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ON SOME PROBLEMS IN THE SCREENING LENGTH DETERMINATION IN HEAVILY DOPED SEMICONDUCTORS

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Four problems that arise in evaluation of the screening length are discussed. (i) According to the existing models the standard deviation begins to decrease with further increase of N. (ii) The normalizing factor in $\int \rho dE = \kappa N$ should be $\kappa=1$ (for $\kappa=2$, $E_F \to E_d$). (iii) The boundary conditions for eqn.(1) should contain a correction ε, according to (14). (iv) The well known incomplete procedure need not be solved self-consistently, a differential equation (15) may be solved instead.

1. INTRODUCTION

We have previously proposed /1/ and elaborated /2/ the complete+) procedure for evaluation of the screening length, λ, that takes into account that, besides the distribution function, f, vs. doping level N dependence (through the Fermi level $\eta \equiv E_F/kT = \eta(N)$), the density of states vs. λ and N (through the standard deviation σ) dependence $\rho = \rho(E;\lambda,N)$ also exists in heavily doped semiconductors. Thus we arrive to the integro-differential equation (with $Y' = dY/d\eta$, $Y''=d^2Y/d\eta^2$)

$$N'' \cdot \int f \frac{\partial \rho}{\partial \lambda} dE = 2(N')^{3/2} \sqrt{\lambda_o} \left[N - \int f^2 \rho dE + N' \left(\int f \frac{\partial \rho}{\partial N} dE - 1 \right) \right] \qquad (1)$$

where we used

$$\lambda^{-2} \equiv \lambda_o \frac{dn}{d\eta} \approx \lambda_o N', \qquad \lambda_o = e^2/\varepsilon\varepsilon_o k_o T \qquad (2)$$

and also

$$f' \equiv \frac{df}{d\eta} = f(1-f), \quad f_{d,c} = \left[1 + K_{d,c} \, e^{E/k_o T - \eta} \right]^{-1} \qquad (3)$$

where indices d and c correspond to impurity and conduction bands.

Taking the appropriate models for σ_d and σ_c (e.g. (4a) and (4b)), and performing the analytical differentiation, $\partial\rho/\partial N$ and $\partial\rho/\partial\lambda$, we have solved eqn.(1) in /2/ (details will be presented elsewhere /3/).

2. DISCUSSION ON SOME PROBLEMS

We shall here discuss on 4 problems arising when solving eqn.(1): the limited validity of models for σ (Ch.2.1), choice of the normalizing factor κ (Ch.2.2),

+) The values obtained by the complete procedure shall be indexed with "co", and those by the incomplete one by "in".

and the determination of boundary conditions for (1) (Ch.2.3). Finally, we shall give a method for $\lambda(N)$ determination from the differential equation by the incomplete procedure (Ch.2.4).

2.1.- The limited validity of models for σ

The mostly used models for σ are those of Kane and Morgan, /4/ and /5/, that use the standard deviations

$$\sigma_{eff} = 1.03\ \sigma_o\ e^{-R_x/\lambda} \quad \text{and} \quad \sigma = \sigma_o\ e^{-r_o/\lambda} \tag{4a,b}$$

for impurity and conduction bands, where the expressions

$$R_x^{-1} = C_3'\sqrt{\lambda N} + C_3 N^{\alpha_K} \quad \text{and} \quad r_o \approx a/2,\ (\sigma_o + C_2 N^{\alpha_K}), \tag{5a,b,c}$$

simulate the scewness of the d-band, i.e. take into account that in a sphere of radius r_o there is no scattering ion, which provides the convergence of integration when evaluating f for the distribution "tail".

