Study of properties of hollow metallic nanoparticles

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Abstract

Hollow nanoparticle structures play a major role in nanotechnology and nanoscience since their surface to volume ratio is significantly larger than that of filled ones. While porous hollow nanoparticles offer a significant improvement of the available surface area, there is a lack of theoretical understanding, and scarce experimental information, on how the porosity controls or dominates the stability. In this contribution, we use classical molecular dynamics simulations to shed light on the particular characteristics and properties of gold porous hollow nanoparticles and how they differ from the nonporous ones.

First, we will study the role of the polycrystalline structure in gold hollow nanoparticles for a wide range of shell thickness and grain sizes [1]. One of the main findings is that the shell thickness necessary for transition from a spherical to a shrunk structure is related to the grain size reduction. The results suggest that to achieve larger hollow nanoparticles, less defective shells are necessary, with single-crystal shells establishing an upper limit in the size that a structure can attain. Second, by including porosity in a hollow gold nanoparticle, we show how, as the temperature increases, the porosity introduces surface stress and minor transitions that lead to various scenarios, from partial shrinkage for small filling factors to abrupt compression and the loss of spherical shape for large filling [2].

Then, we study the thermal stability of eccentric hollow nanoparticles for different sizes and eccentricity values [3]. Our results reveal that eccentricity displays a significant role in the thermal stability of hNPs. We attribute this behavior to the irregular shell contour, which collapses due to the thermal-activated diffusive process from the nanoparticle shell's most thin region. Lastly, we present a study of the mechanical properties of porous nanoshells measured with a nanoindentation technique [4]. Porous nanoshells with hollow designs can present attractive mechanical properties, as observed in hollow nanoshells, but coupled with the unique mechanical behavior of porous materials. Porous nanoshells display mechanical properties that are dependent on shell porosity. Our results show that, under smaller porosity values, deformation is closely related to the one observed for polycrystalline and single-crystalline nanoshells involving dislocation activity. When porosity in the nanoparticle is increased, plastic deformation was mediated by grain boundary sliding instead of dislocation activity.

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