Towards a more Realistic Modeling of Defect - Defect Interactions in Atomistic Simulations of Crystalline Materials

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"Crystals are like people. It is the defects in them which tend to make them interesting."
Colin Humphreys

Real crystals are never perfect, and they always contain some sort of defects. And it is the interaction between these defects which largely determine the mechanical properties of real world materials. Typical examples include the increase in yield strength caused by the interaction of dislocations with solute atoms, precipitates, grain boundaries (GBs) or other dislocations. But also the fracture toughness is governed by the interaction of cracks with dislocations, and crack propagation along GBs is generally easier than transgranular fracture. While the applied stress and long-range elastic interactions between defects provides the driving forces for the nucleation and propagation of defects, their direct interaction is governed by the atomic-scale structure of the defects. Consequently, atomistic simulations play a key role in studying the nucleation and interaction of defects, like GB fracture and the nucleation, pinning, absorption or transmission of dislocations at GBs. However, even though the increase in computational power allows nowadays for massively-parallel simulations of billions of atoms, most of the detailed studies on defect-defect interactions are still performed on simplified, highly idealized scenarios. Typical examples are quasi-two dimensional setups with straight dislocation lines or crack fronts interacting with perfectly planar GBs or the use of Voronoi tessellation to generate polycrystals.
Here we provide an overview of our recent atomistic studies on trans- and intergranular fracture, dislocation – GB interactions and nanocrystal plasticity with the focus on 3D aspects, curved crack fronts, non-planar boundaries and realistic GB topologies and compare them with the results from idealized simulation setups. We furthermore show how using real microstructure morphologies obtained from atom probe tomography allowed to reveal in atomistic simulations dislocation processes hitherto only observed in experiments. While idealized simulation setups will always remain important for the quantitative determination of defect properties, experimentally-informed atomistic simulations provide unique possibilities for the qualitative study of defect-defect interaction mechanisms.