Optical Effects of Extreme Pressure on Silicon

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Abstract:
High-Energy-Density Physics (HEDP) is the study of matter under extreme states of pressure ($\sim$ 1 Mbar to 1000 Gbar, or one million to one trillion times the atmospheric pressure at Earths surface). Earths core, Suns core, igniting Inertial-Confinement-Fusion (ICF) implosions are some examples where these conditions arises. A rigorous computational investigation on the basic nature and properties of the diamond-like silicon structures under extreme conditions was carried out by using density functional theory (DFT) and random phase approximation (RPA). Using DFT in QUANTUM ESPRESSO code, the total energy, stress, band gap, bandwidth and density of states were determined for different compressed silicon structures. The RPA was calculated in BerkleyGW (a massively parallel computational package), which enabled us to evaluate the excited state properties, viz. optical absorption spectra for silicon under those extreme conditions of pressure, which is related to the continuum lowering. This investigation will help us in predicting properties of those structures under extreme pressure before changing their phase. Additionally, these works can help in interpreting some specific experiments of the National Ignition Facility of Lawrence Livermore National Laboratory.

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