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Electron–lattice interaction scattering mobility in $Tl_2InGaSe_4$ single crystals

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Abstract
In this work, the dark electrical resistivity, charge carrier density and Hall mobility of $Tl_2InGaSe_4$ single crystal have been recorded and analyzed to investigate the dominant scattering mechanism in the crystal. The data analyses have shown that this crystal exhibits an extrinsic n-type conduction. The temperature-dependent dark electrical resistivity analysis reflected the existence of two energy levels as 0.396 and 0.512 eV, being dominant above and below 260 K, respectively. The temperature dependence of the carrier density was analyzed by using the single-donor–single-acceptor model. The latter analysis has shown that the above maintained 0.512 eV energy level is a donor impurity level. The compensation ratio for this crystal is determined as 0.96. The Hall mobility of $Tl_2InGaSe_4$ is found to be limited by the scattering of electron–acoustic phonon interactions. The calculated theoretical acoustic phonon scattering mobility agrees with the experimental one under the condition that the acoustic deformation potential is 12.5 eV.

1. Introduction

Ternary semiconducting materials with layered and chain structures possess a number of interesting physical properties. During recent years, much attention has been given to systems that behave in certain respects as if they had less than three spatial dimensions. Such materials are often called quasi-one/two-dimensional solids or chain/layered materials. In particular, $TlGaSe_2$, $TlGaS_2$ and $TlInS_2$ crystals belong to the quasi-two-dimensional solid group (layered crystals) and $TlInSe_2$, $TlInTe_2$ and $TlGaTe_2$ are quasi-one-dimensional solids group which construct a chain parallel to the c-axis. These characters shape the crystals' physical properties. The structural, electrical, optical and thermal properties of these crystals were all considered and studied in [1–13]. As an illustrative example, the visible range photosensitivity, the second-harmonic generation and the high birefringence along with a wide transparency range of 0.5–14 μm make the $TlGaSe_2$ crystals suitable for optoelectronic applications [8, 9]. Similarly, the $TlInSe_2$ compound exhibits, in its electrical behavior, many nonlinear effects, such as S-type characteristics, switching and memory effects [10].

The compound $Tl_2InGaSe_4$ results from the reaction of $TlInSe_2$ and $TlGaSe_2$ crystals, in which half of the trivalent indium (gallium) atoms are replaced by gallium (indium) ones. Recently, the low temperature dependence of the band gap energy of $Tl_2InGaSe_4$ crystals in the temperature region of 10–330 K and the Urbach–Martienssen tail in addition to the low temperature visible photoluminescence spectra have been investigated [11, 12]. The first study [11] allowed the determination of the Debye temperature, dielectric constant, electron and hole effective mass as 373 K, 9.2, 0.42 m_0 and 1.16 m_0, respectively. The room temperature band gap energy value was found to be 2.11 eV. The second study [12] revealed the presence of the donor and acceptor energy levels, being located at 0.355 and at 0.036 eV below and above the conduction and valence bands, respectively. In our previous work [13] we have studied the dispersive optical constants of $Tl_2InGaSe_4$ crystal. Specifically, the refractive index, dielectric constant, dispersion energy and oscillator energy of the $Tl_2InGaSe_4$ crystal were reported.

The main purpose of this work is to study and discuss some more physical properties of the compound

