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Band carriers scattering on impurities

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Abstract. Mobility of band carriers scattered on donors, partially ionized, partially neutral, at low temperatures, is considered in general and calculated for AIII-BV group crystals. It is shown that temperature dependence of mobility is determined by relationship between number of ionized and neutral donors and by average energy of electrons.

Keywords: impurities, scattering potential, quantum kinetic equation, mobility.

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1. Introduction

Investigations of scattering of band carriers by neutral impurities have no noticeable advance for a long time [1–5]. Several approaches to the problem of neutral impurity scattering were used, but only one received wide recognition. There was consideration of interaction of electrons with shallow neutral impurity, which imitates spherically symmetrical hydrogen atom. In this case relaxation time τ for momentum of carriers was constructed on the base of cross-section for scattering process [6]. This time has well-known Erginsoy's form [1]

$$\frac{1}{\tau} = \frac{20\,\varepsilon_L \hbar^3}{m^2 e^2} n_0 \,. \qquad (1)$$

Here ε_L is dielectric constant of lattice, m is effective mass, n_0 is concentration of scattering centers. However, there are serious claims to the method of scalar relaxation time as a whole [7, 8]. The attempts to improve agreement of theory and experimental data by the way of introducing some adjusting factor in Eq. (1) (see, for instance, [4]) should be considered as very naive only.

Other direction of investigations uses model for scattering potential of neutral impurity as rectangular spherically isotropic hole [9]. Limit case of this model is delta-shaped function in space [10, 11]). In this case there is no possibility to evaluate amplitude of interaction. There is also no way to derive rectangular or delta-shaped potential as well-reasoned limit case of physically grounded interaction.

Bellow we shall consider mobility of band carriers, scattered by charged and neutral impurities; calculations will be based on quantum kinetic equation [10, 11]. For simplicity we use here only a model of simple isotropic parabolic dispersion law for band carriers.

We consider shallow donors, which are partially ionized, as a scattering system; degree of donors ionization depends on temperature. So, generally we have both neutral and charged scattering centers; relation between their concentrations depends on temperature. We consider here only low temperatures and do not take into account phonon scattering.

2. Scattering potential

2.1. Delta-shaped potential

The formulation "scattering of band electron on neutral point defect" is completely conditional, because Coulomb interaction of charged particle with really neutral point object does not take place. Therefore neutral scattering center has to be some compact complex structure containing several different charges and has to be neutral as a whole only. In this case range of forces is practically limited by geometrical size of the complex center.

Let us consider delta-shaped potential as the simplest model of a neutral scattering center:

$$\varphi_I(\vec{r}) = \mathrm{Y}\delta(\vec{r}) \,. \qquad (2)$$

Fourier component of this potential is:

$$\varphi_I(\vec{q}) = \int_{-\infty}^{\infty} \exp(-i\vec{q}\,\vec{r})\varphi_I(\vec{r})\, d^3\vec{r} = \mathrm{Y} \,. \qquad (3)$$

Let us note that the value $\varphi_I(\vec{q})$ does not depend on wave vector $\vec{q}$.

2.2. Charged impurity

Fourier component of Coulomb potential generated by charged impurity has the form (see [10, 11]):

$$\varphi_{CI}(\vec{q},\omega) = \frac{4\pi e_I}{q^2 \varepsilon_L}\delta(\omega) . \qquad (4)$$

Taking into account screening of potential of scattering by band carriers, one can obtain:

$$\varphi_{CI}(\vec{q},\omega) = \frac{4\pi e_I}{q^2[\varepsilon_L + \Delta\varepsilon(\vec{q},0)]}\delta(\omega) . \qquad (5)$$

Here ε_L is dielectric constant of lattice, $\Delta\varepsilon(\vec{q},\omega)$ is dielectric function of band carriers.

