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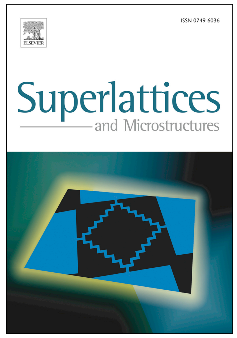

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New explanation of Raman peak redshift in nanoparticles

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Abstract

In this letter, we propose a new model that explains the Raman peak downshift observed in nanoparticles with respect to bulk materials. The proposed model takes into account discreteness of the vibrational spectra of nanoparticles. For crystals with a cubic lattice (Diamond, Silicon, Germanium) we give a relation between the displacement of Raman peak position and the size of nanoparticles. The proposed model does not include any uncertain parameters, unlike the conventionally used phonon confinement model (PCM), and can be employed for unambiguous nanoparticles size estimation.

Keywords: nanoparticles, Raman scattering, phonon confinement
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In nanoparticles the crystalline Raman peak position is downshifted and asymmetrically broadened with respect to bulk materials. Previously the phonon confinement model (PCM) was used to give qualitative and quantitative explanation of this effect. In the PCM the Gaussian-like shape envelope of the atomic displacement wave is introduced and the phonon wave function has a form

$$\psi(\vec{r}) = A_q \exp(-\alpha r^2/L^2) \exp(-i\vec{q}\vec{r}), \tag{1}$$

where $\vec{q}$ is the phonon wave vector, L stands for the diameter of nanoparticles, and α is a dimensionless parameter that regulates strength of confinement of phonons to the center of nanoparticles. According to relation (1) the harmonics with wave vector $-q$ from the envelope allow the momentum conservation

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