

Multiscale modeling of deformation of ultra-fine grained metals at high homologous temperatures

Alexander Hartmaier, Naveed Ahmed
Interdisciplinary Centre for Advanced Materials Simulation (ICAMS)
Ruhr-University Bochum
Stiepeler Str. 129, 44801 Bochum, Germany

Two-dimensional dislocation dynamics (2D-DD) and diffusion kinetics simulations are employed to study the mechanisms of plastic deformation of ultra-fine grained (UFG) metals at high homologous temperatures. Besides conventional plastic deformation by dislocation glide within the grains, we also consider grain boundary mediated deformation and recovery mechanisms based on the absorption of dislocations into grain boundaries. This requires solving the diffusion equation and coupling it to dislocation motion within the model. The material is modeled as an elastic continuum that contains a defect microstructure consisting of a preexisting dislocation population, dislocation sources, and grain boundaries. The temperature dependence of the mechanical response of the model material to an external load is calculated and the contributions of different deformation mechanisms to the total deformation are monitored. We find that at low homologous temperatures the behavior of the model material is well described by a classical Hall-Petch law. At high homologous temperatures, instead, we find a pronounced grain boundary softening and, moreover, a high strain rate sensitivity of the model-material. These numerical findings qualitatively agree very well with experimental results known from the literature. Thus, we conclude that grain boundary sliding although its immediate contribution to plastic slip is only marginal, enables recovery processes at the grain boundary. Hence, grain boundary diffusion is the rate-limiting factor for recovery and plastic deformation of UFG metals and in consequence causes the pronounced strain-rate sensitivity of UFG metals and also the observed tendency towards grain boundary softening at high temperatures.