DOPING DEPENDENCE OF THE DEBYE SCREENING LENGTH IN HEAVILY-DOPED SEMICONDUCTORS HAVING GAUSSIAN BAND-TAILS

By K. P. Ghatak, A. K. Chowdhury*, S. Ghosh and A. N. Chakravarti

Institute of Radio Physics and Electronics, University College of Science and Technology, Calcutta**

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In this work the doping dependence of the Debye screening length of the carriers in the heavily-doped semiconductors having Gaussian band-tails is investigated. It is found, taking heavily-doped *n*-type GaAs as an example, that the screening length decreases with increasing impurity concentration with the exception of much less effective screening over a certain range of impurity concentrations due to the presence of band-tails.

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1. Introduction

It is well-known that the extent of carrier degeneracy influences many of the physical parameters in semiconductors. The Debye screening length is one such parameter which affects many of the physical characteristics of semiconductor devices and electron plasmas in semiconductors. In recent years, the screening length has been studied in degenerate semiconductors under various physical conditions [1–4]. However, these studies have yet to be extended to conditions of degeneracy in heavily–doped semiconductors in which band-tails are invariably formed due to the merging of the impurity band with the free-carrier band. Since, by now, it has become well established [5–9] that the band-tail in heavily–doped semiconductors in the low-density limit (that is near the lower limit of heavy doping where the screening effects are not strong enough to annihilate the impurity states leading to band-tailing mainly by the perturbed free-electron states and also the exchange interaction effects may be neglected) is a merged impurity band with a Gaussian density-of-states function resulting from the random distribution of the impurities, one should consider the presence of such tails in the study of screening in heavily-doped

^{*} On leave of absence from the Dept. of Physics, Patna University, Patna, India.

^{**} Address: Institute of Radio Physics and Electronics, University College of Science and Technology, 92, Acharya P. C. Road, Calcutta 700009, India.

semiconductors unless the level of doping is abnormally high. In the present work, the doping dependence of the Debye screening length in heavily-doped semiconductors is determined in the low-density limit, taking heavily-doped *n*-type GaAs as an example. This dependence is then compared with the monotonous decrease of the screening length with increasing carrier concentration as is observed both under non-degenerate and degenerate conditions in semiconductors in the absence of band-tails to assess the influence of such tails on the doping dependence of the screening length in heavily-doped semiconductors in the low-density limit.

2. Theoretical background

The Debye screening length of the carriers in semiconductors can, in general, be expressed [2] by the relation

$$\frac{1}{L_{\rm d}^2} = \frac{e^2}{\varepsilon} \, \frac{dn_0}{dE_{\rm F}} \,,\tag{1}$$

where e is the carrier charge, n_0 the carrier concentration, e the permittivity and E_F the Fermi energy. It appears, therefore, that the derivation of the expression for the screening length would require expressions for the density-of-states functions for the free-carrier band and the band-tail. In heavily-doped n-type semiconductors having no compensation, the electrons are normally distributed at a finite temperature amongst the energy states of both the conduction band and the band-tail. For the present analysis, we shall assume the dependence of the density-of-states function on energy to be of the standard parabolic type for the conduction band and of the Gaussian type for the band-tail.

For heavily-doped *n*-type semiconductors having Gaussian band-tails, the density-of-states function corresponding to impurity states in the conduction band-tail can be expressed [7] as

$$\varphi_{\rm d} = \varphi_0 \exp \left[-\left(\frac{E - E_{\rm d0}}{\sigma_{\rm d}}\right)^2 \right],$$
 (2)

where φ_0 is the amplitude, σ_d , the half-width, is equal to $\sqrt{2}\sigma$, σ being the standard deviation and E_{d0} is the energy corresponding to the centre of the Gaussian band (the Gaussian function being centred at the hydrogen-model impurity activation energy). The integral over the function φ_d is equal to twice the density N_d of impurity atoms (since spin degeneracy has to be considered [6] also for the impurity states when these merge to form a band-tail), so that we can write

$$\varphi_0 \sigma_{\rm d} = \frac{2N_{\rm d}}{\sqrt{\pi}} \,. \tag{3}$$

According to Kane [8] and Morgan [9], the half-width is expressed as $\sigma_{\rm d} = \frac{e^2}{\varepsilon} \left(4\pi N_{\rm d}/\lambda \right)^{1/2}$, where λ , the reciprocal screening length of the degenerate electron distribution that would

