INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

The ICAMS Seminar presents

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Atomistic Simulations of Nanocrystal Plasticity: From Qualitative to Quantitative Analysis

The high yield strength of nanocrystalline metals makes them interesting candidate materials for technical applications. However, conventional models of polycrystal plasticity can not be used any longer as the deformation mechanisms change when the grain size is reduced from the µm to the nm scale: dislocation-dislocation interactions become less frequent and the interactions of dislocations with grain boundaries (GBs) become more important. Molecular dynamics (MD) simulations have provided considerable insight into the details of deformation mechanisms in face-centered cubic (fcc) nanocrystalline metals. Based on these simulations, it is generally believed that grain boundaries act as both sources and sinks for dislocations, i.e., dislocations are emitted from stress concentrations at GBs, travel through the grain and are absorbed at the GBs. This talk presents results from simulations of tensile tests on different, fully three dimensional nanocrystalline aluminium samples. The detailed analysis of the atomistic configurations showed for the first time the importance of cross-slip which allows the dislocation to avoid local stress concentrations at the GBs that otherwise can act as strong pinning sites for dislocation propagation. The simulations were furthermore analyzed in terms of the grain-averaged shear produced by dislocation slip and the grain-averaged resolved shear stress τ_c at these slip events. Analysis of the atomic processes allowed to correlate the stress signature of slip events with typical dislocation processes related to nucleation and propagation. This analysis showed that the depinning of expanding dislocation loops from obstacles at the GBs rather than the nucleation of dislocations constitutes the rate limiting process in the simulations. A simple crystal plasticity model is presented which captures the main characteristics determined from the atomic scale simulations and highlights the importance of the distribution of τ_c on the plastic deformation of nanocrystalline metals.