Angular-Dispersive Powder X-ray Diffraction from the High Pressure Phase of Fe_2O_3

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Physical properties, *e.g.* crystal structure, magnetic property, of iron oxides of great interest in view of considering interactions between iron-cation and oxide-anion. High pressure technique controls the inter-atomic distances thus the inter-atomic interactions.

Hematite, α-Fe_2O_3, contains only Fe^{3+} and have corundum structure at ambient pressure. Reid and Ringwood[1] point out the possibility that high pressure form of Fe_2O_3 have perovskite structure.

Yagi and Akimoto[2] report X-ray diffraction(XRD) study using diamond anvil cell(DAC) and observe, however, only volume reduction but no structural change at the transition pressure. Suzuki *et al.*[3] also perform XRD study with DAC and observe some extra peaks which cannot be indexed by the corundum structure; They explain all observed peaks using $GdFeO_3$ type orthorombic perovskite structure.

Mössbauer studies using DAC by Suzuki *et al.*[3], Syono *et al.*[4], Nasu *et al.*[5], and Kurimoto *et al.*[6] reveal that the high pressure phase contains two different sites for the iron. Assuming these two iron sites are crystallographically different, ABO_3 type structure is probable structure of the high pressure form

Olsen *et al.*[7] perform powder XRD study of under high pressure up to 65 GPa using DAC and synchrotron radiation(SR). They improve energy-dispersive technique using white incident beam and conclude that transition pressure is about 55 GPa and the $GdFeO_3$ type orthorombic perovskite structure is most probable for the high pressure form of Fe_2O_3.

We report angular-dispersive powder XRD study of high pressure phase of Fe_2O_3 using DAC and SR, instead of the energy-dispersive work by Olsen *et al.*[7].

The DAC used is the same cell for Mössbauer measurements. The gasket used was a Waspaloy with a hole of diameter 0.12 mm. The pressure transmitting medium used was a mixture of methanol and ethanol with the ratio of 4 :1. The pressure was determined to be 68 GPa using pressure dependence of the ruby fluorescence averaging over measurements about 20 points in the gasket hole. The Mössbauer spectrum of this sample contained small amount of sextet from residual low-pressure corumdum phase because of large pressure hysteresis.

Diffraction experiment was performed at BL10XU with in-vacume undulator in SPring-8. The storage ring was operated at 8 GeV. The incident beam with photon energy of 33.2 KeV was monochromatized by Si(111) double monochromater. Diffraction pattern was recorded in a imaging plate.

The observed d-values are listed in Table 1., which are in good agreement with the data of Olsen *et al.*[7].

Table 1. The observerd d-values at 68 GPa

hkl	d / nm	d (at 60GPa) / nm[7]
002	0.329	0.332
111	0.304	0.300
020	0.248	0.248
112	0.241	0.236

References

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