Correlator of screened potentials is:

$$\langle\varphi^2_{CI}\rangle_{\omega,\vec{q}} = \frac{32\pi^3 e^2 N_{CI}}{[\varepsilon_L + \Delta\varepsilon(\vec{q},0)]^2\, q^4}\delta(\omega) , \qquad (6),$$

where (see [10]):

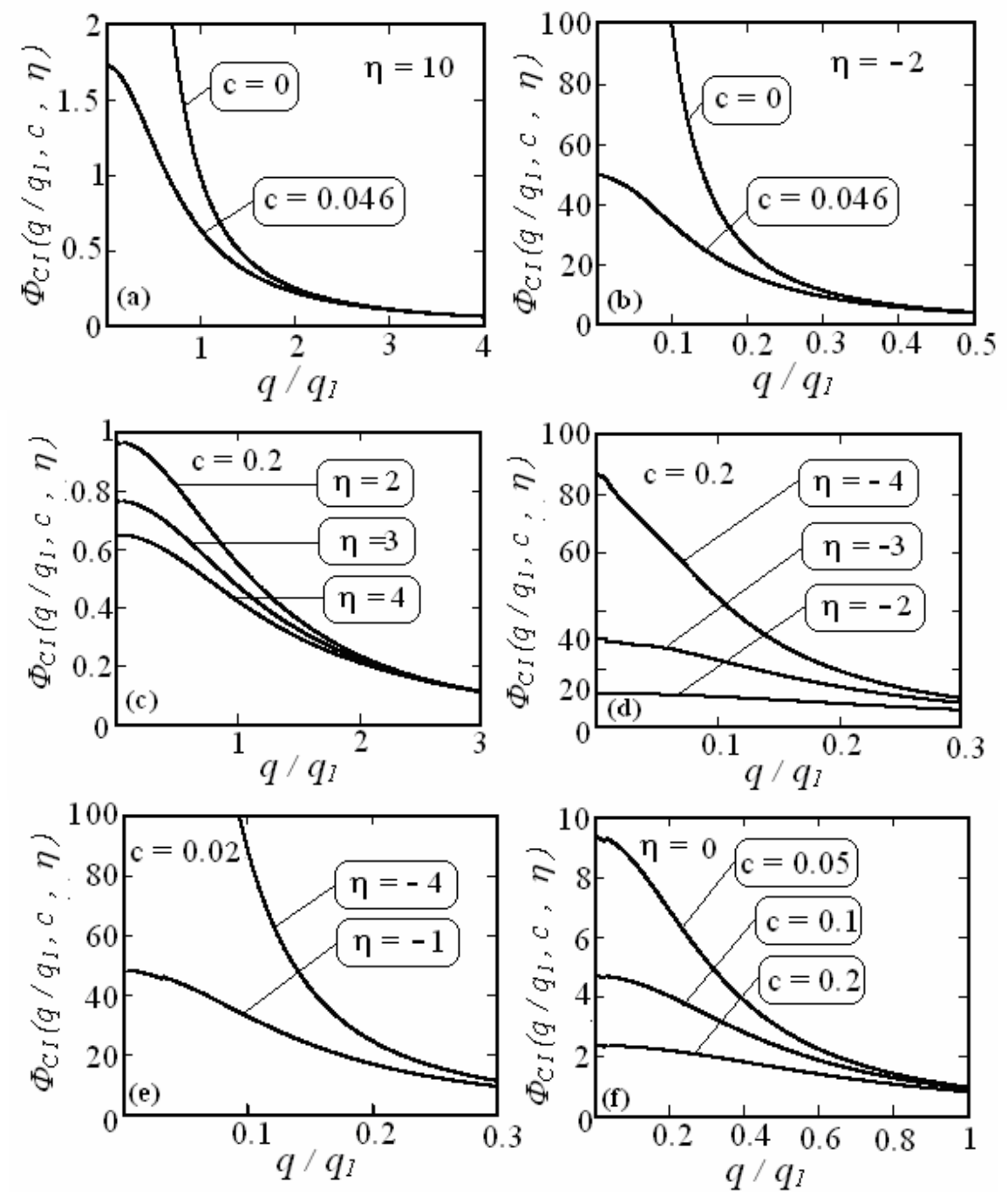

Fig. 1

$$\Delta\varepsilon\ (0,\vec{q}) = \frac{e^2}{\pi^2 q^2} P\int d^3\vec{k}\,\frac{f^0(\varepsilon_{\vec{k}}) - f^0(\varepsilon_{\vec{k}-\vec{q}})}{\varepsilon_{\vec{k}-\vec{q}} - \varepsilon_{\vec{k}}}, \quad (7)$$

and $f^0(\varepsilon_k)$ is equilibrium distribution function; $\varepsilon_k = \hbar^2 k^2/2m$ is dispersion line for this section (we assume that it is simple isotropic parabolic relation).

