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High-pressure structural behavior of α-Fe_2O_3 studied by single-crystal X-ray diffraction and synchrotron radiation up to 25 GPa

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Abstract

In situ X-ray diffraction experiments were carried out at pressures up to 25 GPa on a synthetic hematite (α-Fe_2O_3) crystal using synchrotron radiation in an angle-dispersive setup. Experiments were performed in diamond-anvil cells using neon as a pressure-transmitting medium. Single-crystal diffraction data were collected from omega scans and structural refinements were carried out for 10 pressure points. Bulk and linear incompressibilities were obtained from least-squares fits of refined data to the Eulerian strain based Birch-Murnaghan equation of state. Finite strain analysis suggests a truncation at second order, yielding results of K_0 = 207(3), K_{a0} = 751(17), and K_{c0} = 492(8) for bulk and axial moduli, respectively. The *a*-axis is about 1.5 times stiffer than the *c*-axis. Compression of the main structural feature, the FeO_6 octahedra, is quite uniform, with just slight changes of distortion parameters at higher pressures.

Keywords: Compressibility, diamond-anvil cell, hematite, axial anisotropy, neon pressure medium