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High-pressure study of iron oxide

Shigeaki ONO*[1]
[1] Institute for Frontier Research on Earth Evolution (IFREE), Japan Agency for Marine-Earth Science and Technology (JAMSTEC), Yokosuka, Kanagawa 237-0061, Japan

Introduction

Iron oxide and iron-bearing compounds exist in significant abundance in the Earth's mantle and play an important role in determining the physical properties of the Earth's interior. The investigation of hematite, Fe_2O_3, is useful in providing information that can lead to a better understanding of the group of compounds that crystallize in similar structures. It is generally known that $MgSiO_3$ perovskite, which is a dominant phase in the lower mantle, can contain a significant Fe_2O_3 component. In addition, Fe_2O_3 hematite (*R-3c*), which is the stable phase at ambient conditions, transforms to a perovskite-type structure (*Pbnm*) at high pressures. This high-pressure phase of Fe_2O_3 is an isostructure of $MgSiO_3$ perovskite. The similarity of the structure is likely to affect the solubility of the Fe_2O_3 component and the dissolved Fe_2O_3 must change the stability of $MgSiO_3$ perovskite.

Experimental methods

The high-pressure X-ray diffraction experiments were performed using a laser-heated diamond anvil cell (LHDAC) high-pressure apparatus. The Fe_2O_3 powder was loaded into a hole that had been pre-drilled into a rhenium gasket using a excimer laser. Argon and NaCl were used as the pressure transmitting medium, and ruby chip was placed in the sample chamber for use as an internal pressure calibrant. After each change in pressure, the sample was heated using a multimode YAG laser to overcome potential kinetic effects on possible phase transitions and to reduce the generation of pressure inhomogeneity in the sample. The sample was probed using angle-dispersive x-ray diffractometry using the synchrotron beam line BL13A of the PF, KEK [1].

Results and Discussion

The acquisition time for X-ray diffraction data was typically 3 to 10 min. In addition to the diffraction peaks of the Fe_2O_3 phases, there are several intense diffraction peaks from the pressure transmitting mediums of argon and NaCl. However, diffraction lines that are free from the interferences allow the Fe_2O_3 phase to be identified and its unit cell dimensions to be calculated.

During laser heating, the transition from hematite, which has the corundum-type structure (R3-C), to an orthorhombic structure occurs at about 30 GPa. This high-pressure phase has the orthorhombic perovskite-type structure (Pbnm) and the number of molecules in a unit cell (Z) is 4, which is in agreement with previous studies. Previous studies obtained by room temperature compression experiments reported that the perovskite-type phase appeared at about 50 GPa, which is much higher than 30 GPa obtained here. The pressure discrepancy of this phase transition indicates that the high-temperature heating played a fundamental role to overcome the kinetic effects on the phase transition. On further compression to 70 GPa and laser heating at temperatures up to about 2500 K, reflections from a new high-pressure phase ($CaIrO_3$-type phase) started to grow. The structure of this $CaIrO_3$-type phase (Cmcm) has an orthorhombic symmetry. The number of molecules of this phase in a unit cell (Z) is 4. Failure to observe the $CaIrO_3$-type Fe_2O_3 polymorph in previous static room-temperature studies may simply be due to the metastable persistence of the hematite structure and sluggishness of the transition at low temperatures. Fig. 1 shows a phase diagram for Fe_2O_3 determined by this study [2]. Our experiments show a transition sequence of Fe_2O_3: hematite (corundum-type), perovskite-type, and finally $CaIrO_3$-type. Organov and Ono [3] reported the transition sequence of $MgSiO_3$ was same as that of Fe_2O_3. The similarity of transition sequence between Fe_2O_3 and $MgSiO_3$ provides a useful guide for understanding the layered structure of the Earth's mantle.

References

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[2] Ono et al., J. Phys. Chem. Solids (in press).
[3] Oganov & Ono, Nature (in press).

* sono@jamstec.go.jp

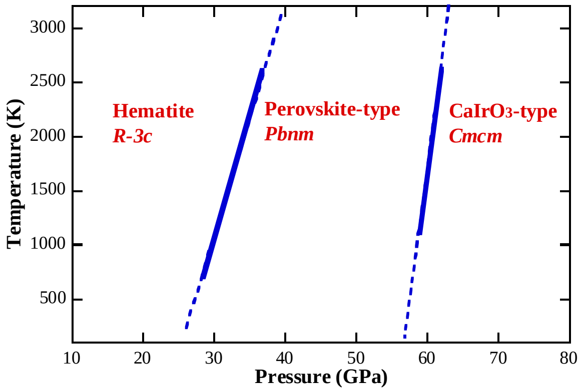

Figure 1

Phase diagram of Fe_2O_3. Solid blue lines represent phase boundaries of Fe_2O_3 phases.