Density and seismic velocities of iron from first principles

Shigeaki Ono[1]

[1] JAMSTEC

The density of the Earth's inner core estimated from seismic observations suggested that it is made predominantly of iron with a certain amount of lighter elements, such as oxygen, hydrogen, carbon, silicon, or sulfur. In order to understand the inner core composition and interpret the observed seismic anisotropy, we have to know stable phase and its physical properties at extreme high pressures and temperatures corresponding to the inner core condition. However, direct observation of the high pressure and temperature behaviour of iron is extremely difficult, with experimental groups getting conflicting results. A recent developed technique from the first principles has a potential to resolve the contradictive results from experiments, because ab initio calculations can provide accurate physical properties of materials at high pressures and temperatures where experiments can not achieve.

In our first principles simulations, the solid is represented as a collection of electrons and atomic nuclei, and ideally, we would like to calculate the energy and forces on every ion as a function of atomic position by solving Schrodinger's equation explicitly. However, this approach is impracticable, because a huge computer resource is needed. In our density functional theory, an approximation is made for the electronic exchange and correlation to predict physical properties of materials [1]. Most previous studies performed simulations to investigate materials at ground state (0 K). We used the molecular dynamics method based on the first principles to directly calculate physical properties of iron at high pressures and temperatures [2].

We calculated three types of structure of iron or iron-nickel alloy (hcp, bcc, and fcc structures). At first, we confirmed that the spin transition from the high-spin to the low-spin state occurred at pressures below 200 GPa. Therefore, the low-spin state is stable in the inner core. According to calculated free energies of the low-spin state, most stable structure was hcp in both pure iron and iron-nickel alloy. The fcc structure is unfavorable compared with the hcp or the bcc structure. In contrast, the energy difference between the hcp and the bcc structure was very small. This indicated that it is difficult to lead the conclusive implication that the hcp structure is dominant in the Earth's inner core.

[1] Ono et al., Earth Planet. Sci. Lett., 272, 481-487 (2008).
[2] Ono et al., J. Appl. Phys., 103, 023510 (2008).