Carrying out integration similar to that in Eq. (3), we obtain:

$$\varphi_{CI}(\vec{q},\omega) = \frac{4\pi e_I}{q_1^2 \varepsilon_L}\left[\Phi\left(\frac{q}{q_1},\ c\ ,\eta\right)\right]^{-1}\delta(\omega).$$

Here $q_1 = \sqrt{8m k_B T}/\hbar$, $\eta = \varepsilon_F/k_B T$, $c = e^2\sqrt{m}/8\pi\varepsilon_L\hbar\sqrt{k_B T}$, and

$$\Phi(q/q_1\ ,c\ ,\eta) = \left(\frac{q}{q_1}\right)^2 + c\left(\frac{q_1}{q}\right)\times$$
$$\times\int_0^\infty \ln\left(\frac{\sqrt{z}+q/q_1}{\sqrt{z}-q/q_1}\right)\frac{dz}{1+\exp(z-\eta)}. \quad (9)$$

The case $c = 0$ corresponds to absence of screening of Coulomb potential by band carriers. Figure 1 represents dependence of Fourier component of potential generated by screened charged impurity on dimensionless wave vector q/q_1 for different values of dimensionless Fermi energy η and screening constant *c*. Comparison of these figures and dependence presented by Eq. (3) shows that screened Coulomb potential cannot imitate delta-shaped potential. The reason for that is evident: the screening cuts Coulomb interaction at long distances and is not important for short distance interaction.

Using Eqs. (8) and (9), let us rewrite correlator (6) in the following form:

$$\langle\varphi_{CI}^2\rangle_{\omega,\vec{q}} = \langle\varphi_{CI}^2\rangle_{\omega,q}\delta(\omega) =$$
$$= \frac{32\pi^3 e^2 N_{CI}}{\varepsilon_L^2\,[q_1^2\Phi(q/q_1,c,\eta)]^2}\delta(\omega). \quad (10)$$

2.3. Hydrogen-shape neutral impurity

Let us consider donor impurity having the structure similar to the spherically symmetrical hydrogen atom. Space density of negative charge χ can be presented by the following relation:

$$\chi(\rho) = -e|\psi(\rho)|^2. \quad (11)$$

Here $\psi(\rho) \sim \exp(-\rho/r_B)$ is wave function of electron of shallow donor;

$$r_B = \hbar^2\varepsilon_L/me^2 \quad (12)$$

r_B is Bohr radius of exterior donor electron; m is effective mass. The charge density $\chi(\rho)$ is normalized by the relation

$$4\pi\int_0^\infty \chi(\rho)\rho^2 d\rho = -e. \quad (13)$$

Electrostatic potential of the positive kernel of impurity atom in crystal is

$$\varphi^+(r) = \frac{e}{\varepsilon_L r}. \quad (14)$$

Electrostatic potential generated by distributed negative charge of exterior donor electron is (8)

$$\varphi^-(r) = -\frac{e}{\varepsilon_L r}\cdot\frac{\int_0^r \rho^2\exp(-2\rho/r_B)\,d\rho}{\int_0^\infty \rho^2\exp(-2\rho/r_B)d\rho}. \quad (15)$$

Total scattering potential of neutral center is:

$$\varphi_{NI}(r) = \varphi^+(r) + \varphi^-(r) =$$
$$= \frac{e}{\varepsilon_L r}\left[1 - \frac{\int_0^r \rho^2\exp(-2\rho/r_B)}{\int_0^\infty \rho^2\exp(-2\rho/r_B)}\right] = \quad (16)$$
$$= \frac{e}{\varepsilon_L r}\left[1 + 2\frac{r}{r_B} + 2\frac{r^2}{r_B^2}\right]\exp(-2r/r_B).$$

Several examples for the space distribution of potential $\varphi_N(r)$ are presented in Fig. 2. Here $K(r,\gamma) = r_0\,\varepsilon_L\,\varphi_{NI}(r)/e^2$; the curves (a), (b), (c), (d) refer to $\gamma = r_0/r_B = 0, 1, 2, 4$ respectively. The value of radius r_B determines range of action for scattering center.

Fourier component of potential (16) has the following form:

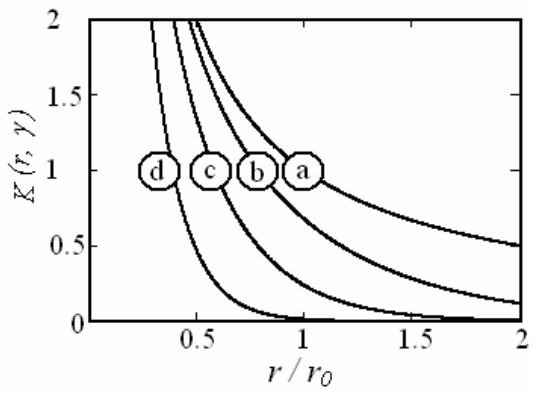

Fig. 2.

