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SOME QUESTIONS OF MOBILITY DETERMINATION IN HEAVILY DOPED SEMICONDUCTORS

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Regarding the non-parabolicity of impurity band energy spectrum the mobility in the range from $5\cdot 10^{18}$ to $10^{20}cm^{-3}$ of the impurity concentrations is calculated for Si at 300 K.

1. INTRODUCTION

Many authors were concerned with the mobility problem, among those is D.L.Rode[1,2]) who worked out the model to determine this quantity in details. His relations, however, implies the proportionality of the density of states, $\rho(E)$, to the square root of energy (E), what is not the case in heavily doped semiconductors. This problem has been also considered in[3]), where the influence of electron-electron scattering was introduced semi-empirically, but again with tacit assumption of the mentioned proportionality, $\rho\sim\sqrt{E}$.

This paper suggests a treatment which takes into account the complex dependence between the density of states and energy in heavily doped semiconductors. The examples for the mobility determination in heavily doped Si show the influence of different ways in the screening length and in the ionized impurities scattering calculations.

2. EXPRESSION FOR CARRIER MOBILITY DETERMINATION

We start from Fermi-Dirac statistics and assuming that equienergetic surfaces are spheric, but not parabolic, it is easy to show that vector of group velocity $\vec{v}$ is colinear with wave vector $\vec{k}$ ($\vec{v}=(1/\hbar)(dE/dk)(\vec{k}/k)$), and that density of states $\rho(E)$ is:

$$\rho(E)=\frac{1}{4\pi^3}\frac{dV_k}{dE}=\frac{k^2}{\pi^2}\frac{dk}{dE}\,. \tag{1}$$

Therefore, $\rho(E)$ and wave vector are related by

$$k^3=\frac{1}{3\pi^2}\int_{-\infty}^{E}\rho(E)dE\;, \tag{2}$$

providing that $\rho(E)$ may have the arbitrary dependence. Electron velocity, according to (1) can be expressed as:

$$v=\frac{1}{\hbar}\frac{dE}{dk}=\frac{1}{\hbar\pi^2}\frac{k^2(E)}{\rho(E)}\,. \tag{3}$$

Taking into account the conventional expression for the mobility (see for example[4])) with spheric equienergetic surfaces and using (1) we obtain

$$\mu = \frac{-e}{3n\pi^2}\int \frac{\partial f}{\partial E}\tau v^2 k^2 dk = -\frac{e}{3n}\int_{-\infty}^{+\infty}\frac{\partial f}{\partial E}\tau v^2 \rho(E)\, dE, \tag{4}$$

where f is Fermi-Dirac's distribution function, $\tau(v)$ total relaxation time, n electron concentration, and energy E is related to the bottom of the conduction band of an intrinsic semiconductor (E_{co}). It is evident that this general expression in the case of a parabolic dependence ($v=\hbar k/m^*$) will reduce to the expression given in[1]).

In fact, in the expression for $\rho(E)$ the constancy of the effective masses is not assumed. However, it is very complicated to find the dependences under the same conditions for the relaxation time, so, for $\tau_i(v)$, we used the expressions from [1,2]) which include m*=const. To examine the applicability of the idea on the influence of charge density redistribution in a heavily doped semiconductor on the ionized impurities scattering[5,6]) we used the expression

$$\tau_i^{-1} = N v \sigma_e = N v \pi \left(\frac{2m^* e^2}{4\pi\varepsilon\varepsilon_0 \hbar^2 k^2}\right)^2 F(2kr_c) \tag{5}$$

where (the same notation as in[6]))

$$F(2kr_c) = \int_0^{2kr_c}\left\{\frac{[3+(R^3/r_c^3 - 1)x^2]\sin x - 3x\cos x}{\frac{R^3}{r_c^3}x^3(1+r_s^2 x^2/r_c^2)} - 1\right\}^2 \frac{dx}{x}. \tag{6}$$

3. SELF-CONSISTENT MODEL FOR SCREENING LENGTH AND FERMI ENERGY DETERMINATION

It is known that the general expression for the screening length has the following form

$$R^{-2} = \frac{e^2}{\varepsilon\varepsilon_0}\int -\frac{\partial f}{\partial E}\rho(E)\, dE. \tag{7}$$

It can be seen that this expression includes the density of states $\rho(E)$ for the calculation of which it is necessary to know the screening length. Generally, the problem of determination of the density of states in a heavily doped semiconductor is very complex and is considered in a number of papers[8-11]). We used the expressions from[9]) with correction of standard deviation introduced in[10]). For the initial screening length value one may use the value obtained according to the expression for the nondegenerate semiconducot or metals,

$$R^{-1} = \frac{e}{(\varepsilon\varepsilon_0)^{1/2}}\left(\frac{N}{k_0 T}\right)^{1/2}, \quad R^{-1} = 2\left(\frac{3}{\pi}\right)^{1/6}\frac{e}{\hbar}\left(\frac{m^*}{4\pi\varepsilon\varepsilon_0}\right)^{1/2} N^{1/6}, \tag{8,9}$$

respectively. With such a value of the R one calculate the density of states $\rho(E)$ recalculating the screening length value according to (7). If the difference between the previous and the present R-s is unsatisfactory, the new screening length value is taken as the initial and the whole procedure repeated.

