Elasticity of Fe-Si 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 unknown light elements (e.g., Mao et al., 1998). Thermoelasticity of iron alloys is therefore a key to interpreting seismological information of the inner core: density, seismic wave velocities, and their anisotropy. So far, several studies reported that pure hcp iron has a shear modulus distinctly larger than that of the inner core and a small P-wave anisotropy (e.g., Mao et al., 1998; Vocadlo et al., 2009). This large V_P/V_S ratio of the inner core is one of the remaining inexplicable features of the deep Earth, and it suggests the presence of mechanisms to lower the S-wave velocity in the inner core, such as a low-velocity component (Prescher et al., 2015), pre-melting effect (Martorell et al., 2013), anelasticity, and so on.

In this study, we perform ab initio molecular dynamics simulations on the thermoelasticity of alloy compositions including potential light element candidate of Si. Computations are conducted at the inner core P,T conditions. The obtained velocities, density and aggregate anisotropies are compared against seismological constraints, and we show the first evidential result on the suitable compositions to the inner core constituents, which can reproduce all of V_P, V_S, V_Φ, and ρ of the inner core simultaneously. We also report why Fe-Si alloy can have a large V_P/V_S ratio.

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