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Modeling Surface and Stress-Anisotropy Effects on Transformations in Lead Sulfide Nanocrystals Under Pressure
CLIVE BEALING, RICHARD HENNIG, Cornell University — The semiconductor PbS, which displays a small band gap and large excitonic Bohr radius, presents an ideal candidate material for such devices as infrared photon detectors and nanocrystal solar cells.[1] This has motivated a number of studies into the effect of pressure on bulk PbS and PbS nanocrystals (NCs), which organize into highly periodic superlattices with interesting mechanical properties.[2] The ambient-pressure NaCl-type structure of PbS undergoes a transformation to an orthorhombic structure close to 2.5 GPa, which itself transforms to the CsCl-type structure at 21.5 GPa. We have identified competitive minimum energy paths between the different modifications of PbS using density-functional calculations, and have calculated the associated enthalpy barriers over a range of pressures. In empirical molecular dynamics simulations of the PbS NC transformation under pressure, the effect on the transformation of anisotropic stresses, applied perpendicular to the {100}- and {111}-type facets of the NC, has been investigated. The effect of the NC surface on the stability of metastable modifications in PbS NCs is also considered.

[1]J. Choi, et al., Nano Lett., **9**, 3749 (2009)
[2]P. Podsiadlo, *et al.*, Nano Lett.,**11**, 579 (2010)

Clive Bealing
Cornell University

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