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Influence of Twin Boundaries on the Mechanical Behavior of fcc-Metallic Nanowires Subjected to Bending

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Metallic nanowires (NWs) display superior mechanical properties compared to their bulk counterparts. Most fcc-metallic NWs are oriented along a <110> axis, and many NWs have one or multiple twin boundaries (TBs) parallel to the wire axis. Such NWs have been studied extensively in tension, where the TBs were shown to lead to an increase in yield stress and to a different deformation morphology compared to single crystalline NWs [1]. The influence of TBs on the deformation in bending, most important for applications in flexible electronics, has, however, so far not been studied in detail.

Here we present our recent results of molecular dynamics simulations on single and bi-crystalline twinned NWs subjected to bending. We show that the presence of a TB not only influences the plastic deformation but also affects the stress state of nanowires. The critical resolved shear stress for dislocation nucleation was determined and the interactions of dislocations with TBs was studied in detail for varying TB location and bending directions.

Keywords: Nanowire, Coherent twin boundary, Bending, Molecular dynamics.

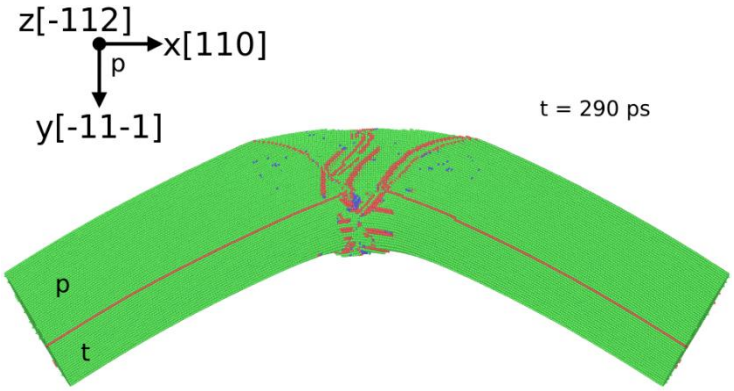

Fig.1 Example of a plastically deformed bi-twinned Ag NW. Atoms belonging to the TB and to stacking faults are colored red.

References:

[1] Zhuocheng Xie, et al, Origins of strengthening and failure in twinned Au nanowires: Insights from in−situ experiments and atomistic simulations, Acta Materialia 187, 2020, 166-175.