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The effect of elastic and structural parameters on phonon transport and thermal properties of a simple cubic nanocrystal

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Abstract

In this paper, we study the phonon and thermal properties of a nanocrystal by using transfer matrix method in the harmonic approximation. The considered system is a mass-spring nanocrystal with a square cross section. At first, for the ideal case, we obtain the phonon spectrum with free boundary conditions. Then we calculate some phonon transport properties of this system, namely, the phonon density of states (modes) and transmission coefficient under different physical and structural conditions. Finally, in the presence of a linear temperature gradient, we obtain the system's thermal conductivity. The results show that the variation in values of physical and structural parameters causes the phonon system properties to strongly change. For example, by decreasing or increasing the typical band frequency of the system, the phonon transmission coefficient increases or decreases, respectively. Moreover, for a mass periodic (for sequential layers) nanocrystal embedded between the two ideal nanocrystals the thermal conductivity decreases with respect to the ideal case.

Keywords: transfer matrix, phonon transport, phonon density of states, thermal conductivity

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