

High-P,T elasticity of hcp iron

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Earth's inner core (329~364 GPa and 5000~6000 K) is known to be composed of hexagonal closed pack (hcp) structured solid Fe-Ni alloy and seismologically anisotropic. Thermoelasticity of hcp (ϵ) iron is therefore a key to interpreting seismological information of the inner core. Since experimental measurements are still technically impractical, theoretical approaches in particular ab initio density functional computation have substantial roles. There are two different ways to simulate high-P,T elastic constants (c_{ij}) of crystals. One is based on the lattice dynamics method + quasiharmonic approximation (Sha and Cohen, 2010a,b) and the other is based on the molecular dynamics method (Vocadlo et al., 2009; Martorell et al., 2013). The former and the latter basically fail to capture higher-order anharmonicity and low-temperature quantum effects, which would be substantial and marginal in subsolidus condition, respectively. Due to these problems, distinct differences can be seen in high-P,T c_{ij} and their temperature dependences calculated by these different approaches. In this study, we performed ab initio molecular dynamics simulations employing a supercell containing 96 Fe, which is 50% larger than in the previous study with 64 atoms (Vocadlo et al., 2009; Martorell et al., 2013), to check the previous results. Technical details for computing high-P,T c_{ij} are basically the same as in our previous studies (Ichikawa et al., 2014; Kawai and Tsuchiya, 2015). We will present temperature dependences of elastic wave velocities and their anisotropies at the Earth's inner core pressures over 300 GPa.

Kawai and Tsuchiya, Geophys. Res. Lett. (2015) under review; Ichikawa et al., J. Geophys. Res., 119, 240 (2014); Martorell et al., Science 342, 466 (2013); Sha and Cohen, Phys. Rev. B 81, 094105 (2010a); Sha and Cohen, Geophys. Res. Lett. 37, L10302 (2010b); Vocadlo et al., Earth Planet. Sci. Lett. 288, 534 (2009)

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