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High-pressure X-ray diffraction and mössbauer spectroscopy study of Fe1.087Te

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The Fe1+xTe compounds are isostructural with FeSe which is the simplest of the iron-based superconducting compounds. In contrast to FeSe, Fe1+xTe does not become superconducting at low temperatures but orders antiferromagnetically. Both Fe1+xTe and FeSe are layered materials composed of layers of edge-sharing FeX4 tetrahedra where X = Te or Se but FeSe is Se deficient while Fe1+xTe is stabilized by excess iron (x) located between the Te layers. The crystal structures of Fe1.087Te have been studied by high-pressure X-ray powder diffraction in the pressure range from 0.0001 to 25 GPa at ambient temperature. Fe1.087Te is tetragonal (space group P4/nmm) at ambient conditions and it was found that the tetragonal symmetry was preserved up to the highest measured pressure. Detailed information on the pressure-induced structural changes of the crystal structure was derived from Rietveld refinements of the recorded powder patterns. The volume of the FeTe4 tetrahedra was found to be less compressible than the entire unit cell volume. Fe1.087Te has also been studied by high-pressure 57Fe Mössbauer spectroscopy at p = 0.0001, 2.9 and 6.5 GPa. The obtained values of the isomer shift (d) and quadrupole splitting (DEQ) indicate that the Fe2+ ions are in the S = 1 spin state, and d and DEQ were found to decrease for increasing pressures. The pressure dependence of these two parameters will be correlated with the observed pressure-induced structural changes and the results obtained in the present study will be compared with the results of low-temperature high-pressure neutron diffraction studies of Fe1+xTe for x = 0.087 and 0.141 [1,2].

[1] J.-E. Jørgensen et al., (2015) Eur. Phys. J. B 88 119-126
[2] J.-E. Jørgensen et al., (2016) Physica Status Solidi B 253 2257

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