High-pressure phase transition of Fe_2O_3

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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*) transforms to a perovskite-type structure (*Pbnm*) at high pressures [1,2]. 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. In this study, structural phase transitions of iron oxide (Fe_2O_3) have been investigated at pressures up to 100 GPa and temperatures above 2500 K. High-pressure X-ray diffraction experiments were performed using a laser-heated diamond anvil cell (LHDAC) high-pressure apparatus. The samples were heated with a TEM01-mode YLF laser or a multi-mode YAG laser to overcome potential kinetic effects on possible phase transitions. The sample temperature was measured using the spectroradiometric method. The samples were probed using an angle-dispersive X-ray diffraction technique at the synchrotron beam lines BL10XU, SPring-8 and BL13A, PF in Japan [3,4]. A phase transition between alpha-Fe_2O_3 (hematite) and perovskite-type Fe_2O_3 was observed at about 30 GPa. At pressures higher than 60 GPa, we also observed the occurrence of a new high-pressure phase of Fe_2O_3[5]. The new phase showed an orthorhombic symmetry (space group: *Cmcm*) that are denser than other known Fe_2O_3 phases and was confirmed to remain stable to 100 GPa. The structure of the new phase was same as that of $CaIrO_3$. The volume change from perovskite-type to the $CaIrO_3$-type phase is about 7 %. Because Fe_2O_3 is an analog material of $MgSiO_3$, it is possible that this new $CaIrO_3$-type structure, *Cmcm*, is also the post-perovskite structure in $MgSiO_3$. Therefore, there is a possibility that the seismic anomaly at the base of lower mantle, D'' layer, is attributable to the transformation from the perovskite to the $CaIrO_3$-type structure in $MgSiO_3$.

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