual dislocation segments relying on the assumption of periodic boundary conditions, which no longer remains valid in elastically anisotropic polycrystalline samples. To address this issue, fundamental changes to the computational approach have to be implemented. In case of successful implementation, polycrystalline samples obtained from 3D microstructural data can be subjected to the new approach and the results shall be compared to experimental results on stress-strain curves. The possibility to directly compute polycrystalline samples with DDD would complete the link between the atomistically-informed mesoscale and the microstructure level. This would also help to explain the empirically motivated Taylor factor which traditionally is used to generalize single-crystal results on the stress-strain behaviour to describe the plastic deformation of polycrystals.