MS20-P2 High-pressure phase transitions in ordered and disordered ternary tetradymite Bi_2Te_2Se

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We report studies of pressure-induced phase transitions of ordered and disordered ternary tetradymite Bi_2Te_2Se by synchrotron powder x-ray diffraction in diamond anvil cells for pressures up to 57 and 48 GPa, respectively. The first sample (SB) was prepared from a single crystal with ordered Se/Te sites (fig. 1a) while the second sample (Q) was prepared from a quenched melt resulting in tetradymite with disordered Se/Te. This allowed for an investigation of the effect of disorder on the phase transitions and the equation of states (EoS) of the tetradymite α-phase.

Fitting the 3rd order Birch-Murnaghan EoS to the tetradymite α-phases yielded bulk moduli K_0 of 36.7(9) and 40.3(19) GPa and K' of 6.0(3) and 4.8(6) for the SB and Q samples, respectively. An electronic topological transition was observed in both samples at pressures of 3.8 and 2.6 GPa, respectively. This was followed by a transition near 10 GPa to a phase that is isostructural with the β-phase of Bi_2Te_3 (fig. 1b).[1] The Se/Te ordering only affected the transition pressure to a small extent.

A cubic phase that resembles the δ-phase observed in high-pressure studies of Bi_2Te_3 (fig. 1c)[1,2] appeared at 16-19 GPa, but the ternary composition lead to a more complex structure. The presence of a low angle diffraction peak in the δ-phase demonstrated that the true structure is not simply body-centered cubic. In this way the samples resemble Bi_2Se_3 where Bi and Se show a high degree of ordering, but the proposed structures in literature[3-5] of δ-Bi_2Se_3 did not fully describe the data for δ-Bi_2Te_2Se. The nature of the partial ordering of the Se/Te in the high-pressure δ-Bi_2Te_2Se is discussed through various short-range ordering models.

References:

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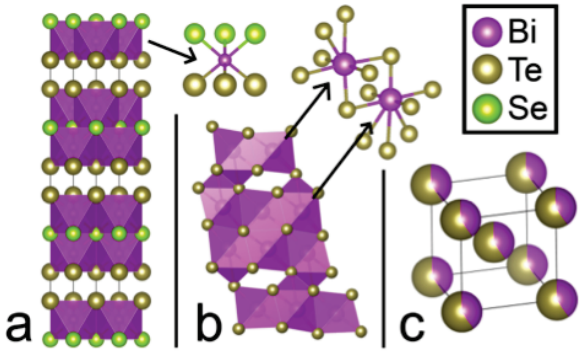

Figure 1. a) α-phase tetradymite Bi_2Te_2Se. b) β-phase Bi_2Te_3. c) δ-phase Bi_2Te_3.

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