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Optical properties and energetic band structure of Tl_3AsS_3, Tl_3AsSe_3 and Tl_3SbS_3 crystals

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Fundamental absorption edge spectra and reflectivity spectra of Tl_3AsS_3, Tl_3AsSe_3 and Tl_3SbS_3 crystals have been investigated in the range 1–6 eV at 300 and 77 K. Polarization dependences of three excitonic series ground states have been found in Tl_3AsS_3 and Tl_3SbS_3 crystals. The energetic band structure of these crystals has been built on the basis of experimental reflectivity spectra and theoretical band calculations for crystals of C_{3v}^5 group.

A number of works dedicated to the investigation of acoustooptical properties of $M_3^1M^5M_3^6$ semiconductor materials were published recently [1]. The semiconductor materials Te, Tl_3AsS_3, Tl_3AsSe_3, Tl_3SbS_3 have the perspective that they can be applied in acoustooptic systems operating in the middle infrared range [1]. Their acoustooptical quality (M_2) is above 1000. These materials have the anisotropy of optical and acoustooptical properties. They are transparent at the near-infrared region and in the operating region of optical fiber communication systems (0.85–1.55 μm). The use of these materials in acoustooptical devices is deterred by the lack of information about optical properties in the transparent region and absorption band. The proustite crystal Ag_3AsS_3 is the analogue of the investigated crystals. Its optical properties are widely investigated and band structure theoretical calculations have been performed. The optical polarized spectra of Tl_3SbS_3 crystals are reported in Ref. [2] for the range 1–5 eV at 300 K but the results given in this work are not exact. The band structure of Tl_3AsS_3, Tl_3AsSe_3 crystals is unknown. In the present work the fundamental absorption spectra and the anisotropy of reflectivity spectra of Tl_3AsS_3, Tl_3AsSe_3 and Tl_3SbS_3 crystals are investigated in the range 1–6 eV at 300 and 77 K. We have found direct electron transitions into the exciton S-states ($n = 1$). Ground states of three exciton series have been discovered. The experimental results are compared with the energetic band structure of Ag_3AsS_3 isomorphous crystals and on the basis of the experimental results the energetic band structure of Tl_3AsS_3 and Tl_3SbS_3 crystals has been proposed. The splittings of the upper valence bands caused by the spin–orbital interaction and the crystal field have been calculated and determined at the points Γ, Σ and Λ of the Brillouin zone.

Single crystals of undoped Tl_3AsS_3, Tl_3AsSe_3, and Tl_3SbS_3 crystals have been grown using a classical Bridgman method. The dimensions of the crystals were $10 \times 10 \times 20$ mm^3. The freshly cleaved surfaces of the crystals have been investigated. The Tl_3AsS_3, Tl_3AsSe_3 and Tl_3SbS_3 compounds crystallize in a lattice with the space group C_{3v}^5 with $z = 3$ molecules per unit cell and one molecule in the primitive cell.

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