3D discrete dislocation dynamics simulation of polycrystalline films and silicon electrostatics

Hareesh TUMMALA

Supervisor: Marc Fivel and Thomas Pardoen (Univ. Catholique de Louvain)

Monday, December 12th at 9:30 am

Amphitheater Jean Besson – Phelma Campus

Abstract: Plastic deformation of classical crystalline materials is essentially dominated by dislocations and their mutual interactions. In nanocrystalline (nc) metals, different grain boundary mechanisms may exist in addition to the dislocation-based mechanisms. The dependency on, among others, the grain shape, grain orientation, initial dislocation density, grain boundary structure and external conditions will promote one or two deformation mechanisms over others. These dominant mechanisms dictate the overall response of nc metals. The influence of microstructural features in promoting these dominant mechanisms need to be better understood individually and collectively.

In the scope of the thesis, 3D discrete dislocation dynamics (DDD) simulations were performed on three micron-sized single grains of same volume but differing in aspect ratios to understand the influence of grain morphology. A decrease in localization of plastic deformation with increasing grain aspect ratio was observed. Due to the enhanced cross-slip mechanism, grains with higher aspect ratio exhibit a lower strain hardening behaviour. The anisotropic plastic response of elongated grains was quantified in terms of the magnitude of backstress on each slip system.

Further, a polycrystalline version of dislocation dynamics code coupled with a finite element method was used to study the mechanical behaviour of free-standing palladium thin films with columnar grains. The initial dislocation density considered in the simulations is close to the one measured experimentally. DDD simulations of a polycrystal with hexagonal grains properly reproduce the strain hardening behaviour. For a heterogeneous grain size distribution of the polycrystal, an increase in strength with decreasing film thickness was observed. The key element is that the probability of smaller grains with no initial dislocations is increasing with decreasing thickness of the film.

Finally, by adapting Read's model, the influence of a static, electrically-charged dislocation on electrical properties in semiconductors was studied.