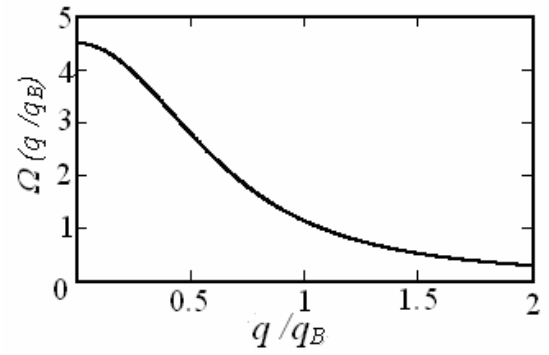

Fig. 3.

$$\varphi_{NI}(\vec{q},\omega)=\frac{4\pi}{\varepsilon_L}\frac{e}{q^2+q_B^2}\times$$
$$\times\left[1+\frac{3q_B^2/2}{q^2+q_B^2}+\frac{2q_B^4}{(q^2+q_B^2)^2}\right]\delta(\omega)\equiv \qquad (17)$$
$$\equiv\frac{4\pi}{\varepsilon_L}\frac{e}{q_B^2}\Omega(q/q_B)\delta(\omega)\,.$$

Here

$\Omega(p)=(1+p^2)^{-1}[1+(3/2)(1+p^2)^{-1}+2(1+p^2)^{-2}]$ (see Fig. 3), and $q_B=2/r_B=2me^2/\varepsilon_L\hbar^2$.

