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The change of electrical conduction in the valence/conduction band to the impurity band in CdSe x Te1−x thin films

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The parameters α_{0BT} and α_{0BB} are related to the density-of-tail-states pre-exponent as follows

$$\alpha_{0BT}/\alpha_{0BB} = |M_{\rm env}|^2 \rho_0.$$

An estimate of $|M_{\rm env}|^2 \cong 1 \times 10^{-17}$ cm^3 is obtained from the calculations of Casey and Stern.[14] This gives an order of magnitude value of ρ_0 for the undoped sample $\cong 1 \times 10^{18}$ eV^{-1} cm^{-3} and for the doped sample $\cong 1 \times 10^{19}$ eV^{-1} cm^{-3}.

In conclusion, we have analyzed the absorption spectra of Ge-doped $\rm In_{0.72}Ga_{0.28}As_{0.60}P_{0.40}$ by including contributions from band-to-band transitions and valence-band tail to conduction-band transitions. Different types of disorders that produce the band tailing have been considered. In the doped samples, the absorption from the tail states is considered with multiphonon emission and calculated within the framework of the configuration coordinate model.

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The change of electrical conduction in the valence/conduction band to the impurity band in $\rm CdSe_xTe_{1-x}$ thin films

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Reported here are the results of investigations carried out on the mechanism of electrical conduction in $\rm CdSe_xTe_{1-x}$ thin films between 300 and 125 K in vacuum. All the films showed a transition from grain boundary limited conduction in the conduction/valence band to phonon assisted hopping via the impurity band (impurity band conduction) at around 280–290 K. The grain boundary limited conduction showed an activation energy equal to about 0.14 eV and conduction via impurity band showed an activation energy of about 0.02 eV, which is characteristic of phonon assisted hopping conduction.

$\rm CdSe_xTe_{1-x}$ are a class of very important materials used in semiconductor device technology, but the number of investigations carried out to understand the electrical conduction mechanism in thin films of this material are few.[1-9] Belyaev *et al.*[6,7] have studied the electrical conduction in these films at high and low temperatures, but their reports do not give anything regarding the phonon-assisted hopping conduction at low temperatures. We have analyzed the results after taking into consideration the behavior of CdSe and CdTe films at low temperatures. The high-temperature data have been interpreted based on Seto's[10] polycrystalline model of thermionic emission across grain boundaries and the low-temperature behavior has been explained by the Mott model.[11] A conclusion has been reached regarding the temperature at which valence band (conduction band) conduction changes to impurity band conduction and the activation energies required, at the two sides of the transition temperature.

The experimental techniques regarding preparation and characterization of bulk, as well as thin films, measurements of film resistance and substrate temperature, rate monitoring, etc. have been described in our previous paper.[8] A bath-type cryostat was used for low-temperature studies in vacuum.

Films deposited at a pressure of 10^{-5} Torr and at various substrate temperatures and deposition rates when cooled down to 125 K in vacuum showed two regions of different slopes in the $\log(R/\sqrt{T})$ vs $1/T$ plot, where R is the

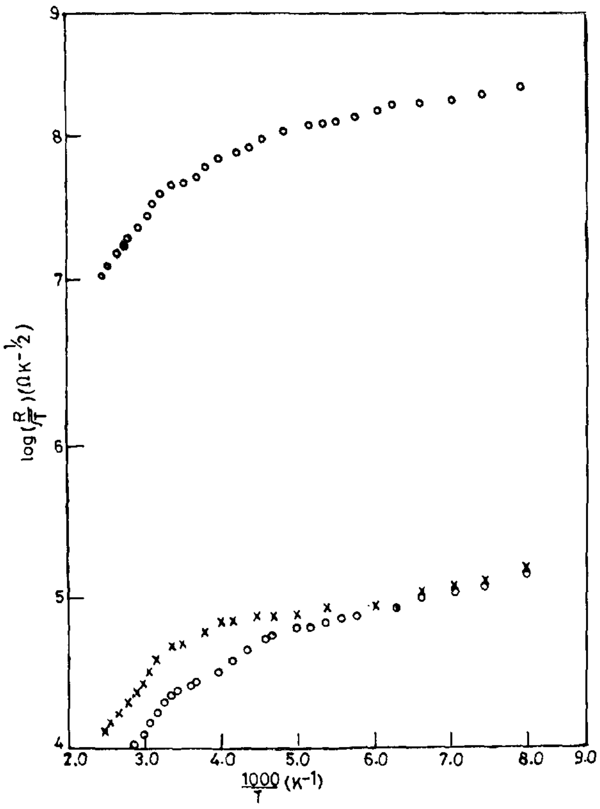

FIG. 1. log($R/\sqrt{T}$) vs $1/T$ plot for the films: O: CdSe(0.2)Te(0.8); ×: CdSe(0.6)Te(0.4); ●: CdSe(0.8)Te(0.2).

