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Toward an accurate ab initio estimation of compressibility and thermal expansion of diamond in the [0, 3000 K] temperature and [0, 30 GPa] pressures ranges, at the hybrid HF/DFT theoretical level

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Abstract

The isothermal bulk modulus, together with its temperature dependence, and the thermal expansion of diamond at various pressures were calculated from first principles in the [0, 30 GPa] and [0, 3000 K] pressure and temperature ranges, within the limits of the quasi-harmonic approximation (QHA). The hybrid HF/DFT functional employed (WC1LYP) proved to be particularly effective in providing a very close agreement between the calculated and the available experimental data. In particular, the bulk modulus at 300 K was estimated to be 444.6 GPa ($K' = 3.60$); at the same temperature, the (volume) thermal expansion coefficient was 3.19×10^{-6} K^{-1}. To the authors' knowledge, among the theoretical papers devoted to the subject, the present one provides the most accurate thermo-elastic data in high-pressure and temperature ranges. Such data can confidently be used in the determination of the pressure of formation using the "elastic method" for minerals found as inclusions in diamonds (recently applied on different minerals included in diamonds), thus shedding light upon the genesis of diamonds in the Earth's upper mantle.

Keywords: Diamond, thermo-elastic properties, thermal expansion, ab initio calculations