On the role of amorphous overlays on the mechanical properties of Ni nanoparticles under compression

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Abstract

Nano-objects like nanowires, nanoparticles and thin films are used in various fields of applications as nano-electronics, pharmaceutics, catalysis or additives and lubricants. Nano-crystals exhibit particularly promising mechanical properties: they show a size-dependent elastic regime as well as increased yield strength and ductility compared to their bulk counterpart that is associated to surface dislocation nucleation. However, a significant data spread is observed and the sample surface state has to be taken into account. For example, *in situ* TEM experiments have identified the presence of an amorphous overlay at the top of metallic, ceramic or semi-conductor nano-structures. Very few studies investigate the role of these amorphous shells on the mechanical properties of nano-crystals. In this context, we use Molecular Dynamics (MD) simulations to investigate the influence of amorphous overlays on the mechanical properties of nanoparticles under compression. To avoid glass composition complexity, we choose to make a Ni monoatomic system for both the crystalline and amorphous phases. The first part of the study will focus on the sample fabrication methodology *i.e.* making a monoatomic bulk metallic glass and then creating a core/crystalline-shell/amorphous Ni nanoparticle. Based on multiple EAM potentials and fabrication method tests, a unique methodology that stabilizes the monoatomic amorphous-crystalline interface is proposed. Then, compression MD tests using a flat punch virtual indenter will be presented. In particular, we will discuss the mechanical response disparities between crystalline, core-shell and purely glassy 20 nm nanospheres. A specific attention will be paid to address the major differences in terms of dislocation-based plastic deformation processes.

Keywords: nanoparticles, amorphous, crystalline interface, monoatomic glass, Molecular Dynamics, compression

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