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Contribution of Lattice Parameter and Vacancies on Anisotropic Optical Properties of Tin Sulphide

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Abstract

Theoretical investigations were made into the band gap, band structure and optical properties of tin sulphide (SnS) crystal with C2mb symmetry. The SnS crystal with this symmetry though has many properties similar to the well documented SnS crystal with Pnma symmetry, it does exhibit some uniqueness in band structure. The purpose of this study was to verify and confirm the recent experimental results of p-SnS thin films with C2mb symmetry. The p-type conductivity in SnS films is obtained due to Tin vacancies. These defects invariably gives rise to residual stress in the crystal. Theoretical investigations allow to address the question as to which of the two factors, stress or vacancies with stress, influences the electrical and optical properties more. Results of our calculations confirm that reported p-SnS films were oriented such that the incident light of UV-visible spectroscope fell perpendicular to the 'ab' plane and that shallow levels appear just above the valence band edge along with a spread in the conduction band edge on introduction of defects in the lattice. The spread in conduction band edge and appearance of shallow levels manifest themselves as Urbach spread or tail in UV-visible absorption spectra, which results in a decrease in band-gap with increasing number of Tin vacancies. Calculations also show that while optical properties are essentially due to the Tin vacancies,