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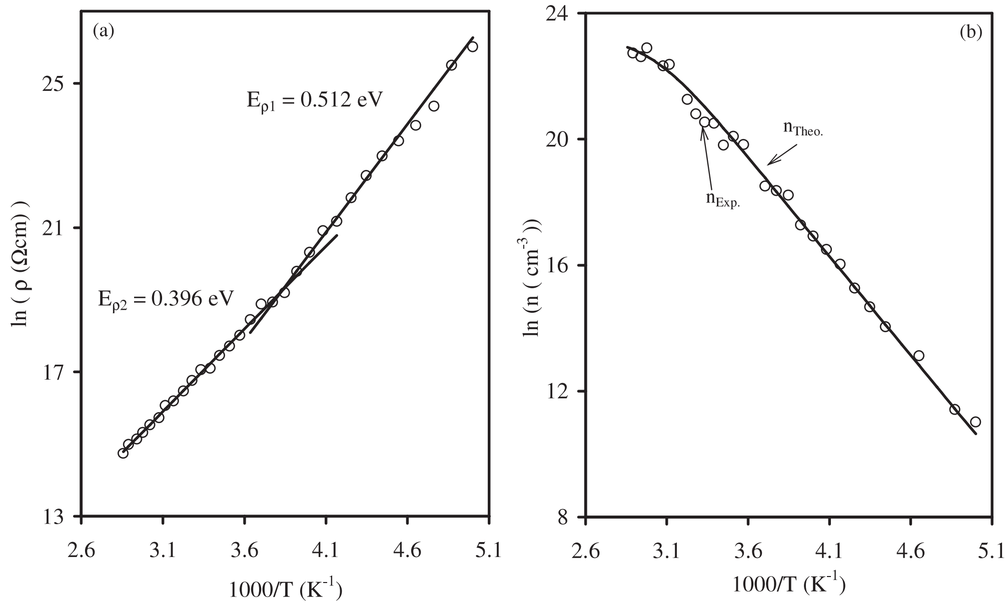

Figure 1. (a) The $\ln(\rho)$–T^{-1} variation for $Tl_2InGaSe_4$ crystal. (b) Variation of $\ln(n)$ versus T^{-1}. The solid lines represent the fits according to the related equation.

$Tl_2InGaSe_4$. In particular, the physical interpretation of the Hall properties, the single-donor–single-acceptor model analysis of the temperature-dependent carrier density in addition to the analysis of the Hall mobility will be reported for the first time.

2. Experimental details

$Tl_2InGaSe_4$ polycrystals were synthesized from the high purity elements (at least 99.999%) taken in stoichiometric proportions. The single crystals were grown by the modified Bridgman method. The x-ray diffraction patterns show that these crystals have monoclinic structure with the lattice parameters $a = 0.772\,44$, $b = 0.649\,45$, $c = 0.922\,05$ nm and $\beta = 95.03°$. Crystals suitable for measurements were obtained by easy cleavage along the (001) plane, which is perpendicular to the c-axis. The resulting single-crystal layers were not subjected to any additional annealing. Typical dimensions of Van der Pauw-type samples were $3 \times 3 \times 2$ mm^3. For reliable electrical measurements, the electrical contacts were made by painting high purity silver paste using suitable masks. The ohmic nature of the contacts was confirmed by the I–V characteristic, which is found to be linear and independent of the reversal current for low applied voltages ($V < 4.0$ V). The temperature-dependent dark electrical resistivity and Hall coefficient measurements were carried out in the temperature range 200–350 K in an automated closed-cycle Lakeshore cryogenic system. The temperature-dependent Hall mobility was measured using the same system at a magnetic field ranging from 0.1 to 1.4 T.

3. Results and discussion

Accurate dark electrical resistivity (ρ) and Hall mobility (μ_h) measurements parallel to the layer on $Tl_2InGaSe_4$ crystals were possible in the temperature range of 200–350 K. The sign of the Hall coefficient, R_h, indicates that the crystals exhibit n-type conduction. A view of the measured temperature-dependent electrical resistivity is shown in figure 1(a). The figure displays the sharp increase in the resistivity values with decreasing temperature at two different rates above and below 260 K. Namely, the resistivity increased from 2.53×10^6 Ω cm at 350 K to 2.00×10^{11} Ω cm at 200 K. The measured $\rho(T)$ data can be represented by the formula

$$\rho(T) = \rho_0 \exp\left(-\frac{E_\rho}{kT}\right), \quad (1)$$

where ρ_0 is the pre-exponential factor and E_ρ is the resistivity activation energy in a related temperature range. Typical best fits for the experimental data are illustrated by the solid lines in figure 1(a). The values of $E_{\rho1}$ and $E_{\rho2}$ calculated from the slopes of these lines are found to be 0.512 and 0.396 eV in the temperature regions of 200–260 and 270–350 K, respectively. These values are close to those that we have previously reported for Tl_2InGaS_4 crystals [14]. It is interesting to note that both crystals Tl_2InGaS_4 and $Tl_2InGaSe_4$ exhibited the extrinsic type of conductivity while $Tl_2InGaTe_4$ crystal [15] exhibited the intrinsic type in the same temperature range. The existence of these different energy levels in the band gap of these crystals and the change in the conduction type may be due to the structural defects such as Tl, In(Ga) or/and S(Se, Te) vacancies and stacking faults present during the growth process.

