Atomistic simulations of plasticity in small dimensions: Nanocrystals, nanowires and nanofoams

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It is well known that at reduced length scales, metallic materials often show enhanced mechanical properties, particularly an increase in strength, leading to the so-called “smaller is stronger” paradigm. Understanding such behavior is currently a central topic of research in materials science. Atomistic simulations which have now become the cornerstone of computational materials science, are increasingly used to gain deeper insights into small scale plasticity.

Here, we report on the results of large scale atomistic simulations of both single crystalline and polycrystalline materials. In particular, we look into the influence of interface curvature, topology and network, and the presence of notches or slits in nanocrystalline microstructures, on the detailed plastic deformation mechanisms at small scales. The results show the activation of twins in microstructures that evidence curved grain boundaries (GBs), which also show reduced GB mediated plasticity. Subsequently, to assess the importance of twins, we study the deformation behavior of nano-twinned nanowires under tensile loading.

In the final part of the talk, we present a state-of-the-art method to obtain realistic atomistic samples directly from experimental datasets. Exemplarily, we construct atomistic samples of nanoporous Au using STEM tomography data, and subject them to compressive loading. By comparing the results of these simulations to those obtained from geometrically constructed samples, we can study the effect realistic curvature and topology, and the distribution of ligament size on the deformation behavior.

The atomistic simulations are carefully analysed in terms of dislocation activity, twin nucleation, and stress state, amongst others. The results are finally discussed in the context of meso-scale and continuum scale models.