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DEFORMATION MECHANISMS OF TWINNED NANOPARTICLES AND NANOWIRES

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The plastic deformation of nanoscale metallic specimens has recently attracted a lot of interest due to the reported changes of deformation mechanisms with reduced size. Similarly, the interaction of dislocations with twin boundaries has received lots of attention in the context of the ultrahigh strength and ductility of nanotwinned metals. Here, we present experiments and atomistic simulations of compression test on twinned gold nanoparticles to study dislocation processes and -storage in nanosized volumes and dislocation-twin interaction mechanisms and compare them with the deformation behavior of twinned silver and gold nanowires. Compression experiments were performed on triangular shaped, facetted particles using a nanoindenter with a flat punch tip. During compression along the [111] direction, all particles assume a characteristic asymmetric “mushroom” shape, which has not been reported in the case of uniaxially compressed single crystalline Au nanoparticles. Post-mortem TEM-analysis in cross-sectional and plan-view geometry reveal the storage of full dislocations. Dislocations were also observed on the (111) plane parallel to the twin plane, which should not experience any resolved shear stress during compression.

Molecular Dynamics simulations of Au nanoparticles of same shapes as in the experiments were performed using different types of indenters, boundary conditions, strain rates and potentials. The processes of dislocation nucleation, interaction with the twin boundary, dislocation-dislocation reactions, cross-slip and dislocation escape through the free surfaces are studied in detailed and analyzed in terms of the stress state. Comparison with the experimental microstructure of the compressed particles allows to draw conclusions about the dominating dislocation processes during the deformation of the twinned nanoparticles. In particular, the presence of dislocations on the (111) planes provides indirect evidence for transmission of dislocations through the twin boundary onto {100}-type planes. The dislocation – twin interaction mechanisms are compared to single and multitwinned gold and silver nanowires. The results highlight the importance of boundary conditions and internal interfaces on the nucleation, escape, storage and interactions of dislocations in nano-objects.