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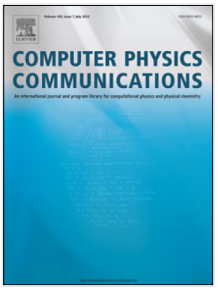

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Direct anharmonic correction method by molecular dynamics

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Abstract

The quick calculation of accurate anharmonic effects of lattice vibrations is crucial to the calculations of thermodynamic properties, the construction of the multi-phase diagram and equation of states of materials, and the theoretical designs of new materials. In this paper, we proposed a direct free energy interpolation (DFEI) method based on the temperature dependent phonon density of states (TD-PDOS) reduced from molecular dynamics simulations. Using the DFEI method, after anharmonic free energy corrections we reproduced the thermal expansion coefficients, the specific heat, the thermal pressure, the isothermal bulk modulus, and the Hugoniot P-V-T relationships of Cu easily and accurately. The extensive tests on other materials including metal, alloy, semiconductor and insulator also manifest that the DFEI method can easily uncover the rest anharmonicity that the quasi-harmonic approximation (QHA) omits. It is thus evidenced that the DFEI method is indeed a very efficient method used to conduct anharmonic effect corrections beyond QHA. More importantly it is much more straitforward and easier compared to previous anharmonic methods.

Keywords: Anharmonic corrections, Molecular dynamics, Thermal properties, Equation of states

1. Introduction

The materials design guided by theoretical methods is developing to pioneer in the discovery of new materials, with the advantages of reduction of materials development time and cost, and the rapid promotion of new materials to products [1]. While theoretical methods often include pressure effects only, hardly taking into account the effects of temperature. This is resulted from the fact

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