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Calculated elastic constants at arbitrary temperature and pressure beyond the quasiharmonic approximation

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The prediction of elastic constants (Cij) of materials under extreme conditions of pressure and temperature is important for developing geochemical and geophysical models of planetary interiors. The experimental determination of Cij has its own complications, and coupling those measurements with extreme conditions of PT is extremely challenging. For this reason, the computational prediction of Cij is fundamental. In the past, density functional theory (DFT), ab initio molecular dynamics (AIMD) and the quasi-harmonic approximation (QHA) have been used to compute the elastic constants at arbitrary conditions of pressure and temperature. Nevertheless QHA is inaccurate at high temperatures, while AIMD calculations are in general more complex and demand higher computational resources.

In this work, we explore the use of the recently implemented quasiparticle approximation (QP) [1], proposed by Allen[2], to calculate thermodynamic properties at high temperature. In the QP approach, nth order force constants are used to derive volume- and temperature-dependent entropies, which are fitted with a Debye-like model to generate the rest of the thermodynamic properties, including the elastic constants.

In this work, we compare the use of QHA and QP for the calculation of Cij at arbitrary conditions of pressure and temperature. Some results for the elastic constants of simple and geologically relevant systems are presented.

[1] Blancas, E.J., Lobato, Á., Izquierdo-Ruiz, F. *et al., npj Comput Mater* **10**, 267 (2024).

[2] Allen, P. B., *Mod. Phys. Lett. B* **34**, 2050025 (2020).