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Magnetic transition of hcp-Fe

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Introduction

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. Previous Mössbauer experiments have been interpreted to show the absence of magnetism in hcp-Fe. In contrast, a recent theoretical study based on density functional theory has shown that the antiferromagnetic state is stable at pressures below 50 GPa. As it is generally accepted that a change in the magnetic state of iron and its alloys causes a change in their physical properties, an understanding of the magnetic state of hcp-Fe is important to understand the dynamics of the inner core. The stable structure of iron under ambient conditions is bcc. The phase transition from the bcc to the fcc structure has been confirmed to occur at a temperature of 1185 K. Under high pressure, the bcc-Fe transforms into the hcp structure, and this structure seems to be stable over a wide range of pressures and temperatures approaching those existing in the inner core. Therefore, pure Fe under high pressure has been the subject of numerous experimental studies.

Experimental

High-pressure X-ray diffraction experiments were performed using a laser-heated diamond anvil cell high-pressure apparatus. The starting materials of pure iron have a bcc structure. High-pressure X-ray diffraction experiments were carried out in a motor-driven diamond anvil cell [1]. 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. A few grains of powdered ruby were also loaded into the sample chamber to carry out a preliminary pressure calibration. The NaCl acted as both a pressure-transmitting medium and as a thermal insulation medium, and was also used as the primary pressure calibrant. The sample was heated after compression or decompression using an infrared laser to minimize any pressure inhomogeneity in the sample, and to overcome the effect of any potential kinetics on a possible magnetic transition. A typical annealing time of the sample to produce data of sufficient quality to determine accurate cell parameters was 5-10 min. The sample was probed using angle-dispersive X-ray diffraction, employing the NE1A synchrotron beam line at KEK. The angle-dispersive X-ray diffraction patterns were obtained on an image plate system (Rigaku-RAXIS, Japan). The pressure was calculated from the NaCl unit cell volume using the equations of state for NaCl developed by Ono (2010) [2].

Results and Discussion

The sample was compressed to pressures > 15 GPa in the high-pressure experiment, where hcp-Fe is stable at room temperature. Before laser heating was carried out, the diffraction patterns of both the hcp-Fe and the NaCl pressure-transmitting medium showed broad peaks, reflecting the presence of a compression-related differential stress. The sample was then heated for a period of 5~10 mins to relax the differential stress for each pressure increment. After the required annealing period, the temperature was gradually decreased by controlling the laser power. This was carried out to avoid any differential stress during temperature quenching. After annealing, the strain broadening of each peak in the diffraction pattern had decreased, implying that the differential stress in the sample had decreased. Only diffraction data after annealing were used in this study. No structural phase transition in hcp-Fe was observed up to a maximum pressure of 110 GPa. The diffraction peaks of the sample were reasonably indexed to a hexagonal unit cell (space group = $P6_3/mmc$). As the pressure increased up to approximately 50 GPa, the c/a ratio decreased. At pressures greater than 50 GPa, the ratio was approximately constant at 1.6. Although the change in the cell parameter ratio was observed at approximately 50 GPa, no corresponding changes in the X-ray diffraction pattern were observed. Our experimental data explain that a magnetic transition from the antiferromagnetic to nonmagnetic state occurs at 50~55 GPa, and that the nonmagnetic state is stable at high pressures corresponding to those in the inner core [3]. These results agree with previous theoretical calculations.

References

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