Figure 1(b) illustrates the behavior of the carrier concentration, $n(T)$, as a function of the reciprocal temperature for $Tl_2InGaSe_4$ crystals. The carrier concentration was calculated from the Hall coefficient by assuming a Hall factor of unity. As can be seen in the figure, $n(T)$ drastically decreases with decreasing temperature. The temperature

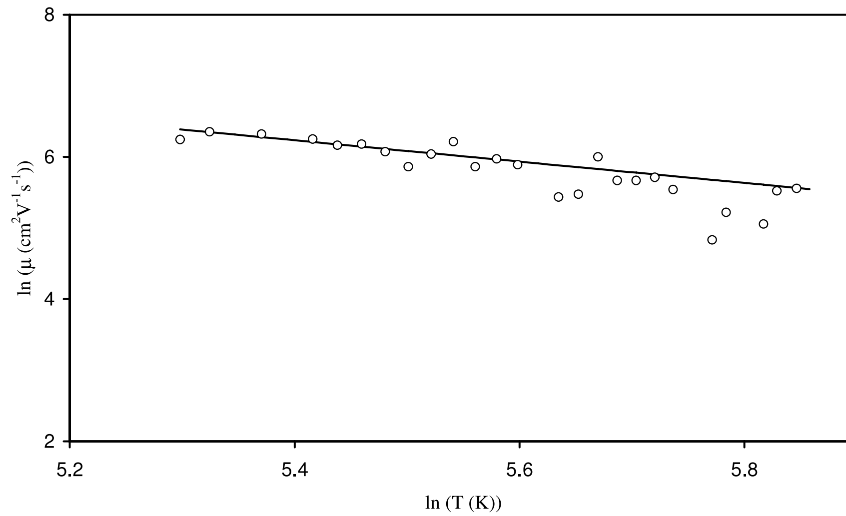

Figure 2. The $\ln(\mu)$–$\ln(T)$ plot for $Tl_2InGaSe_4$ crystal. The solid line represents the fit according to equation (4).

dependence of the carrier concentration is analyzed by using the single-donor–single-acceptor model in which the dependence of the carrier concentration on the temperature is given by [16]

$$\frac{n\,(n+N_a)}{N_d-N_a-n}=\beta N_c\exp\left(-\frac{E_d}{kT}\right) \tag{2}$$

where β is the degeneracy factor, N_c is the effective density of states of the conduction band, N_a and N_d are the acceptor and donor impurity concentrations present in the crystals. Assuming both types of impurities to be present in the crystals and using the three-dimensional expression for N_c, the temperature dependence of n in equation (2) can then be rewritten as

$$n=2\,(N_d-N_a)\left\{1+\frac{N_a}{\beta N_c}\exp(E_d/kT)+\left[\left(1+\frac{N_a}{\beta N_c}\exp\,(E_d/kT)\right)^2+\frac{4\,(N_d-N_a)}{\beta N_c}\exp\,(E_d/kT)\right]^{1/2}\right\}^{-1}. \tag{3}$$

By substituting in the degeneracy factor $\beta = 2$, $m_e^* = 0.42\ m_0$ [11] and $E_d = 0.512$ eV, which is the value of the donor ionization energy calculated from the resistivity measurement, a computer numerical analysis was handled using equation (3). The best fitting curve for the experimental data, obtained from the temperature-dependent Hall effect measurements, is represented by the solid line in figure 1(b). As a result of this fitting procedure, data regressions provide the determination of the acceptor–donor concentration ratio (N_a/N_d) as 0.96 and a donor–acceptor concentration difference of $N_d - N_a = 1.25\times10^{10}$ cm^{-3}.

