Atomistically motivated interface modeling to account for coupled plasticity and damage

S. Reese*, S. Rezaei*, T. Brepols*, M. Fassin* and S. Wulfinghoff†

* RWTH Aachen University, Institute of Applied Mechanics
D-52074 Aachen, Germany
e-mail: stefanie.reese@rwth-aachen.de, web page: http://www.ifam.rwth-aachen.de

† Kiel University, Institute for Materials Science – Computational Materials Science
D-24143 Kiel, Germany

ABSTRACT

Grain boundary (GB) characteristics play an important role in the determination and prediction of material behavior, especially when it comes to nanocrystalline metals and ceramics. The main goal of this contribution is to develop a general interface model to accurately incorporate grain boundary sliding as well as intergranular fracture as two main phenomena in characterizing the grain boundary. To gain a deeper insight into the behavior of different grain boundaries, molecular dynamics (MD) simulations are utilized for mode I and mode II loadings. Current MD investigations motivate a model which accounts for anisotropic plasticity and damage within the grain boundary to capture the complex interface behavior. Therefore, a two-surface formulation is developed in which damage and plasticity at the interface are coupled in a thermodynamically consistent way. The parameters for the introduced interface model are determined using the MD simulations based on an embedded atom potential. Finally, the calibrated interface model is implemented into a cohesive zone (CZ) element [1].

It is observed by numerical simulations of representative material samples that the macroscopic material behavior is anisotropic. This motivates the development of an anisotropic continuum mechanical plasticity-coupled damage model (see e.g. [2]). One important finding is the treatment of the second order damage tensor as structural tensor [3]. It is further interesting that the theoretical formulation of the model shows strong analogies to models of Armstrong-Frederick kinematic hardening and for fibre-reinforced materials.

REFERENCES

