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An Investigation of Temperature Effect on Phonon Dispersion Spectra of Ni by Molecular Dynamics Simulation

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Abstract: Lattice vibrations have great influences on physical and mechanical properties of materials. In this study, changes of acoustic phonon frequencies of Ni model system with temperature was investigated by Molecular Dynamic (MD) simulation for [100], [110] and [111] high symmetry directions of the Brillouin zone. To model the interactions between atoms, Sutton-Chen type of Embedded Atom Method (SCEAM) based on many-body interactions were used. The obtained results show that the increase of temperature causes a decrease in longitudinal and transverse acoustic phonon frequencies because of thermal expansion.

Key Words: Molecular dynamics simulation, embedded atom method, phonon dispersion spectra, dynamical matrix

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