Resolution of the Intermediate High Pressure Phase of PbTe

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The lead chalcogenides PbX (X=Te, Se, S) are narrow-gap semiconductors (group IV-VI), which crystallise at ambient conditions in the cubic NaCl (B1) structure. It has been known for 20 years that they transform at \sim 3-6 GPa to an intermediate phase, and at higher pressures to the 8-fold coordinated CsCl (B2) structure. There has been much controversy on the crystal structure of the intermediate high pressure phase [1,2,3].

We report recent X-ray powder diffraction obtained at synchrotron sources under pressure, that allowed us to solve the structure of the intermediate phase of PbTe, from simulated annealing techniques and Rietveld refinement : the phase transition at 6 GPa is not to the GeS (B16) or TII (B33) type structures as previously reported, but to an orthorhombic Pnma structure, with cell parameters a=8.157(1), b=4.492(1), c=6.294(1) Å at 6.7 GPa. This structure corresponds to a distortion of the low pressure NaCl structure with a coordination intermediate between the six-fold B1 and the eightfold B2 structure. These new results may modify the admitted paths of phase transitions between the B1 (NaCl) and B2 (CsCl) structures.

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