sheet resistance in Ω/□ and T is the substrate temperature in degrees kelvin. Figure 1 gives the log($R/\sqrt{T}$) vs ($1/T$) plot for three films of compositions CdSe(0.2)Te(0.8), CdSe(0.6)Te(0.4), and CdSe(0.8)Te(0.2) between 300 and 125 K. Referring to Fig. 1, it is seen that there is a slope change at about 280–290 K for all the compositions. Above the transition temperature an activation energy of about 0.14 eV and below around 0.02 eV was observed. The value 0.14 eV is typical of high-temperature conduction activation energy observed in CdTe,[12] CdSe,[13] and $\text{CdSe}_x\text{Te}_{1-x}$[8,9,14] thin films. This value has been attributed to Cd vacancy in CdTe[12] and Se vacancy in CdSe[13] films. Hence, one of these can give rise to the observed value in CdSe(x) Te($1-x$) thin films.

CdSe, CdSe(0.8)Te(0.2), and CdSe(0.6)Te(0.4) were found as n-type and CdTe and CdSe(0.2)Te(0.8) as p-type conductors. This may be attributed to the presence of Cd donor impurities in the first three cases and Te acceptor impurities in the last two cases. Also, Te acts as a trap in the first three cases and Cd forms trap states in the last two cases.

According to Seto's[10] model, if N is the impurity concentration per unit volume of a grain size L and if there are Q_t traps per cm^2 of the grain boundary, film conductivity is given by

$$\sigma = [\eta_{av} L q^2/(2\pi m^* kT)^{1/2}]\exp(-E/kT), \qquad (1)$$

where η_{av} is the average carrier concentration in the film, q is the electronic (hole) charge, and m^* is the effective mass of the carriers. This case is applicable when the film is not heavily doped, i.e., if $LN > Q_t$, which is true in the case of $\text{CdSe}_x\text{Te}_{1-x}$ films. From the linearity of log($R/\sqrt{T}$) vs ($1/T$) plot above the transition temperature of Fig. 1, it may be assumed that Eq. (1) is applicable in the case of $\text{CdSe}_x\text{Te}_{1-x}$ films.

Referring to Fig. 1 again, it is seen that below the transition temperature, log($R/\sqrt{T}$) vs ($1/T$) has a linear relationship with a low value of slope quite different from that obtained from the high-temperature region. In all the compositions an activation energy of about 0.02 eV was obtained in the low-temperature region. This value is characteristic of the activation energy required for phonon-assisted hopping conduction.

According to Mott and Davis,[11] impurity band conduction takes place as a result of hopping of charge carriers from one impurity level to an adjacent one activated by phonons. At low temperatures, sufficient energy is not available for the charge carriers to be excited to the conduction/valence band. Hence carriers move from one impurity level to the other with the help of phonons. The energy needed in this type of charge conduction is very small. The activation energy obtained in the case of $\text{CdSe}_x\text{Te}_{1-x}$ (0.02 eV) agrees with the theory.

