

Theoretical studies of thermodynamic and elastic properties of diamond under Earth's mantle conditions

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ABSTRACT

Diamonds are crucial in understanding the deep Earth's carbon cycle, offering essential insights into the composition and processes of the deep mantle. To effectively explore diamond-rich regions, it is essential to understand their unique seismic signatures. In this study, we employed *ab initio* PBEsol methods to calculate thermodynamic and elastic properties of diamonds under Earth's mantle conditions. Our findings showed good agreement with experimental data at lower pressures and temperatures. Then we extended the analysis up to 140 GPa and 4000 K, allowing for a comprehensive examination of the entire mantle. The elastic moduli of diamonds exhibit notable nonlinear responses to pressure and temperature variations. Additionally, the elastic anisotropy of $A_S^{P_0}$ of diamonds is significantly pronounced. We calculated density and wave velocity profiles for diamonds along mantle geotherms, revealing that diamond has higher bulk and shear moduli and lower density compared to the reference state (PREM) of the lower mantle. We also calculated the density and seismic wave velocities (V_P , V_S) of a peridotitic mantle mixture as a function of the diamond content. The results indicate that even minimal amounts of diamond integrated with the background mantle can substantially reduce density and enhance seismic velocities in the lower mantle. Consequently, we predict that diamond may accumulate in the upper mantle over time. The diamond-rich regions will exhibit exceptionally high and anisotropic seismic velocities under Earth's extreme pressure and temperature conditions, as well as within other planetary bodies. These findings provide new approaches for probing diamond-rich zones and investigating the role of carbon in Earth's geological history.

Keywords: Diamond, thermodynamics, elasticity, density functional theory, Physics and Chemistry of Earth's Deep Mantle