

High-P,T elasticity of Fe-Si and alloy

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Earth's inner core thought to be composed of solid Fe-Ni alloy with some unknown light elements is characterized by having a large VP/VS ratio. This is originated in its slow S-wave velocity (Dziewonski and Anderson, 1981) but studies on hcp iron alloys so far reported not so small shear moduli (e.g., Li et al., 2018). This large VP/VS ratio of the inner core is one of the major remaining mysteries of the deep Earth, suggesting the presence of somewhat complicated mechanisms to lower VS in the inner core, such as a low-velocity components (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 Fe-Si alloys. Computations are conducted at the inner core P,T conditions. The obtained velocities, density and anisotropy are compared against seismological constraints, and we show the first evidential result on the suitable composition to the inner core constituents, which can reproduce all of VP, VS, $V\Phi$, and ρ of the inner core simultaneously in a reasonable temperature range.