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The microscopic origin of size-dependent lattice contraction and expansion

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With a decrease in the particle size, the lattice parameters in a large class of metallic nanoparticles (Ag, Al, Au, Cu, Ni, Pd, Pt, Bi, Sn, etc.) show a contraction as compared to their corresponding bulk values. Interestingly, among the metal nanoparticles listed above that exhibit a lattice contraction, all except Bi and Sn have a face centered cubic (fcc) crystal structure. The size dependence of the lattice parameter in fcc metals can be generally fitted to a Laplace-Young type equation, which suggests that they can be represented by a simple liquid-droplet model in which surface-tension-like forces are the most dominant. On the other hand, the few metals known to exhibit a systematic lattice expansion in the nanoparticle form include Cr, Fe, Nb, V and Ta, each of which happens to have a body centered cubic (bcc) structure. To understand the physical basis for this striking empirical correlation, we have carried out a detailed microscopic study based on *ab-initio* density functional theory (DFT). Our simulations on representative bcc (Nb) and fcc (Cu) nanoclusters elucidate the importance of a capping layer on the metal nanoparticles and succeed in provide a consistent understanding of this apparently puzzling observation. It is important to appreciate that size-driven changes in the lattice parameters is a non-trivial effect with significant consequences, in some cases dominating over quantum size effects and other types of surface effects. Thus, size-induced lattice expansion has been invoked to understand the (a) persistence of superconductivity down to unexpectedly small sizes, (b) appearance of a magnetic moment in isolated Fe atoms embedded in a nanocrystalline metals, and (c) destruction of ferroelectricity in nanocrystalline oxides.

Recent Publications:

1. D Nafday et al. (2018) A reduction in particle size generally causes body-centered-cubic metals to expand but face-centered-cubic metals to contract. ACS Nano. 12(7):7246-7252. Doi:10.1021/acsnano.8b03360.
2. S Sarkar et al. (2017) Is there a lower size limit for superconductivity? Nano Letters. 17:7027-7032.
3. S K Mohanta et al. (2016) Size-induced crossover from itinerant to localized magnetism observed for isolated Fe impurities embedded in different structural polymorphs of silver. Physical Review B. 94:184431.
4. S Chattopadhyay et al. (2015) Local structure, composition and crystallization mechanism of a model two-phase “composite nanoglass”. J. Chemical Physics. 144(6):064503.
5. S Bose and P Ayyub (2014) A review of finite size effects in quasi-zero dimensional superconductors. Reports Progress Physics. 77(11):116503.

Biography

Pushan Ayyub is a Senior Professor and Chair in the Department of Condensed Matter Physics at the Tata Institute of Fundamental Research, Mumbai, India. He has over 160 publications in the general area of nanoscience. He was a Member of the International Committee on Nanostructured Materials (1998-2008) and is currently a Member of the Nano Mission Council of the Government of India. He is a Fellow of the Indian National Science Academy. His research interests include the size dependence of superconductivity and ferroelectricity. He is particularly interested in size-induced structural phase transitions and stabilization of novel crystal structures.

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