The modeling of the electron scattering on the short-range potential in chlorine doped cadmium telluride

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Abstract. The processes of the electron scattering on the short-range potential caused by interaction with polar and nonpolar optical phonons, piezoelectric and acoustic phonons, static strain and ionized impurities in Cl-doped CdTe samples with impurity concentration ~5×10^{16} ÷ 5×10^{17} cm^{-3} are considered. The temperature dependences of the electron mobility and Hall factor in temperature range 25 ÷ 590 K are calculated.

Keywords: transport phenomena, charge carrier scattering, cadmium telluride.

Introduction

Chlorine doped cadmium telluride is widely used in the highly sensitive uncooled detectors of nuclear radiation. Further progress in the design and optimization of CdTe-based devices requires a thorough adequate approximation of the material parameters. One of the important material parameter is the electron mobility. Usually the electron scattering in cadmium telluride was considered in relaxation time approximation. The common feature of this method is the using of the long-range charge carrier scattering models for the description of the transport phenomena in this semiconductor. In these models it is supposed that either the charge carrier interacts with all the crystal (electron -phonon interaction) or it interacts with the defect potential of the impurity the action radius of which is equal to ~10 – 1000 a_0 (a_0 – lattice constant). However, such an assumption has next contradictions: a) it contradicts the special relativity according to which the charge carrier would interact only with the neighbouring crystal region; b) it contradicts the atomistic hypothesis according to which the charge carrier interacts (and transfers the energy respectively) only with one atom but not simultaneously with many atoms which are situated in different points of space. To eliminate these contradictions it is necessary to consider the following question – what object in the crystal absorbs the energy during the charge carrier scattering process? It can be either ionized (neutral) impurity atom or an atom which oscillates in the lattice site. During the scattering process all of these objects do not leave the boundaries of the elementary cell. Therefore the short-range charge carrier scattering models in II-VI [1,3] and in III-V [2] semiconductors were proposed where it has been supposed that the carrier interacts with the defect potential only within the limits of one elementary cell. Here the following physical reasons were used: during the scattering the electron interacts only with neighboring crystal region (the short-range principle), after the scattering on this region the electron interacts with the next neighboring crystal region, etc. The aim of the present paper is the use of short-range models to describe the electron scattering on the various crystal lattice defects in cadmium telluride.

Discussion

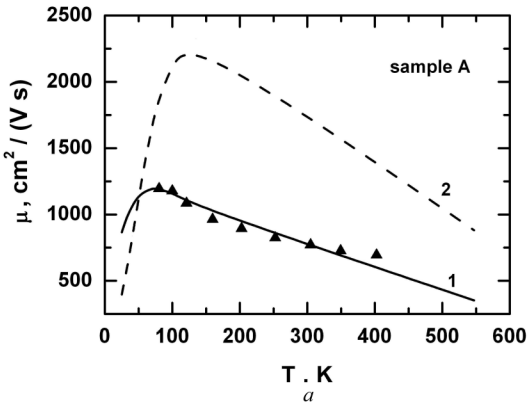
For the electron scattering on the nonpolar optical (NPO), acoustic (AC) phonons and static strain (SS) centre the interaction radius of the short-range potential is limited by one unit cell. For the electron scattering on the ionized impurity (II), polar optical (PO) and piezoelectric (piezoacoustic (PAC and piezooptic (POP)) phonons the interaction radius of the short-range potential is founded in a form $R=\gamma\ a_0$ (a_0 - lattice constant, γ – the respective fitting parameters).

It must be noticed that the strong power dependence of parameters γ sharply limits the choice opportunities of their numerical values.

The respective electron transition probability from state $\boldsymbol{k}$ to state $\boldsymbol{k'}$ caused by the interaction with defect potential was chose from [1,3]. To calculate the conductivity tensor components the method of an exact solution of the stationary Boltzmann equation was used [4]. Using this formalism one can obtain additional fitting parameter $\gamma_{SS}N_{SS}$ (we put γ_{SS}=1) for SS- scattering mode. The material parameters used for calculation are listed in Table 1.

A comparison of the theoretical temperature dependences of the electron mobility was made with the experimental data presented in [5] for two CdTe samples with Cl concentration 5×10^{16} (sample A) and 5×10^{17} cm^{-3} (sample B). The Fermi level was obtained from the electroneutrality equation $n=1/e\ R$, where R– experimental value of Hall coefficient. The obtained fitting parameters for different scattering modes are listed in Table II.

Theoretical curves for CdTe:Cl are presented in Fig. 1a, b. The solid lines represent the curves calculated on the basis of short-range models in the framework of the exact solution of the Boltzmann equation. Dashed lines presented the curves calculated in the relaxation time approximation.



