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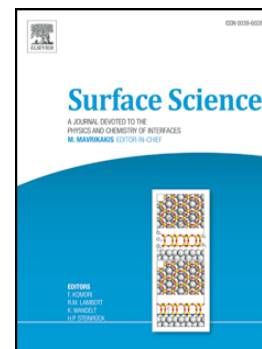
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Yin Yao, Yaochi Wei, Shaohua Chen

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Size effect of the surface energy density of nanoparticles

Yin Yao Yaochi Wei Shaohua Chen^{*}

LNM, Institute of Mechanics, Chinese Academy of Sciences, Beijing, 100190, China

Abstract

The surface energy density of nanoparticles exhibits an obviously size-dependent behavior. However, how the surface energy density changes with the diameter of nanoparticles is still ambiguous. Based on a recently developed continuum theory considering the size effect in nanomaterials, theoretical analysis is carried out for various fcc metallic nanoparticles. Surface lattice contractions of nanoparticles are predicted and compared with the existing experimental data. As a result, the surface energy density decreases with the increase of nanoparticle diameter. Such a variation trend of surface energy density is contrary to the prediction of existing theoretical models, but consistent well with the previously atomistic simulations and density functional calculations. The results in this paper provide a further understanding of the surface effect of nanoparticles, which should be helpful for the design of nanoscale devices or nanomaterials related to nanoparticles, such as NEMs and nanoparticle-reinforced composites.

Keywords: Metallic nanoparticles; Size effect; Lattice contraction; Surface energy density.

^{*} Corresponding author.

E-mail addresses: chenshaohua72@hotmail.com; Tel.: 86-10-82543960; fax: 86-10-82543977.

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