# The modeling of the electron scattering on the short-range potential in cadmium sulfide

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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 centers, ionized and neutral impurities in CdS crystals with impurity concentration ~$5.6\times10^{16}$ ÷ $8.7\times10^{17}$ $cm^{-3}$ are considered. The temperature dependences of the electron mobility and Hall factor in temperature range 10 ÷ 400 K are calculated.

**Keywords:** transport phenomena, charge carrier scattering, cadmium sulfide.

**Introduction**

Cadmium sulfide is widely used in the manufacture of the thin film solar energy converters. Further progress in the design and optimization of CdS-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 sulfide 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 sulfide.

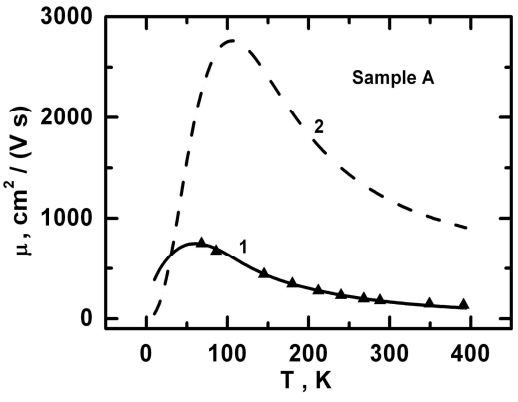
**Discussion**

The structure of wurtzite CdS lattice contains four atoms in the unit cell which leads to existence of 12 vibration modes. According to group theory these oscillations may be represented as a sum of irreducible representations : $\Gamma = 2A_1 + 2B_1 + 2E_1 + 2E_2$. One $A_1$ mode and one $E_1$ mode pair present the acoustical branches of oscillations. Therefore, the sum $\Gamma_{opt} = A_1 + 2B_1 + E_1 + 2E_2$ represents the optical phonon eigenmodes. The optical vibrations are classified by displacement of the atoms along $c_0$ - axis and in directions perpendicular to the $c_0$ - axis. As a result one can obtain that $A_1$ and $E_1$ represent the polar phonon modes and $B_1^{(1)}, B_1^{(2)}, E_2^{(1)}, E_2^{(2)}$ represent the non-polar modes.

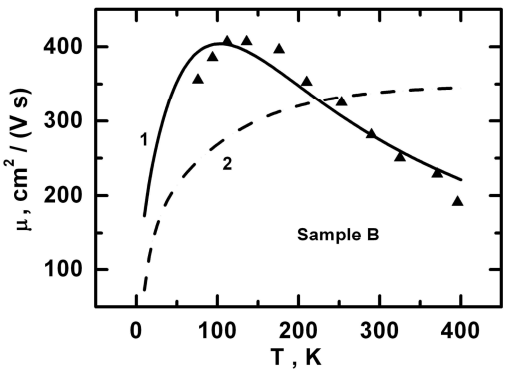
The respective electron transition probability from state $\boldsymbol{k}$ to state $\boldsymbol{k'}$ caused by the interaction with defect potential was chose from [3]. To calculate the conductivity tensor components the method of an exact solution of the stationary Boltzmann equation was used [4]. Using this formalism one can obtain additional fitting parameter $\gamma_{SS}N_{SS}$ (we put $\gamma_{SS}$=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 CdS samples with defect concentration $5.6\times10^{16}$ (sample A) and $8.7\times10^{17}$ $cm^{-3}$ (sample B). The obtained fitting parameters for different scattering modes are listed in Table II.

Theoretical curves for CdS samples 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.




*a*




*b*

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

MATERIAL PARAMETERS

*Table I.*

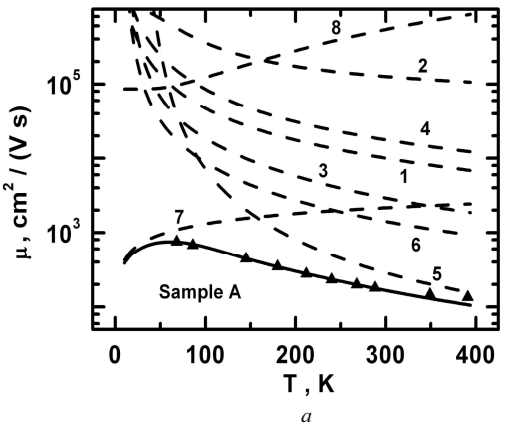
| Material parameter | Value |
|---|---|
| Lattice constant, $a_0$ ; $c_0$(m) | $4.1365\times10^{-10}$ ; $6.716\times10^{-10}$ |
| Energy gap, $E_g$ (eV) | $2.579 - 4.7\times10^{-4} T^2/(T+230)$ |
| Energy equivalent of matrix element, $E_p$ (eV) | 21 |
| Spin-orbit splitting, $\Delta$ (eV) | 0.062 |
| Density, $\rho_0$ (gm cm$^{-3}$) | 4.82 |
| Optical deformation potential, $d_0$ (eV) | 6.9 |
| transverse phonon frequency, (rad) | $2.63\times10^{13}$ |
| Acoustic deformation potential, (eV) | 3.3 |
| Piezoelectric tensor component, $e_{13}$ (C m$^{-2}$) | -0.262 |
| $e_{33}$ | 0.385 |
| $e_{15}$ | -0.183 |

PARAMETERS γ FOR DIFFERENT SCATTERING MODES

*TABLE II.*

| Sample | $\gamma_{PO}$ | $\gamma_{PZ}$ | $\gamma_{ID}$ | $\gamma_{SS}$ Nss $\times 10^{-14}$ cm$^{-3}$ |
|---|---|---|---|---|
| *A* | 0.58 | 0.50 | 1.0 | 27.0 |
| *B* | 0.72 | 0.52 | 1.0 | 12.0 |

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 CdS compared with the relaxation time

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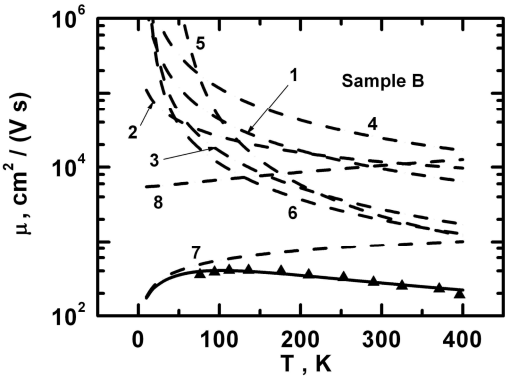


*b*

Fig.2. The contribution of different scattering modes into electron mobility inCdS . Solid line - mixed scattering mechanism; 1,2,3,4,5,6,7,8 – AC-, II-, NPO-, PAC-, PO-, POP-, SS, NI - 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.

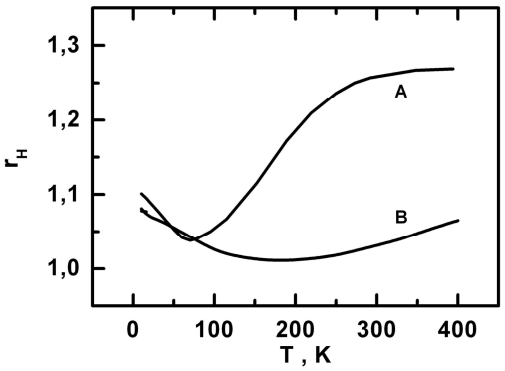


Fig.3. Temperature dependence of electron's Hall factor in CdS

**Conclusion**

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


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