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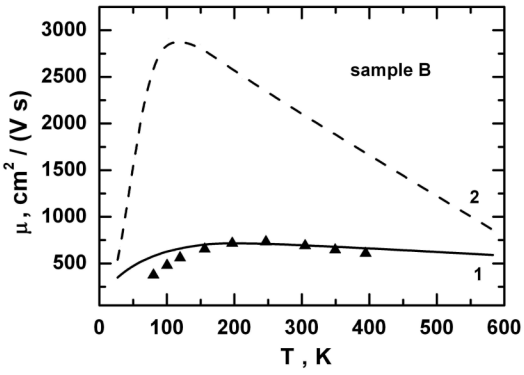

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Fig.1. Temperature dependence of electron mobility in CdTe:Cl. 1-short-range models, 2- relaxation time approximation.

MATERIAL PARAMETERS

Table I.

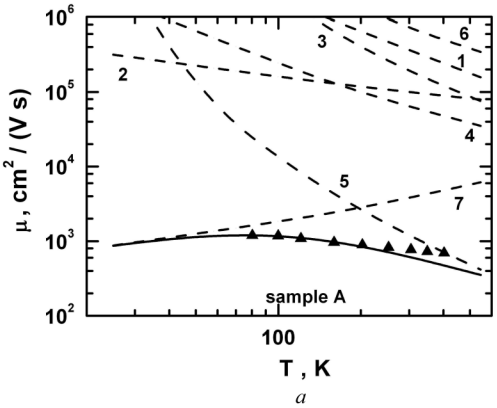
Material parameter	Value
Lattice constant, a_0 (m)	6.481×10^{-10}
Energy gap, E_g (eV)	$1.65 - 5.35\times10^{-4}$ T
Energy equivalent of matrix element, E_p (eV)	21
Spin-orbit splitting, Δ (eV)	0.92
Density, ρ_0 (gm cm^{-3})	5.75
Optical deformation potential, d_0 (eV)	22
transverse phonon frequency, (rad)	2.63×10^{13}
Acoustic deformation potential, (eV)	1.85
Elastic constants, (N m^{-2})	
C_l	6.32×10^{10}
C_t	1.538×10^{10}
Piezoelectric tensor component, e_{14} (C m^{-2})	$0.03457-1.39\times10^{-5}$ T

PARAMETERS γ FOR DIFFERENT SCATTERING MODES

TABLE II.

Sample	γ_{PO}	γ_{PZ}	γ_{ID}	γ_{SS} Nss $\times 10^{-14}$ cm^{-3}
A	0.67	0.47	1.0	7.5
Б	0.60	0.49	1.0	19.5

It must be noticed that during the calculation of these curves the same scattering mechanisms was used. It is seen that in all investigated temperature interval the short-range scattering models give sufficiently good agreement of theory and experiment while the relaxation time approximation gives the deviation of the theory from experiment 2 ÷ 5 times. It means that short-range models more adequately describe the processes of electron scattering in CdTe compared with the relaxation time



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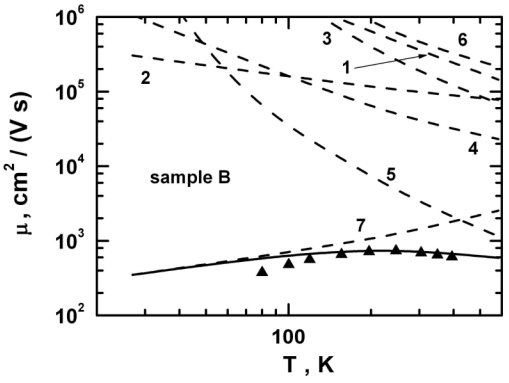

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Fig.2. The contribution of different scattering modes into electron mobility in GaN. Solid line - mixed scattering mechanism; 1,2,3,4,5,6,7 – AC-, II-, NPO-, PAC-, PO-, POP-, SS - scattering mechanism respectively.

approximation. To estimate the role of the different scattering mechanisms in Fig. 2a,b the dashed lines represent the appropriate dependences. It is seen that at low temperatures (T<100 K) the main scattering mechanism is static strain scattering. At high temperatures the contribution of the polar optical phonon scattering becomes dominant. Other scattering mechanisms give negligibly small contributions.

On the base of the obtained scattering parameters the temperature dependences of electron's Hall factor were calculated (see Fig.3). It is seen that the minimums of these dependences observe at the temperature where the transition from SS-scattering (low temperatures) to PO-scattering (high temperatures) occurs. The transition temperature depends on the impurity concentration: the higher doping level determines the higher transition temperature.

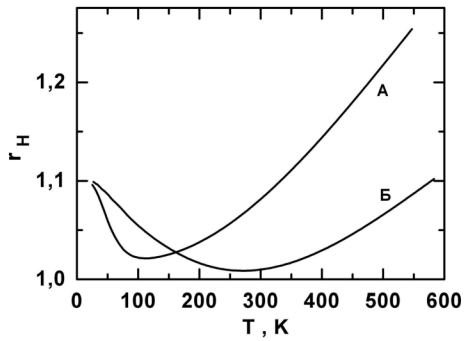

Fig.3. Temperature dependence of electron's Hall factor in CdTe:Cl.

Conclusion

On the base of the short-range principle the electron scattering processes on the various crystal lattice defects in chlorine doped cadmium telluride were considered. A good agreement between the theory and experimental data in investigated temperature range was established.

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