High-*P*,*T* Elasticity of Iron-Light Element Alloys

*土屋 卓久[1]、桑山 靖弘[2]、石井 水晶[3]、河合 研志[2]
*Taku Tsuchiya[1], Yasuhiro Kuwayama[2], Miaki Ishii[3], Kenji Kawai[2]

1. 愛媛大学地球深部ダイナミクス研究センター、2. 東京大学、3. ハーバード大学
1. Geodynamics Research Center, Ehime University, 2. University of Tokyo, 3. Harvard University

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 light elements such as carbon (e.g., Chen et al., 2014). In this study, we perform ab initio molecular dynamics simulations of iron-light element alloys with potential candidates of Si, C, and H and examine their high-P,T elasticity to identify the viability of iron alloys in the inner core.

Research supported by KAKENHI JP15H05834 and JP26287137.

キーワード：鉄軽元素合金、第一原理計算、内核
Keywords: Iron-light element alloy, Ab intio computation, Inner core

