Combined Diffraction and Raman Studies on Incommensurately Modulated Host-guest Structures of Elements

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Since their discovery in Ba in 1999 [1], the incommensurate host-guest structures have been found in a series of elemental metals at high pressures [2], consisting of two interpenetrating components incommensurate with each other along one direction. The group-V elements Bi, Sb and As are shown to have similar host-guest structures in their high-pressures phases [3], where both components exhibit displacive modulations [4].

Using synchrotron x-ray diffraction and diamond anvil cells, we study the host-guest structures of Sb and As under pressure [5-6], and find an incommensurate-to-incommensurate phase transition with change in symmetry from monoclinic to tetragonal in both host and guest components. In our Raman spectroscopy studies on lattice dynamics of these metallic phases we observed five modes with the frequencies in the range of 90-200 cm^{-1} for Sb, shifting to higher values with pressure increase. We analyze the Raman modes with the help of first-principles calculations for commensurate approximants [6].

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