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Lattice Dynamics and Thermal Equation of State of Platinum
TAO SUN, Dept. of Physics and Astronomy, Stony Brook University, KOICHIRO UMEMOTO, ZHONGQING WU, Dept. of Chemical Engineering and Materials Science, University of Minnesota, JINCHENG ZHENG, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, RENATA WENTZCOVITCH, Dept. of Chemical Engineering and Materials Science, University of Minnesota — Platinum is widely used as a pressure calibration standard. However, the established thermal EOS has uncertainties, especially in the high P-T range. We use density functional theory to calculate the thermal equation of state of platinum, up to 550 GPa and 5000 K. The static lattice energy is computed by using the LAPW method, with LDA, PBE, and the recently proposed WC functional. The electronic thermal free energy is evaluated using the Mermin functional. The vibrational part is computed within the quasi-harmonic approximation using density functional perturbation theory and pseudopotentials. Special attention is paid to the influence of the electronic temperature to the phonon frequencies. We find that in overall LDA results agree best with the experimental ones. To provide accurate thermal EOS for pressure calibration, we combine the computed temperature dependence of the Gibbs energy with the room temperature Gibbs free energy corrected by experiments. The resulting thermal EOS seems reasonably accurate and can be used as a reference for pressure calibration.

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