

Effect of high pressure on the crystal structure and electronic properties of magnetite below 25 GPa

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ABSTRACT

We report results from high-pressure single-crystal X-ray diffraction and Mössbauer absorption experiments on magnetite. Based on high-quality diffraction data, we have obtained accurate information on the crystal structure of magnetite below 25 GPa, which enables an unambiguous interpretation of the Mössbauer data using constrained area ratios and a full transmission integral fit that avoids area distortion due to thickness effects. Based on our analysis, all aspects of the electronic and magnetic properties of magnetite reported previously below 25 GPa at ambient temperature can be explained solely by the enhanced delocalization of $3d$ electrons of iron atoms. For instance, we present evidence that the compression-induced metallization changes the sign of the charge carrier spin polarization at 15 GPa.

Keywords: Magnetite, high pressure, Mössbauer spectroscopy, single-crystal X-ray diffraction