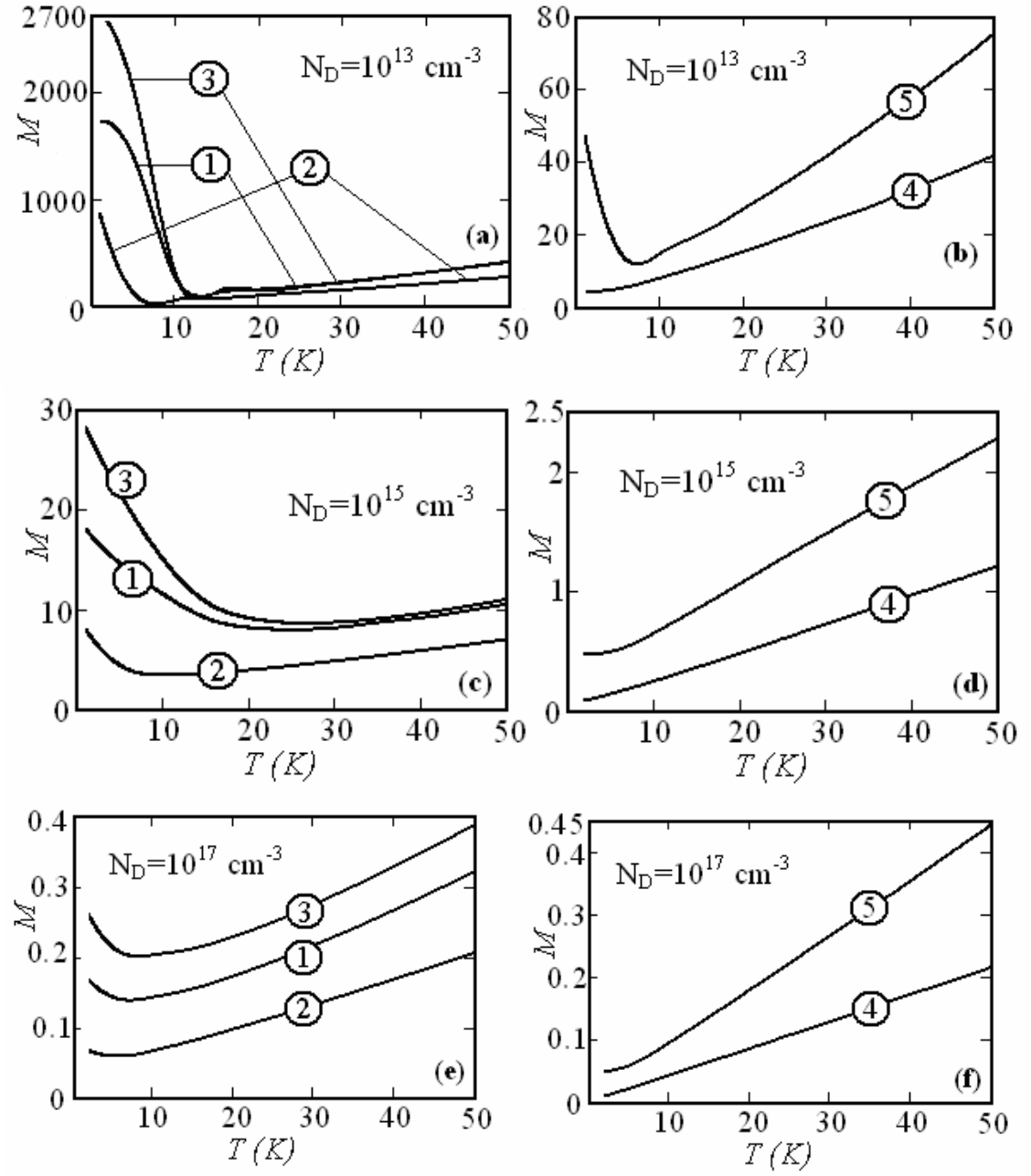

Fig. 4.

One can see that wave vector q_B is natural measure for distribution of scattering potential, generated by neutral impurity, in *q*-space. For *n*-GaAs we have: $m = 0.067 m_0$, and $\varepsilon_L = 12.5$; therefore we obtain: $q_B^2 = 4.108 \cdot 10^{12} cm^{-2}$. Hence it follows that noticeable screening of the short-range potential (16) by band electrons takes place in this crystal at concentrations $n > 10^{17} cm^{-3}$. Assuming $q_B = 0$ (that is $r_B \to \infty$) in expression (17), we obtain form (4).

As follows from Eq. (17), the correlator of scattering potentials for neutral centers is:

$$\langle \varphi^2_{NI} \rangle_{\omega, \vec{q}} = \langle \varphi^2_{NI} \rangle_q \delta(\omega) = \frac{32\pi^3 e^2 N_{NI}}{\varepsilon_L^2 (q^2 + q_B^2)^2} \times \left[1 + \frac{3 q_B^2 / 2}{q^2 + q_B^2} + \frac{2 q_B^4}{(q^2 + q_B^2)^2} \right]^2 \delta(\omega) . \quad (18)$$

Here N_{NI} is concentration of neutral impurities. Due to short range of considered scattering center, there is no need to involve screening of scattering potential by band electrons into consideration.

3. Mobility of band carriers

Let us consider impurity system as partially ionized, partially neutral donors. The degree of ionization depends on temperature *T*. Let us write the relation between concentrations of ionized and neutral impurities as

$$N_D = N_{DN} + N_{DI} = N_{NI} + N_{CI} \quad . \quad (19)$$

Below we shall assume that band electrons concentration n is equal to concentration of ionized donors

$$n = N_{DI} = N_{CI} = N_D \left[1 + \exp\left(\frac{\varepsilon_F - \varepsilon_D}{k_B T} \right) \right]^{-1} . \quad (20)$$

Here ε_F is Fermi energy, $\varepsilon_D < 0$ is energy level for donors.

We calculate mobility μ of band carriers using the formula (see Ref. [11])

$$\beta = \frac{1}{\mu} = \beta_{CI} + \beta_{NI} . \quad (21)$$

Here

$$\beta_{CI} = \frac{em^2}{24\pi^4 \hbar^3 n} \int_0^\infty \frac{q^3 d\ q}{1 + \exp\left(\hbar^2 q^2 / 8m\ k_B T - \eta \right)} \langle \varphi^2_{CI} \rangle_q . \quad (22)$$

$$\beta_{NI} = \frac{em^2}{24\pi^4 \hbar^3 n} \int_0^\infty \frac{q^3 d\ q}{1 + \exp\left(\hbar^2 q^2 / 8m\ k_B T - \eta \right)} \langle \varphi^2_{NI} \rangle_q . \quad (23)$$

The value β_{CI} represents contribution of charged impurities in reverse mobility of band carriers, the value β_{NI} refers to neutral impurities.

