Deformation of Single- and Bi-Crystalline Au Nanowires

Nanowires (NW) have gained great attention in recent years as basic building blocks for reliable nano- and micro-electromechanical devices (NEMS/MEMS) owing to their unique properties, in particular due to their ultrahigh-strength and super-ductility. One of the recent approaches to tailor mechanical properties of NWs is to introduce an initial microstructure a-priori during their growth process, creating ordered structures of grains separated by planar defects called twin boundaries. For instance, NWs with twin boundaries perpendicular to the NW’s axis exhibit high yield stress and a ductile-to-brittle transition with distinct correlation to the boundary spacing. Additionally, five-folded twinned NWs, a stable structure consisting of five identical grains separated by twin boundaries parallel to NWs axis, exhibit high strength and low ductility compared to pristine single-crystalline NWs. In the current research, we examine how an initial single longitudinal twin boundary, i.e. a NW with two identical grains, affects mechanical properties. We performed Molecular Dynamic (MD) tensile simulations of both single- and bi-crystalline Au NWs in order to reveal the influence of the individual longitudinal twin boundary on mechanical properties and the governing microstructural mechanisms. We show that deformation of both types NWs takes place either via deformation twin or through ordinary dislocation plasticity. Single-crystalline NWs deform mainly by deformation twin and can elongate in a few tens of percent before fracturing. Twinning of the bi-crystalline NWs require a coordinated deformation twin in both grains since the longitudinal twin limits the deformation twin in each grain. Consequently, limited detwinning of the longitudinal twin was observed and shorter lengths of deformation twin were identified. Eventually, fracture occurred in the twinned region via ordinary dislocation plasticity in both types of NWs. The simulation results rationalize experimental observations performed in a frame work of a joint research project with Georg-August-Universität Göttingen.