NANOINDENTATION OF GOLD NANOPARTICLES – A COMBINED EXPERIMENTAL/COMPUTATIONAL MULTISCALE STUDY

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Key Words: nanoindentation, nanoparticles, molecular dynamics, discrete dislocation dynamics, dislocation nucleation

The idea of dimensionality and size effect the strength of metallic specimen as their typical size is pushed into the sub-micrometer scale is well established. The importance of the shape at the nanoscale was demonstrated on Au thin-films and nanoparticles in nanoindentation experiments. It was shown that nanoparticles are substantially softer than thin-films of the same height and the smallest nanoparticles are softer than the largest ones [1]. We propose that the size effect arises from the interaction between the lateral free surfaces on the plastic zone. However, experiments alone cannot provide the understanding on the governing microstructural dislocation mechanisms and we demonstrate here a combined experimental/computational study, by developing a multiscale frame to study nanoindentation of nanoparticles from the atomic- to the macro-scale.

Using molecular dynamics (MD) simulations, we revealed how dislocations are nucleated beneath the indent and interact with the free surfaces. In small nanoparticles all dislocations were starved shortly after nucleating while in the larger nanoparticles a portion of the nucleated dislocations accumulated around the indent. Nonetheless, the MD simulations are limited in size and to bridge between the scales, discrete dislocation dynamics (DDD) were performed. Inspired by the MD simulations, a nucleation criterion was introduced in the DDD simulations. The nanoindentation was introduced by applying the elastic stress field distribution inside the nanoparticle, obtained from finite element simulations. The DDD simulations complemented the MD simulations and revealed that the amount of dislocations escaping at the free surfaces increases for smaller particles, i.e., the plastic zone beneath the indent increases with the size of the nanoparticle. The simulations allowed us to identify the different dislocation mechanisms by which dislocations are escaping from the nanoparticle and we shall discuss them in this talk. The study on both scales, in combination with the experimental results, furnish and elucidate the underlying dislocation mechanisms that controlled the effect of size in nanoindentation and can be served to construct a dislocation-based continuum law for the nanoscale.

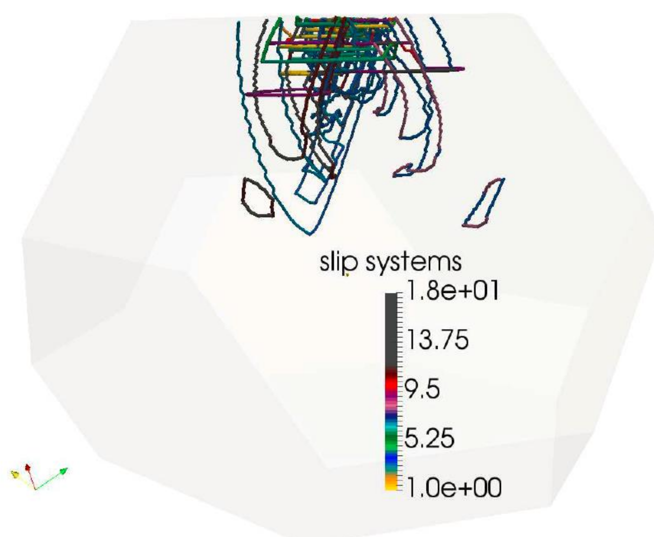

Figure 1 – DDD simulation of nanoindentation of a 90 nm high Au nanoparticle

References:

[1] Mordehai, D., Kazakevich, M., Srolovitz, D.J. and Rabkin, E., Nanoindentation size effect in single-crystal nanoparticles and thin films: a comparative experimental and simulation study, Acta Mater. 59 (2011), 2309 – 2321