We carried out the following numerical calculations for set of AIII-BV-group crystals (see Ref. [12] and Table 1):

Table 1

	AIII-BV	m/m_0	ε_L	$-\varepsilon_D$ (eV)
1	GaAs	0.067	12.5	0.008
2	GaSb	0.05	15	0.003
3	InP	0.07	14	0.008
4	InSb	0.013	17	0.0007
5	InAs	0.02	14	0.002

Results of calculations of mobility based on formulae (21)–(23) are presented in Fig. 4 (a – l). Here

$$\mu = \frac{3\pi \varepsilon_L^2 \hbar^3}{2 e^3 m^2} M \quad . \quad (24)$$

Numbers on curves correspond to numbers in Table 1.

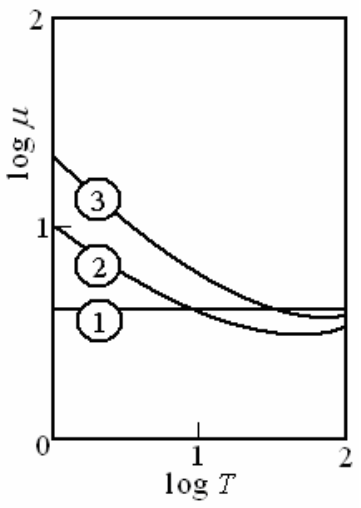

Fig. 5

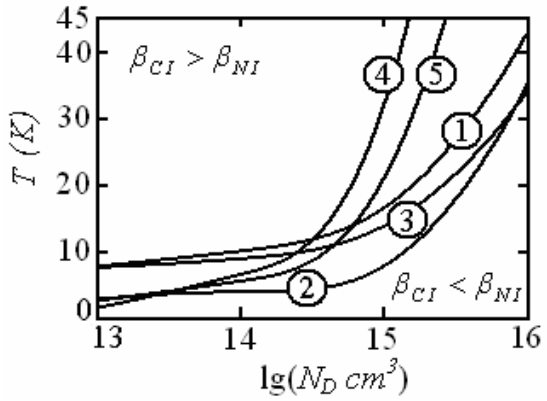

Fig. 6

Temperature dependence of mobility μ for considered crystal appears as a result of competition of two processes: change of ionized centres number and change of average energy of electrons. The first process dominates at lower temperatures, the second one — at higher temperatures. Therefore calculated dependence of dimensionless mobility M on temperature T is non-monotonous.

Figure 5 is presented here for comparison, which reproduces Fig. 4.5(b) from Ref. [9]. Here curve 1 is constructed on the base of Erginsoy's theory [1], curves 2 and 3 — on the base of theoretical calculations of N. Sclar [12] and T. McGill with R. Baron [13] respectively. Our curves shown in Fig. 4 have the same shape as curves 2 and 3 in Fig. 5.

