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ACCEPTED MANUSCRIPT

New quaternary thallium indium germanium selenide TlInGe₂Se₆: Crystal and electronic structure

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Abstract

Crystal structure of a novel quaternary thallium indium germanium selenide TlInGe₂Se₆ was investigated by means of powder X-ray diffraction method. It was determined that the compound crystallizes in the trigonal space group *R*3 with the unit cell parameters $a = 10.1798(2)$ Å, $c = 9.2872(3)$ Å. The relationship with similar structures was discussed. The as-synthesized TlInGe₂Se₆ ingot was tested with X-ray photoelectron spectroscopy (XPS) and X-ray emission spectroscopy (XES). In particular, the XPS valence-band and core-level spectra were recorded for initial and Ar⁺ ion-bombarded surfaces of the sample under consideration. The XPS data allow for statement that the TlInGe₂Se₆ surface is rigid with respect to Ar⁺ ion-bombardment. Particularly, Ar⁺ ion-bombardment (3.0 keV, 5 min duration, ion current density fixed at 14 μA/cm²) did not cause substantial modifications of stoichiometry in topmost surface³ layers. Furthermore, comparison on a common energy scale of the XES Se Kβ₂ and Ge Kβ₂ bands and the XPS valence-band spectrum reveals that the principal contributions of the Se 4p and Ge 4p states occur in the upper and central portions of the valence band of TlInGe₂Se₆, respectively, with also their substantial contributions in

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