American Journal of Materials Science and Application
2015; 3(4): 54-58
Published online August 30, 2015 (http://www.openscienceonline.com/journal/ajmsa)

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The Band Structure of $TlGaSe_2$ Crystals

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To cite this article

N. N. Syrbu, V. V. Zalamai, I. G. Stamov, L. N. Nemerenco. The Band Structure of $TlGaSe_2$ Crystals. *American Journal of Materials Science and Application.* Vol. 3, No. 4, 2015, pp. 54-58.

Abstract

Energies of electron transitions for the energy diapason 2 - 6 eV were identified from the analysis of reflection and wavelength modulated reflection spectra measured at temperature 30 K. Bands parameters were determined in framework of theoretically calculated band structure. The spectral dependencies of optical functions were calculated and the interpretation of observed electron transitions was suggested.

Keywords

Semiconductor Compound, Optical Absorption and Reflection Spectra, Kramers-Kronig Relations, Optical Constants, Band Structure

1. Introduction

$TlGaSe_2$ crystals are a group of triple thallium chalcogenide compounds with a well pronounced layered structure. $TaGaSe_2$, $TlGaS_2$ and $TlInS_2$ semiconductors crystallize as a layered structure and have monoclinic lattice at room temperature and atmosphere pressure according literature data [1, 2]. These crystals have a strong anisotropy of physical characteristics due to the specificity of the crystal structure [1 -3].

The temperature and pressure influence on the optical spectra near the absorption edge in $TlGaS_2$ crystals was studied [4 - 11]. The Raman scattering at different geometries and temperatures (from 77 to 400 K) was investigated [12]. Polar vibrational LO and TO modes and their main parameters were extracted from reflection vibrational spectra measured for 4000 - 50 cm^{-1}. Calculations of anions and cations relative effective charges for E||a and E||b polarizations show the difference in iconicity degree of cations and anions along axes a and b [12]. The switching phenomenon in current-voltage and optoacoustic characteristics was discovered in these crystals [13 - 15]. There are a lot of references dedicated to investigations of these materials (see Ref. [4 - 16]).

Spectra of wavelength modulated reflection and transmission for energies 2 - 6 eV were investigated in present work. The new data of excitonic states and electron transitions in intrinsic region for $TlGaSe_2$ crystals were received. The spectral dependencies of optical functions for investigated energies were calculated.

2. Experimental Methods

Low-temperature spectra of $TlGaSe_2$ crystals were measured by high-aperture spectrometer MDR-2 with linear dispersion 7Å/mm and aperture ratio 1:2. Photoelectric multiplier PMP-136 was used as detector. The optical systems are computerized. Wavelength modulated spectrawere registered at frequencies 89 Hz. The optical system allows registering data with bandwidth 0.2Å (±0.1 meV). Transmission and reflection interference spectra were registered with accuracy ±0.2 meV. The cleaved crystals of $TlGaSe_2$ with different thicknesses were mounted into the LTS-22 C 330 optical helium cryogenic system.

3. Experimental Results and Discussion

3.1. Electron Transitions and Optical Functions of $TlGaSe_2$ Crystals in the Absorption Band Depth

Figure 1 shows the spectral dependence of reflectivity of