Defect structure and kinetic properties of $CdSe_xTe_{1-x}$ solid solution: ab initio calculation

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INTRODUCTION

$CdSe_xTe_{1-x}$ solid solution possesses unique physical properties necessary for photovoltaic converters of solar energy and infrared detectors, namely, a required band gap width and needed absorption coefficient value. It is known that the structure of intrinsic and impurity defects of the crystal lattice largely determines the optical and electrical properties of this material, in particular, the absorption coefficient and the transport phenomena. Therefore, the study of the $CdSe_xTe_{1-x}$ defects structure is an actual applied problem. In the proposed study the point defects in n-$CdSe_{0.1}Te_{0.9}$ are considered, namely: Cd_{Te}, Cd_{Se}, Te_{Cd}, Se_{Cd}, V_{Te}, V_{Se}, V_{Te}–Cd_{Te}, V_{Se}–Cd_{Se}. A connection between the defect structure and the kinetic properties of the crystal was established.

RESULTS

The energy spectra of ideal CdTe and CdSe supercells in corresponding sublattices were calculated based on the approach proposed in [1]. The calculation was carried out in such a way as to ensure the coincidence of the theoretical band gap with the experimental value at 0 K and 300 K. This was achieved by choosing a certain mixture of usual exchange-correlation GGA potentials of Cd, Se and Te (pseudopotentials) and the Hartree-Fock exchange potential. A similar procedure was used to calculate the energy spectra of the above-mentioned defective supercells. Having

Fig. 1. Electron mobility versus temperature in $CdSe_xTe_{1-x}$ solid solution crystals with different intrinsic defects concentration.

the energy spectra of ideal and above-mentioned defective supercells at 0 K and 300 K, it was possible to determine the temperature dependences of the ionization energies of the corresponding donor defects. Defects with the lowest ionization energy make the largest contribution to transport phenomena, namely: Cd_{Te} –E_{D1} = 0.048 -2.667×10^{-4}T eV, E_{D1} = 0 at T = 179.9 K; V_{Se}-Cd_{Se} – E_{D2} = 0.018 – 1.1×10^{-4} T eV, E_{D2} = 0 at T =163.6 K. Using these dependencies, neutrality equations take the form: 1

$$T<163.6K: n-p=(1-x)N_D\Big/\left[1+2\exp\left(\frac{F-E_{D1}}{k_BT}\right)\right]+\frac{1}{2}xN_D+\frac{1}{2}xN_D\Big/\left[1+2\exp\left(\frac{F-E_{D2}}{k_BT}\right)\right];\quad 163.6<T<179.9K: n-p=(1-x)N_D\Big/\left[1+2\exp\left(\frac{F-E_{D1}}{k_BT}\right)\right]+\frac{1}{2}xN_D+\frac{1}{2}xN_D;\quad T>179.9K: n-p=N_D.$$

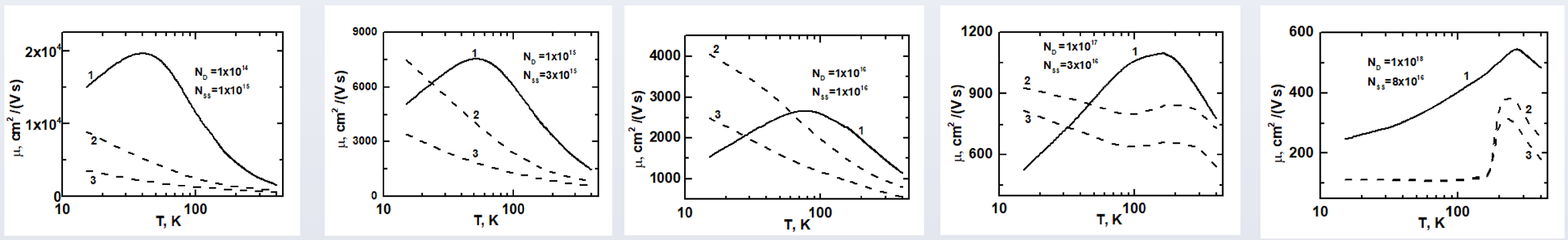


Fig. 2. Comparing of theoretical curves obtained in framework of short-range (curve 1) and long-range (curves 2 and 3) scattering models.