Fermi energy is calculated according to

$$N_D = n_0 = \int_{-\infty}^{\infty} f \rho(E)\, dE. \qquad (10)$$

Evidently, to use (10) it is necessary to know the density of states, for the calculation of which one should previously know the Fermi energy (E_f). Therefore, it is necessary to apply the self-consistent method similar to that for the calculation of the screening length. The initial Fermi energy value may be evaluated in such a way that $\rho(E)$ for the impurity band (having Gaussian character) is assumed to be proportional to delta-function of $(E-E_D)$, and that $\rho(E)$ for the conduction band is $\rho(E)\sim\sqrt{(E)}$. Thus we obtain a quadratic equation on $\exp(E_f/k_oT)$ and the solution is approximately

$$\exp(E_f/k_oT) \approx n/(B_c + 2n\exp(W_D/k_oT)) \qquad (11)$$

where $B_c=2(m_n k_o T/(2\pi\hbar^2))^{3/2}=n(\exp(-\tilde{W}_f)-2\exp(-\tilde{W}_D))$, and $W_D=E_{co}-E_D$ is the depth of the basic impurity level $(\tilde{x} \equiv x/k_oT)$.

4. NUMERICAL DESULTS

Using (4) the mobility μ in n-type Si was calculated (for phosphorous, W_D=0.046 eV) in dependence of the impurity concentration N_D ($5\cdot10^{18}$ - 10^{20}cm^{-3}) at room temperature. There were included acoustic, intervalley and ionized impurity scattering. The last one was calculated according to two models: the one based on (25) in[1]) - MODEL 1, and the one based on (6) of this paper (according to[6])) - MODEL 2. The screening length was calculated in three ways: by self--consistent model, according to the expression (9) for metals, and according to the approach in[6])

$$R^{-2} = e^2N/(\varepsilon\varepsilon_o k_o T_f), \qquad (12)$$

where T_f is the "freezing" temperature (T_f=1400 K).

The obtained results, for the considered concentrations, are shown in Fig. 1 (curves 2-7) parallel with the results of the experiment according to[12]) and theoretical curve (curve 1) obtained in[13]). They show that the mobility (obtained by means of both models) is dependent of the screening length. One can notice that the greatest deviation from the experiment is obtained when expression (9) is used, because it holds for the conditions of the extreme degeneracy, so that for the concentration $N_D \leq 2\cdot10^{19}$cm^{-3} are even obtained the unreal values for μ. On the other hand, value of R according to eqn (12) fits most favourably with experimental values of μ in both models.

Analysing the consequences of the calculations according to two models one can conclude that model 2 gives better, both quantitative and qualitative results (curves 5 and 7 in Fig. 1) than model 1 (curves 2 and 4). This results from the fact that the charge density redistribution reduces the scattering effects of the ionized impurities. The best results are obtained by model 2 using the screening length according to (12) (curve 7).

5. CONCLUSION

The suggested procedure for the mobility calculation enables us to take into account the complex dependence between the density of states and energy in heavily doped semiconductors, while the model 2 is much more adequate then the model 1.

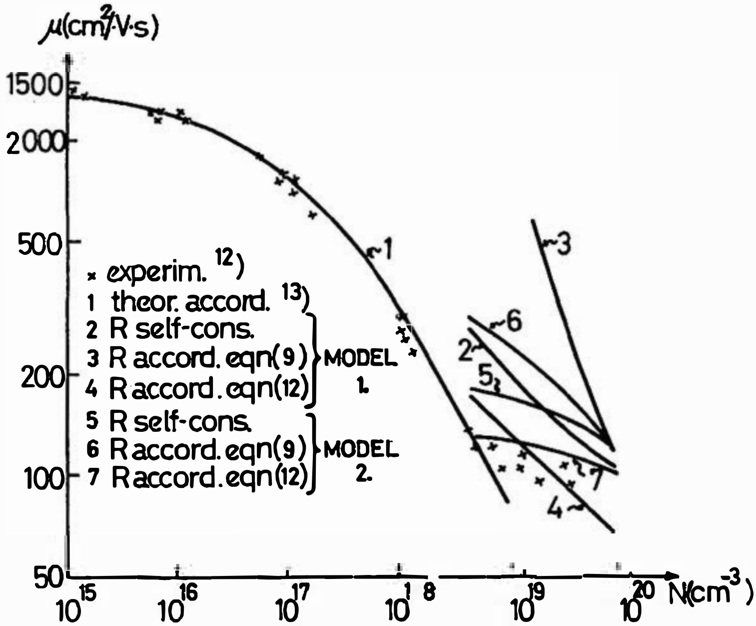

Fig. 1

The developed procedure enables us to follow the influence of complex dependence $\rho(E)$, as well as the screening length and scattering mechanisms to the curve $\mu=f(N_D)$.

Our further investigations will comprise electron-electron scattering and criteria enabling us to avoid the singularities in numerical calculations in an area between nondegenerated and strongly degenerated semiconductors.

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