Interactions of dislocations and twins with grain boundaries: unraveling the mechanisms of plastic deformation in polycrystals

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Grain boundaries play a critical role in the plastic deformation of metallic materials. They may hinder slip transfer, leading to the formation of dislocation pile-ups and to size effects (Hall-Petch) or allow slip transfer, allowing the localization of deformation in suitably oriented grains clusters. They can also absorb and/or emit dislocations, nucleate twins, induce fracture, etc. As a result, interaction of dislocations and twins with grain boundaries as well as the role of grain boundaries in the nucleation of twins has received a lot of attention from the scientific community. However, most of experimental results are limited to surface observations in which the 3D nature of grains boundaries is not accounted for while atomistic simulations are mostly focused on coincidence lattice site boundaries that are different from the disordered grain boundaries of polycrystals. Thus, reliable criteria to quantify the role of grain boundaries in polycrystal deformation are still lacking.

In this talk, large experimental data sets of the interaction of dislocations with grain boundaries were obtained using state-of-the-art characterization techniques to assess the influence of grain boundary orientation in 3D on the possibility of slip transfer/blocking in Ti and Mg. Similarly, in situ mechanical tests within the scanning electron microscope were carried to study the nucleation of tensile twins in Mg near grain boundaries. This information was analyzed using statistical methods and machine learning tools to determine the critical microstructural parameters that dominate slip transfer/blocking and twin nucleation. This information was then implemented in crystal plasticity finite element models to predict the mechanical behavior of polycrystals.