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**First-principles temperature-dependent phonons and elastic constants**

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Calculations of thermodynamic properties of materials from first-principles are critical for equation of state and materials strength modeling. Here we present the thermodynamic properties of a select set of metals based on density functional theory. In particular, we present elastic constants and lattice dynamics for body-centered cubic metals obtained from first-principles molecular dynamics and a self-consistent phonon approach. In order to calculate the thermodynamic properties, we make use of fluctuation formulas associated with the canonical ensemble form of *ab initio* molecular dynamics (AIMD). This procedure is efficient and takes into account the anharmonic contributions to the equilibrium thermodynamic properties. In the self-consistent lattice dynamics approach, the phonon dispersions at finite temperature are determined from small displacements along normal modes associated with the chosen temperature. This method provides an efficient and accurate technique for phonon spectrum and finite-temperature acoustic sound speeds and elastic constants. We found that both methods provide consistent results for the temperature- and pressure-dependent elastic moduli. The AIMD include full anharmonicity but suffers from statistical errors of the order of 5%. The self-consistent phonon method, on the other hand, has less statistical uncertainty but does not explicitly account for electron-phonon coupling. At ambient pressure, our calculations (both methods) agree quite well with experimental data.

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