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Experimental and ab-initio study of the structural, electronic and vibrational properties of ZnTe

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Abstract

Polycrystalline ZnTe thin films have been deposited by industrially viable electron beam evaporation technique. The effect of substrate temperature on its structural, vibrational and optoelectronic properties has been investigated. The results are complemented with the ab initio calculations performed using density functional theory for bulk ZnTe. X-ray diffraction studies reveal that the films crystallize in zinc blende structure and the highest crystallinity has been observed for the films deposited at 373 K. The surface morphology and roughness of the films have been studied through scanning electron microscopy and atomic force microscopy. Raman spectroscopy has been used to study the vibrational properties of the films and the frequency of the optical phonon modes are in close agreement with that of the ab initio calculations. Optical absorption and photoluminescence spectroscopy has been used to investigate the optoelectronic properties of ZnTe thin films. The individual orbital contributions to the valence and conduction band edges have been analysed through the density functional theory.

Keywords: Zinc Telluride; Semiconductors; Thin films; Electron beam evaporation; Ab initio calculations