The energy level being 0.396 eV obtained from the analysis of the resistivity is comparable to the donor energy level being 0.355 eV revealed from the temperature-dependent photoluminescence spectra [12]. Although these energy levels (0.355 and 0.396 eV) may have a contribution to the conduction mechanism of the crystal under investigation, their effect can not be easily observed through Hall effect experiment. This may be due to the dominant contribution of the deep donor energy level (0.512 eV) to the conduction mechanism. When the value of the energy level being 0.396 eV was used in equation (3), it was not possible to reproduce the experimental data even for a compensation ratio of ∼0.999. On the other hand, since the 0.512 eV was able to fit the experimental data one may expect that a sharp absorption peak should appear near this energy value. However, our absorption spectra measurements on $Tl_2InGaSe_4$ crystals in the frequency region of 2000–4800 cm^{-1} revealed a weak (slightly noticeable) wide absorption band near 3900 cm^{-1} which corresponds to an energy level of 0.48 eV.

The Hall mobility ($\mu_{exp} = (ne\rho)^{-1}$), calculated from the experimental resistivity and carrier concentration data, exhibits a magnitude of 290 cm^2 V^{-1} s^{-1} at room temperature. The experimental data for the Hall mobility as a function of temperature are illustrated in figure 2. The mobility increases with decreasing temperature. The slope of the logarithmic μ–T plot is found to be $\sim -3/2$. This value is an indication of thermal lattice scattering domination in the crystals. Following our previous works on Tl_2InGaS_4 crystals [15], we attempt to explain the Hall mobility assuming the domination of acoustic phonon scattering in $Tl_2InGaSe_4$ crystals.

The acoustic phonon scattering mobility is given by the relation [16]

$$\mu_{ac}=3.17\times10^{-5}\frac{du^2}{\left(m_c^*\right)^{5/2}E_{ac}^2\,T^{3/2}}\ \text{cm}^2\ \text{V}^{-1}\ \text{s}^{-1}, \tag{4}$$

where d is the density in g cm^{-3}, E_{ac} is the deformation potential in eV for acoustic phonons, and u is the average sound velocity, which can be estimated from the formula

$$u=\frac{k\theta_D}{\hbar}\left(\frac{V}{6\pi^2}\right)^{1/3}\ \text{cm s}^{-1}. \tag{5}$$

Here θ_D is the Debye temperature estimated using Lindemann's melting rule and V is the average atomic volume. In computing the acoustic phonon scattering mobility, the values of d and V were calculated as 6.59 g cm^{-3} and 4.61×10^{-22} cm^3, respectively, using the x-ray results (reported in the experimental part of this paper) for the $Tl_2InGaSe_4$ crystal. θ_D was estimated as 142 K for a melting temperature of 1065 K.

It is important to notice that the Debye temperature reported by Abay *et al* [11] as 373 K, which was calculated as one of five fitting parameters for the absorption spectra, cannot be used to reproduce the Hall experimental data because it is so far from the phonon frequencies, detected from Raman spectroscopy as 18–240 cm^{-1} and from IR spectroscopy as 30–230 cm^{-1}. The mean frequencies of the phonon excitation are 111 and 100 cm^{-1} for Raman and IR spectroscopy, respectively. $\theta_D = 373$ K corresponds to a mean phonon frequency of 195 cm^{-1} which is very high as compared to experimental ones.

When the above experimentally determined parameters were used to calculate the theoretical acoustic phonon scattering mobility (see equation (4)), the acoustic deformation potential which provides the best fit to the experimental data in figure 2 was found to be $E_{ac} = 12.5$ eV. The consistency of the experimentally determined and theoretically evaluated acoustic phonon scattering mobility data (solid line) is displayed in figure 2.

4. Conclusions

The resistivity and the Hall effect data for $Tl_2InGaSe_4$ crystals in the temperature region of 200–350 K are presented and analyzed. The crystal is observed to exhibit extrinsic n-type conduction. The temperature dependences of the electrical resistivity and carrier concentration predict the existence of the donor level located at 0.512 eV below the conduction band. The single-donor–single-acceptor model analysis on the temperature dependence of the carrier concentration reveals a compensation ratio of 0.96 and a donor and acceptor concentration difference of $N_d - N_a = 1.25 \times 10^{10}$ cm^{-3}. The Hall mobility is found to be limited by the scattering of electron–acoustic phonon interactions. The data analysis revealed an acoustic phonon deformation potential of 12.5 eV.

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