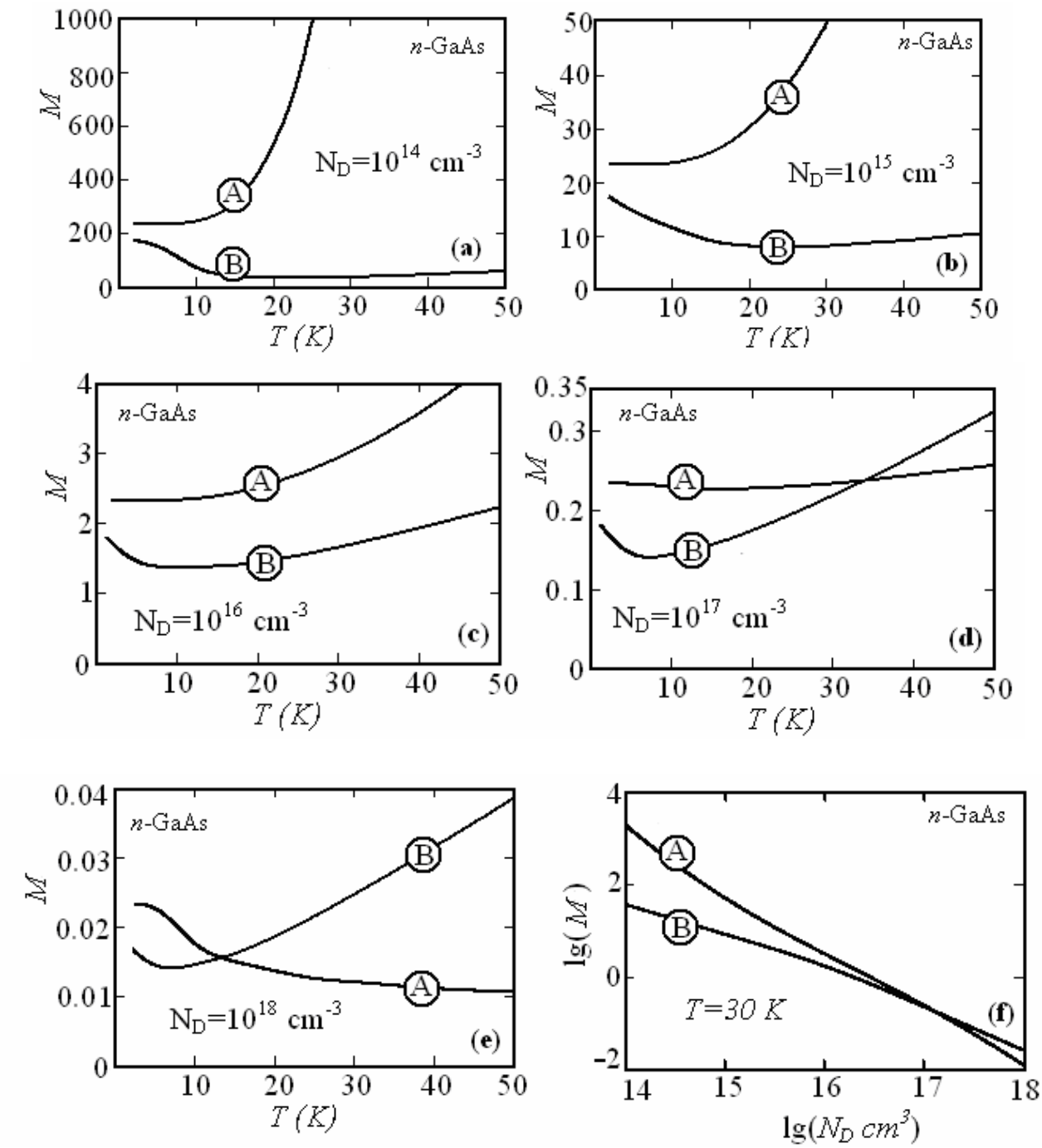

Fig. 7.

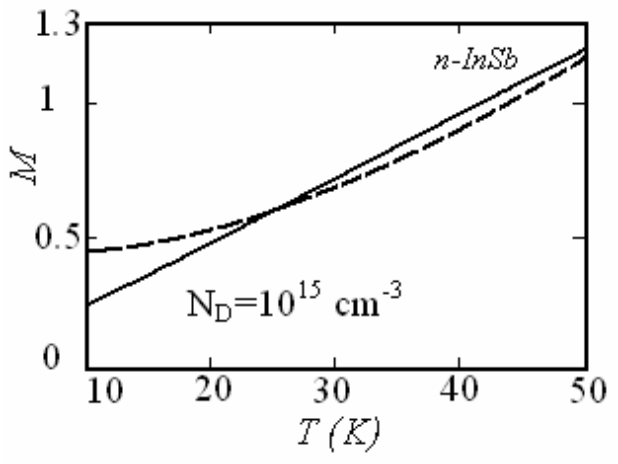

Fig. 8.

4. Discussion

To compare contributions of neutral and charged impurities in mobility, let us introduce border temperature T^* by the relationship $\beta_{CI}(T^*) = \beta_{NI}(T^*)$. Connection between temperature T^* and donor concentration N_D is presented in Fig. 6 by five lines (corresponding to five different crystals). These lines divide the plane $\{N_D, T\}$ in two areas. In top area ($T > T^*$) the scattering on charged donor prevails; in lower area ($T < T^*$) scattering on neutral impurities dominates. The numbers of curves correspond to Table 1.

Let us now compare results obtained in this article with results which can be obtained on the base of calculations carried out on the base of tau-approximation (see Ref. [5]). Result of comparison is shown in Fig. 7. Here B-lines refer to the calculations of this article, A-line are constructed with the help of corresponding formulae represented in monograph of Anselm (see Ref. [5]). One can see that their divergence is quite noticeable.

In Fig. 8 our theoretical curve (solid line) and experimental curve (dashed line) obtained for InSb by H.J. Hrostowski et al. are presented (see Refs. [14, 15]). It is seen that these lines are in gratifying agreement.

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