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Changes in physical properties of iron on high spin-low spin transition

Shigeaki Ono[1*]

[1]JAMSTEC

The properties of the major constituents of the Earth's inner core, i.e., iron and its alloys, have long been of great interest to geophysicists. Therefore, pure Fe under high pressure has been investigated by numerous theoretical and experimental studies. Under high pressure, the body-centered cubic (bcc) structure transforms into the hexagonal close-packed (hcp) structure, and this structure seems to be stable over a wide range of pressures and temperatures approaching those existing in the inner core. The magnetic state of iron has a major influence on the physical properties of iron and its alloys, including the relative stability of iron polymorphs. Although the magnetic structure of hcp-Fe has been investigated for over three decades, contradictory results from experimental and theoretical studies have been reported. We made use of a high-pressure diamond anvil cell apparatus and first-principles calculations using density functional theory, to investigate the physical properties of hcp-Fe at high pressures and high temperatures.

First-principles simulations were performed using the projector augmented wave implementation of the density functional theory using the Vienna ab initio simulation software package. For the Brillouin zone sampling at 0 K calculations, we used a large number of k-point grids, which provided the convergence of the total energy to within 1 meV/atom. We also used super-cells, gamma-point for the Brillouin zone sampling, a time step of 1 fs for the first-principles morecular dynamics simulations at high temperatures. High-pressure X-ray diffraction experiments were performed using a laser-heated diamond anvil cell. The samples were heated with a laser to overcome any potential kinetic effects on the possible phase transitions. The heated samples were probed using an angle-dispersive X-ray diffraction technique at the synchrotron beam lines. The angle-dispersive X-ray diffraction patterns were obtained on an imaging plate. The pressure was estimated from the observed unit cell volume of NaCl that was used as the pressure-transmitting medium, using the equation of state for B2-NaCl [1].

In high-pressure experiments, no structural phase transition in hcp-Fe was observed up to a maximum pressure of 110 GPa. An interesting variation in the ratio of the cell parameters (c/a) of hcp-Fe as a function of pressure was observed. As the pressure increased up to approximately 50 GPa, the c/a ratio decreased from 1.61 to 1.60. At pressures greater than 50 GPa, the ratio was approximately constant. According to our first-principles calculations, the magnetic moment of iron and the c/a ratio decrease up to approximately 55 GPa, and then the calculated c/a ratio increases slightly with increasing pressure. These calculated results were in good agreement with experimental observations. This indicated that the transition pressure of high spin-low spin state is approximately 50 GPa. As the spin state of iron could be estimated accurately using our calculations, we also calculated elastic properties of different spin states. For example, our calculations predict that the bulk modulus of the high spin state is 10% less than that of the low spin state [2]. Such change in elastic property should be considered to investigate the dynamic of the inner core.

[1] Ono et al. (2006) Structural property of CsCl-type sodium chloride under pressure. Solid State Communications, 137, 517-521.
[2] Ono et al. (2010) High-pressure magnetic transition in hcp-Fe. American Mineralogist, 95, 880-883.

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