Elastic properties of Cerium Oxide nanocubes

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Cerium oxide (CeO_2) nanoparticles are used in several industrial applications, among which photocatalysis, or biomedical applications [1]. For these applications, CeO_2 can undergo compressive stresses, inducing plastic deformation. *In situ* TEM mechanical tests bring interesting pieces of information as it can provide simultaneously quantitative mechanical data (force-displacement curves) and images of the sample during deformation [2]. In the case of cerium oxide, the sensitivity to electron irradiation has to be taken into account prior to the experiments. Indeed, oxygen vacancies and changes in the cerium valence state have been evidenced [3], and may affect the materials mechanical response. Fortunately, the introduction of an oxygen gaseous environment is a rapid way to stop or even reverse *in situ* reduction. If is therefore possible to probe the same objects with stoechiometries ranging from Ce_2O_3 to CeO2.

We will present results obtained on cerium oxide nanocubes, of sizes ranging from 20 to 50 nm, with a Hysitron PI 95 fitting in a Cs-corrected FEI Titan Environmental TEM operating under vacuum or with a partial pressure of oxygen. we will focus on the elastic regime and compare the elastic moduli obtained on the same nanocube tested under different environments (under vacuum or with O_2).

To better characterize the reduction/oxidation process and its effect on the mechanical properties, we will also present DFT+U simulations on bulk systems with various CeO_x stoechiometries ($1.5 < x < 2$). The stability of each crystallographic phase appears to be in agreement with the literature [4] and with experimental observations. Significant changes in the calculated elastic moduli are obtained and compared with experimental results [5].

References:

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