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Structure and properties of metastable phases of m-Sb2Te3 and m-Bi0.4Sb1.6Te3

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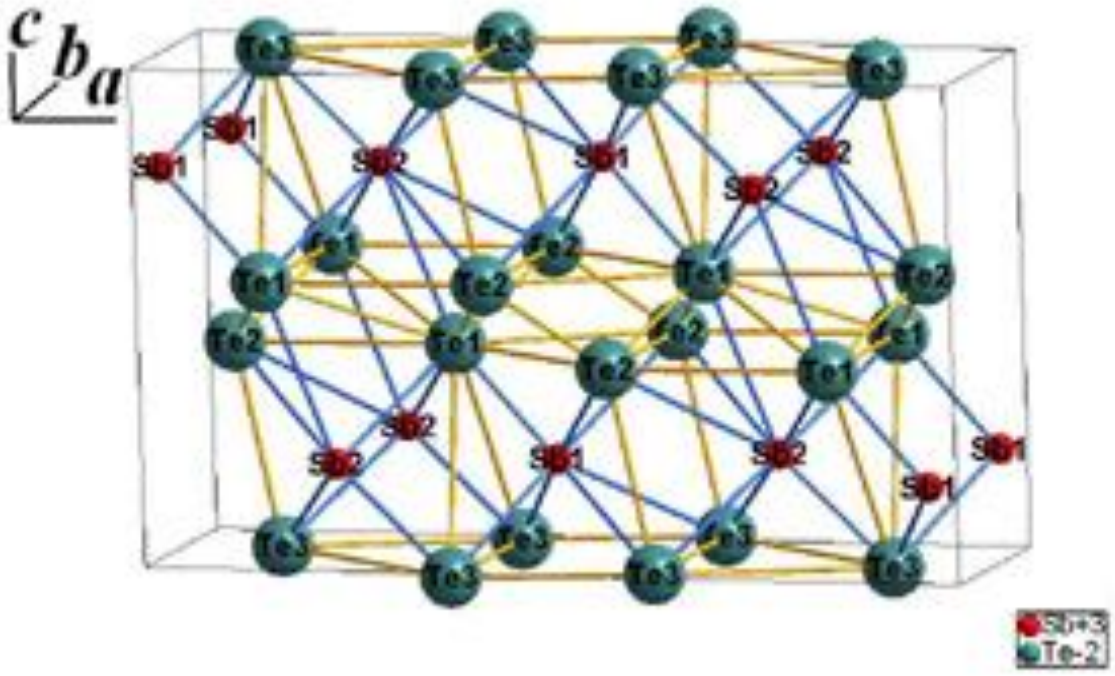
The m-Sb2Te3 and m-Bi0.4Sb1.6Te3 metastable phases were found after high-pressure (4 GPa) and high-temperature (873 K) treatment of initial rhombohedral Sb2Te3 and Bi0.4Sb1.6Te3. These metastable phases crystallize in the same structure because they have almost identical diffraction pattern. The crystal structure of metastable phases, determined by the powder X-ray and electron diffraction methods, is monoclinic (C2/m). The cell dimensions of m-Sb2Te3 are: a=15.64(8) Å, b=4.282(8) Å, c=9.38(2) Å, β=89.70°(5). The reliability factors are: RBragg=0.12, RF=0.13, χ2=4.35. There are two different types of Sb atoms: with seven-coordinated by Te atoms for Sb1 and for Sb2 – eight-coordinated by Te atoms forming composite coordination polyhedra. A comparison with the structure of pressure-induced β-Sb2Te3-phase, observed in situ under high pressure, has been made. Pressure-induced β-Sb2Te3-phase can be retained at ambient conditions as m-Sb2Te3. The annealing of m-Sb2Te3 and m-Bi0.4Sb1.6Te3 samples at 673 K during 2, 5 hours returns their structures to initial symmetry. This fact was supported by the exothermal peak found by differential scanning calorimetry. The ab initio study verified metallic character of quenched phases: the energy spectrum is consistent with the proposed monoclinic structure with short interlayer distances. The electrical resistivity and the Hall coefficient in the temperature range of T = 1.8−450 K have been measured. m-Sb2Te3 phase is superconductive at T < 2K.



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