The calculation of the temperature dependences of the electron mobility was performed on the basis of short-range scattering models [2-4] within the framework of the exact solution of the Boltzmann's kinetic equation. On Figure 1 the calculation of the temperature dependences of the electron mobility in $CdSe_xTe_{1-x}$(x=0.1) was performed for the defects concentration of 1×10^{14} ÷ 1×10^{18} cm-3. In order to cover all possible values of the electron mobility at low temperature for each concentration of the donor defects the corresponding values of concentration of the static strain centers (*Nss*) was selected. Unfortunately in the literature the experimental data for the abovementioned interval of the intrinsic donor concentrations are absent. Figure 2 presents a comparison of two competing approaches: short-range scattering models and long-range scattering models (relaxation time approximation). The dashed lines 2 and 3 represent the results of calculation of the dependence μ(T) obtained in the relaxation time approximation: curve 3 describes the high-temperature region ($h\omega<<k_BT$), curve 2 describes the low-temperature region ($h\omega>>k_BT$). As it can be seen, these curves demonstrate significant qualitative and quantitative differences of the temperature dependences of the charge carrier's mobility throughout the studied range of defect concentrations and temperatures. For $CdSe_xTe_{1-x}$(x=0.1) the Debye temperature is θ_D = 245 K. It means that the low-temperature region will be determined by the condition T <24 K, and the high-temperature region will be determined by the condition T >2400 K. From this point of view, the application of the relaxation time approximation (elastic scattering) in the range of 24 K <T <2400 K is incorrect. At the same time, the short-range scattering models allow to describe inelastic scattering. Thus, it can be argued that short-range models give a more adequate description of physical reality than long-range models. To establish the role of different scattering mechanisms on Fig. 3, the dashed curves represent the corresponding mobility for the samples with minimum and maximum defect concentration. In the case of minimum defect concentration at low temperatures the main scattering mechanism is static strain (SS) scattering. At high temperatures the influence of polar optical (PO) scattering becomes predominant, however, the effect of piezoacoustic (PAC) scattering becomes also significant. Other scattering mechanisms – acoustic (AC), ionized impurity (II), nonpolar optical (NPO), piezooptical (POP), neutral impurity (NI)scattering mechanisms – give neglected contribution to the total mobility. In the case of the maximum defect concentration in all investigated temperature range up to T ~400 K the main scattering mechanism is SS- scattering. However, in contrast to the previous case, an additional mechanism of NI-scattering is significant in this temperature range. At *T > 300 K* the PO- and PAC-scattering mechanisms dominate. Other scattering mechanisms in this case also minimally influence on the total mobility.

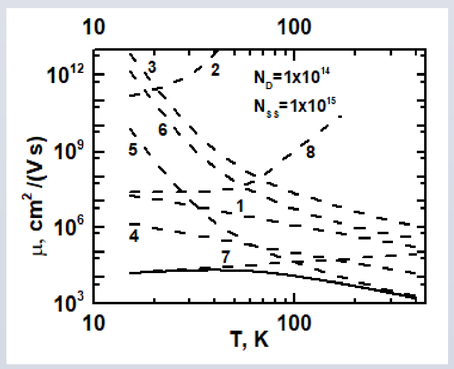
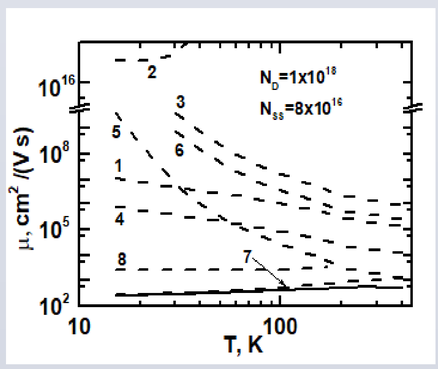


Fig. 3. Contribution of different scattering modes to electron mobility in $CdSe_xTe_{1-x}$ solid solution.



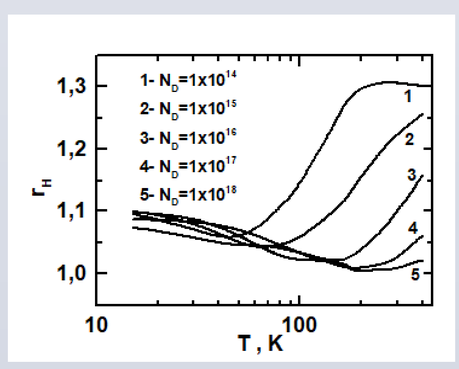


Fig. 4. Electron's Hall factor versus temperature in $CdSe_xTe_{1-x}$ solid solution.

Calculated on the basis of the proposed method the dependences of Hall factor on temperature are presented on Figure 4. It is seen that these dependencies have minimums, which are situated as follows - the higher the concentration of donor defects, the higher the temperature of minimum.

CONCLUSIONS

The authors propose a new scheme for calculating the energy spectrum, wave function and potential energy of an electron in a $CdSe_xTe_{1-x}$(x=0.1) crystal at a given temperature. Based on this, the temperature dependences of the defects parameters and kinetic coefficients are calculated. It should be noted that the proposed calculation method can be applied to all semiconducting solid solutions with a sphalerite structure.

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