The 488th Geodynamics Seminar

High-P,T elasticity of iron-light element alloys



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Abstract

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; Kuwayama et al., 2008; Sha & Cohen, 2010). 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 Vp/Vs ratio of the inner core is one of the major 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), premelting effect (Martorell et al., 2013), anelasticity, and so on. In this study, I perform ab initio molecular dynamics simulations of several alloy compositions including potential light element candidates of Si, S, C, and H. The obtained density and P and S wave velocities are compared against seismological constraints and we discuss what composition can reproduce the inner core properties most.

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