Influence of spin transition on elastic properites of hcp-Fe

SHIGEAKI ONO[1]

[1]JAMSTEC,, Yokosuka 237-0061, Japan (sono@jamstec.go.jp)

It is known from experiments that the pressure-induced transition of Fe from body-centered cubic (bcc) to hexagonal close-packed (hcp) is accompanied by a simultaneous magnetic transition from the ferromagnetic to nonmagnetic states, because Mössbauer effect experiments have never detected the presence of a hyperfine magnetic field in the hcp structure. However, some experimental observations of the structural variation, x-ray emission spectroscopy, or Raman mode splitting indicated that hcp-Fe could have remnant magnetism. It is known that the magnetic transition accompanied by the spin transition induces changes in the physical properties of Fe or its alloys. In this study, we investigated the pressure-induced spin transition by the theoretical calculations and the high-P experiments.

In our theoretical calculations, the VASP code was used to calculate total energy, atomic forces, and stresses in the samples, by solving electronic quantum-mechanical equations using the density functional approach with the generalized gradient approximations of Perdew-Burke-Ernzerhof (PBE). In our hig-P experiments, a small sample of polycrystalline Fe was sandwiched between pellets of NaCl powder, and this was loaded into a 50-100 μm diameter hole in a rhenium gasket of the diamond anvil cell. The sample was heated using an infrared laser. The sample was probed using angle-dispersive X-ray diffraction, employing the AR-NE1A synchrotron beam line at the KEK and the BL10XU beam line at the SPring-8.

The high-pressure and high-temperature behavior of the spin state in hcp-Fe has been examined up to 180 GPa pressure and 2000 K temperature. The spin transition of hcp-Fe from high to low state was confirmed. A significant change in the *c/a* ratio of the cell parameters of hcp-Fe was observed at the transition boundary. This change was in good agreement with that predicted by the theoretical calculations [1]. The spin transition pressure, *P*, increased as the temperature increased. The transition boundary was estimated to be *P (GPa) = 51 + 0.045 x T (K)* [2]. A significant influence of this spin transition on the elastic properties was confirmed.

[1] Ono et al (2010) *Am. Mineral.* **95**, 880-883. [2] Ono (2015) *Solid State Commun.* **203**, 1-4.