High-*P*,*T* elasticity of iron and iron-carbon alloy

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Earth’s inner core (329~364 GPa and 5000~6000 K) is thought to be composed of solid Fe-Ni alloy with some light elements. Thermoelasticity of iron and iron-light element alloys is therefore a key to interpreting seismological information of the inner core: density, seismic wave velocities, and their anisotropy. However, several studies reported that pure hcp iron has a shear modulus distinctly larger than that of the inner core (e.g., Mao et al., 1998; Vocadlo et al., 2009). This large Poisson ratio of the inner core is one of the remaining inexplicable features of the deep Earth, and some studies recently proposed this be explained by alloyed with carbon (e.g., Chen et al., 2014).

In this study, we perform ab initio molecular dynamics simulations of iron and iron-carbon alloy. Also computations are conducted in a wide *P*,*T* range including, but not limited to, the inner core conditions to clarify the *P*,*T* effects on their elasticity more comprehensively, and to provide an internally-consistent thermoelastic model. In addition to checking the validity of the Birch’s law, the obtained Poisson ratio and aggregate anisotropy, with and without the pre-melting effect, are compared against seismological constraints to reinvestigate the viability of iron and iron-carbon alloy in the inner core.

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