result from the complete ionization of the impurities in the absence of band-tailing effects, can be calculated from the Thomas-Fermi model and is given [6] by

$$\lambda = \left[2 \left(\frac{3}{\pi} \right)^{1/6} \left(\frac{m^*}{\varepsilon} \right)^{1/2} \frac{e}{\hbar} N_{\rm d}^{1/6} \right], \tag{4}$$

 m^* being the effective electron mass and \hbar the Dirac constant. Under the assumption stated above, when the electrons are distributed in both the conduction band and the band-tail, we can express the electron concentration according to Fermi-Dirac statistics as

$$n_0 = N_c F_{1/2}(\eta) + \frac{2kTN_d}{\sqrt{\pi} \sigma_d} \int_{-\infty}^{\infty} \exp\left[-\left(\frac{kT}{\sigma_d}\right)^2 x^2\right] \left[1 + \exp\left(x - \frac{\zeta + E_{di}}{kT}\right)\right]^{-1} dx,$$
 (5)

where

$$N_{\rm c} = 2(2\pi m^* kT/h^2)^{3/2}, \quad \eta = \frac{E_{\rm F}}{kT},$$

$$x = \frac{E - E_{d0}}{kT}, \quad \zeta = E_{F} - E_{c0},$$

k being the Boltzmann constant, T the temperature, E_{c0} the energy corresponding to the bottom of the unperturbed conduction band, $E_{d_i} = (E_{c0} - E_{d0})$ and $F_j(\eta)$ stands for Fermi-Dirac integrals of order j defined elsewhere [10]. Introducing the variables $kT/\sigma_d = a$

and
$$\eta' = \eta - \left(\frac{E_{d0}}{kT}\right)$$
, we can write

$$n_0 = N_c F_{1/2}(\eta) + \frac{2aN_d}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp(-a^2 x^2) dx}{1 + \exp(x - \eta')},$$
 (6)

$$\frac{dn_0}{dE_F} = \frac{N_c}{kT} F_{-1/2}(\eta) + \frac{2aN_d}{\sqrt{\pi} kT} \int_{-\infty}^{\infty} \frac{\exp(-a^2x^2 + x - \eta')dx}{\{1 + \exp(x - \eta')\}^2}.$$
 (7)

The integrals in equations (6) and (7) can conveniently be expressed in terms of a converging series which enables one to convert these equations into the following forms:

$$n_0 = N_c F_{1/2}(\eta) + \frac{2aN_d}{\sqrt{\pi}} I_1, \tag{8}$$

$$\frac{dn_0}{dE_F} = \frac{N_c}{kT} F_{-1/2}(\eta) + \frac{2aN_d}{\sqrt{\pi} kT} I_2, \tag{9}$$

where

$$I_{1} = \frac{\sqrt{\pi}}{2a} \exp\left(-a^{2} \eta'^{2}\right) \left[\sum_{r=0}^{r=n} (-1)^{r} \{F(\alpha_{1}) + F(\alpha_{2})\} \right],$$

$$I_{2} = \frac{\sqrt{\pi}}{2a} \exp\left(-a^{2} \eta'^{2}\right) \left[\sum_{r=0}^{r=n} (-1)^{2r} \{F(\alpha_{3}) + F(\alpha_{4})\} \right],$$

 $r = 0, 1, 2, \dots$ being the index of summation, and

$$\alpha_{1} = \left(\frac{r - 2a^{2}\eta'}{2a}\right)^{2}, \quad \alpha_{2} = \left(\frac{1 + r + 2a^{2}\eta'}{2a}\right)^{2},$$

$$\alpha_{3} = \left(\frac{1 + 2r - 2a^{2}\eta'}{2a}\right)^{2}, \quad \alpha_{4} = \left(\frac{1 + 2r + 2a^{2}\eta'}{2a}\right)^{2},$$

$$F(\alpha_{i}) = \exp(\alpha_{i})\left[1 - \frac{g(\frac{1}{2}, \alpha_{i})}{\sqrt{\pi}}\right], \quad i = 1, 2, 3, 4,$$

