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Impact-response study of lattice waves and phonons in metallic fcc nanoclusters using the Sutton-Chen potential

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We suggest a novel approach to investigate phonon propagation in an FCC lattice through bond length oscillations in response to a single atom velocity perturbation. The lattice is modelled using the Sutton-Chen embedded atom model (EAM) without any energy loss mechanisms. We begin by showing that the concept of the cut-off distance must be abandoned to meaningfully simulate the transient behavior of nanoclusters. Oscillations are shown to arise and propagate through the lattice as a result of the interatomic potential. The waves, which have fundamental frequency and velocity, are put into the context of Debye theory and are shown to aptly postulate bulk and surface phonons. Calculations of the C11, C12 and C44 directional moduli of elasticity calculated along the <100>, <110> and <111> directions on a thin, nanosized slab-shaped Cu lattice consisting of 2281 Cu atoms are in good agreement with the literature values at the attained simulated temperature. We also show how the cluster temperature is affected by the passage of the wave.

Apply to be
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No

Level for award
 (Hons, MSc,
   PhD, N/A)?

No

Primary author: Dr OCAYA, Richard (UFS, Department of Physics)

Co-author: Prof. TERBLANS, JJ (Koos) (UFS)

Presenter: Dr OCAYA, Richard (UFS, Department of Physics)

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