According to the Mott theory, film conductivity may be written as

$$\sigma = \sigma_0 T^{-1/2}\exp[-(T_0/T)^{1/4}], \qquad (2)$$

where

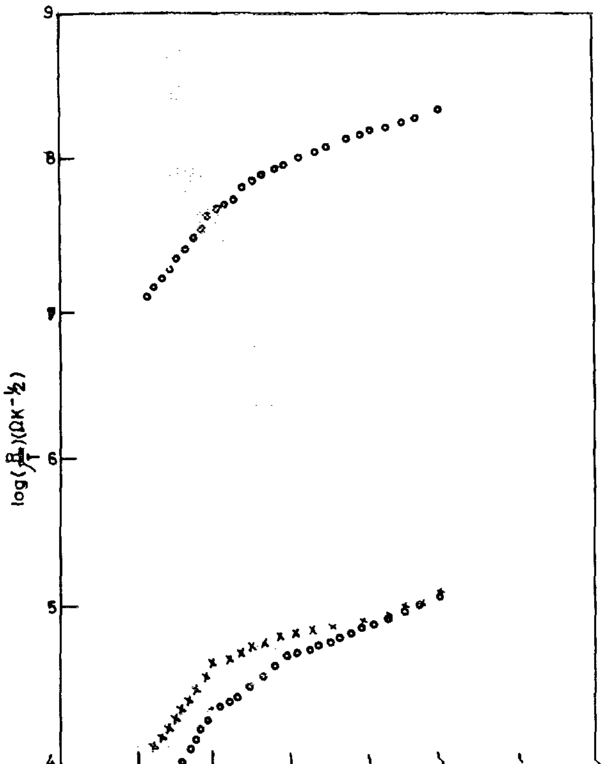

FIG. 2. log($R/\sqrt{T}$) vs $T^{-1/4}$ plot for the films given in Fig. 1.

$$\sigma_0 = 3q^2\nu[N(E_f)/8\pi\alpha k]^{1/2}, \tag{3}$$

$$T_0 = \lambda\alpha^3/kN(E_f), \tag{4}$$

$$d = [9/8\pi\alpha kTN(E_f)]^{1/4}, \tag{5}$$

where $N(E_f)$ is the density of states near the Fermi level, λ is a dimensionless constant, ν is the frequency factor taken as Debye frequency, α is the decay constant of wave function of localized states near the Fermi level, q is the electronic (hole) charge, k is the Boltzmann constant, and d is the hopping distance.

The data in Fig. 1 were replotted in Fig. 2 as $\log(R/\sqrt{T})$ vs $(T^{-1/4})$ and the figure shows a linear relationship. This result shows that electrical conduction in $CdSe_xTe_{1-x}$ below the transition temperature may be explained by the Mott theory for disordered systems.

Hence from the above discussion it may be concluded that in $CdSe_xTe_{1-x}$ thin films there exists a transition temperature of around 280–290 K, above which electrical conduction is effected by charge carriers excited to the conduction/valence band from the impurity levels and may be explained by Seto's polycrystalline model of thermionic emission across the grain boundaries. Below the transition temperature conduction occurs by phonon-assisted hopping via an impurity band and may be explained by the Mott model.

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Infrared study of Fe-B-pair behavior in iron-implanted Czochralski silicon

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A Fourier transform infrared study of Fe-donor B-acceptor complexes formed in iron-implanted B-doped Czochralski-grown silicon crystals is performed by monitoring the behavior of boron-acceptor excitation spectrum lines. The effect of the iron presence on absorption spectra due to B-acceptor hydrogenlike systems, related to electronic transitions from the ground to excited states associated with the silicon $P_{3/2}$ valence band, was analyzed in a wide range of fluences. Low-temperature optical data are reported and discussed comparing optical results with secondary-ion mass spectroscopy and spreading resistance measurements, supporting the existence of a fluence threshold that controls iron diffusion into the bulk.

It is well established that iron is one of the most important heavy metal impurities in silicon. Because of its high solubility and fast diffusion, one needs to take into account its behavior in order to prevent the detrimental effects of metallic contamination on structural and electrical properties of silicon devices during technological processes.

The interstitial iron atoms introduce a deep-donor level in the band gap at $E_v + 0.38$ eV and can form Fe-acceptor pairs[1–5] with B ($E_v + 0.1$ eV), Al, Ga, In, and Tl. Fe-acceptor complexes, acting as recombination centers, decrease the minority-carrier lifetime, are effective in degrading *p-n* junction characteristics, and limit the photovoltaic efficiency of solar cells.[6,7]

In recent works, particular attention has been paid to the importance of reducing iron solubility and improving intrinsic iron gettering in order to remove transition-metal impurities[8–10] from electrically active regions. In this framework it is interesting to study Fe behavior in as large a concentration range as possible and to correlate it with oxygen- and dopant-related centers.

In our previous works[11,12] we analyzed effects of the

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