 $g(\frac{1}{2}, \alpha_i)$ being the incomplete Gamma function [11]. Thus, using the above equations, we can express the Debye screening length of the carriers in heavily-doped *n*-type semiconductors having Gaussian band-tails as

$$\frac{1}{L_{\rm d}^2} = \frac{e^2 N_{\rm c}}{\varepsilon k T} \left[F_{-1/2}(\eta) + H \sum_{r=0}^{r=n} (-1)^{2r} \{ F(\alpha_3) + F(\alpha_4) \} \right],\tag{10}$$

where

$$H = N_{\rm d} \exp{(-a^2 \eta'^2)}/N_{\rm c}$$

In the absence of the band-tails or when most of the carriers are in the conduction band under degenerate conditions, $H \to 0$ and equation (10) simplifies into the form:

$$\frac{1}{L_{\rm d}^2} = \frac{e^2 N_{\rm c}}{\varepsilon k T} F_{-1/2}(\eta). \tag{11}$$

For $\eta < 0$, i.e. under non-degenerate conditions, $F_j(\eta)$ can be replaced [10] by exp (η) leading to the following well-known expression for the screening length:

$$\frac{1}{L_a^2} = \frac{e^2 n_0}{\varepsilon k T} \tag{12}$$

3. Results and discussion

Using equation (10), together with the other related equations and parameters, and taking for GaAs, for example, the relative permittivity to be 11.8 (neglecting its doping dependence), $m^* = 0.067 m_0$, m_0 being the free electron mass, and $E_{d_1} = 6$ meV (as a typi-

cal figure for donors in GaAs), we have computed the doping dependence of the Fermi energy and the Debye screening length of the carriers corresponding to different temperatures for heavily-doped n-type GaAs having Gaussian band-tails as shown in Figs. 1 and 2, respectively.

It is known that the rate of change of the Debye screening length with increasing impurity concentration is faster in degenerate semiconductors than that in non-degenerate

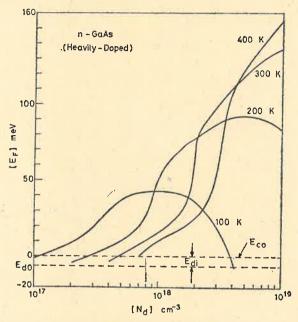


Fig. 1. Doping dependence of the Fermi energy corresponding to different temperatures in heavily-doped n-type GaAs having Gaussian band-tails

semiconductors. This fact alone explains well the doping dependence obtained here. It is apparent from Fig. 1 that the Fermi level enters into the band-tail both for relatively high and low levels of doping and remains in the conduction band for the intermediate range of impurity concentrations. Thus, the conditions are non-degenerate at relatively low and high levels of doping since the density-of-states in the conduction band is much larger than that in the band-tail resulting in the Boltzmann distribution of the electrons raised at a finite temperature to the conduction band when the Fermi level is in the band-tail. However, conditions are always degenerate in the intermediate range of impurity concentrations when the Fermi level is situated in the conduction band. Thus, for relatively low and high levels of impurity concentration, the rates of decrease of the screening length with increasing impurity concentration would more-or-less be the same and would be slower than that corresponding to the degenerate condition. The link between relatively slow and fast rates followed again by a relatively slow rate of decrease of the screening length with increasing impurity concentration has, therefore, resulted in the particular natures of the curves with the peaks shown in Fig. 2. It is observed that the peak shifts

with increasing temperature towards higher impurity concentrations. The height of the peak is also observed to decrease with increasing temperature.

It is further concluded that, over a certain range of impurity concentrations, the screening length becomes quite large resulting in much less effective screening. This particular feature of the doping dependence can only be obtained from the consideration of

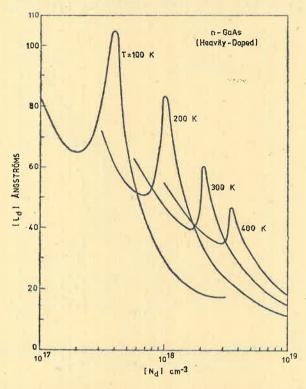


Fig. 2. Doping dependence of the Debye screening length of the carriers corresponding to different temperatures in heavily-doped *n*-type GaAs having Gaussian band-tails

band-tails as are invariably formed in heavily-doped semiconductors in the low-density limit. The present analysis would also be applicable to heavily-doped p-type semiconductors provided that the different parameters are defined as appropriate for the valence band. These conclusions may be of much interest in the study of degenerate plasmas in semi-conductors having different impurity concentrations. However, the conclusions would not be meaningful in the high-density limit for the reasons already stated.

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