Using the δ-model /2/, with f calculated from (3b), we get the following asymptotic expressions for the screening length (for $G \gg 1$)

$$\lambda_{co} \cong \lambda_{nd}\, F_{co}(y;K,\kappa) \to C_{\kappa K}^{co} N^{-\beta_\kappa^{co}}, \text{ and } \lambda_{in} = \lambda_{nd}\, F_{in}(y;K,\kappa) \to C_{\kappa K}^{in} N^{-\beta_\kappa^{in}} \tag{6a,b}$$

where, with $\phi = E_d/k_oT - \eta$, $G = N/N_{cd}$ and $N_{cd} = N_c\, exp(E_d/kT)$ (7a,b)

$$y \equiv e^{-\phi} = \frac{1}{2}(\sqrt{b^2+4GK} - b), \text{ with } b = K + (\kappa-1)G \tag{8a,b}$$

and $\lambda_{nd} = \sqrt{1/\lambda_o N}$ is the nondegenerate semiconductor ($G \ll 1$) screening length, while "→", as in (4-5) denotes the asympthotic values for large $N(G \gg 1)$. In this case, using the asympthotic values from (8) in (6), we first evaluate the exponents in (6) and subsequently in (5), as given in T1. It is obvious, for physical reasons that the standard deviation has to increase with increasing N, the case (co, $\kappa=2$)

The exponents α_κ and β_κ from (6) and (7) Table T 1

Procedure	β_κ		α_κ		γ_κ		For n-Si at 300 K
	$\kappa=1$	$\kappa=2$	$\kappa=1$	$\kappa=2$	$\kappa=1$	$\kappa=2$	
in-incompl.	1/4	1/2	3/8	1/4	-1/8	1/4	λ_o = 636 Å
co-complete	1/2	1	1/4	0	1/4	1/2	N_{cd} =5.23·10^{18}cm^{-3} E_d ≅ -44 meV

is meaningless, because here we have $\alpha_\kappa=0$ ($\sigma_o = const$), which is one of the reasons that this case is not physically real (see also Ch.2.2), although $\beta=1$ is acceptable for evaluation of λ.

It is straightforward to differentiate σ and σ_{eff} by N, and, using the condition that they are positive or zero, we get

$$N_\sigma^{\alpha_\kappa} \le \frac{C_{\kappa K}}{2r_o}\left(\frac{1}{\beta_\kappa} - 1\right) \quad \text{and} \quad N_{\sigma_{eff}}^{\alpha_\kappa} \le \frac{1-\beta_\kappa}{2\beta_\kappa C_4} \tag{9a,b}$$

with

$$C_4 = 1/C_3 C_{\kappa K} = 1/6\ C_{\kappa K}^{3/2},\ \gamma_\kappa = \beta_\kappa - \alpha_\kappa \text{ and } \alpha_\kappa = (1-\beta_\kappa)/2 \tag{10a,b,c}$$

Using the values from T1, and r_o = 1 Å and β_κ = 1/2, we get

$$C_{\kappa K}^{in} = \sqrt{2}/\lambda_o = 2C_{\kappa K}^{co}\ ,\ N_\sigma \lesssim 2\cdot 10^{20} \text{ and } N_{\sigma_{eff}} \lesssim 6.3\cdot 10^{17} cm^{-3} \qquad (11a,b,c)$$

where the sign of equality corresponds to the maximum. As one can see from Fig.1, the agreement with (11c) is very good. The decrease of σ_{eff} (and σ) with further increase of N lacks a physical explanation, and is a consequence of inadequacy of the used model, especially for $N_{\sigma_{eff}}$.

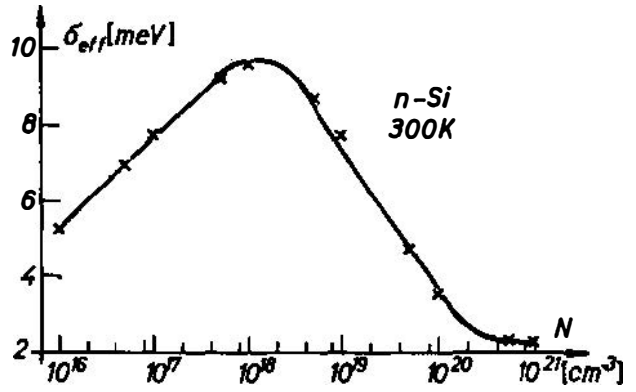

Fig.1.- $\sigma_{eff}(N)$, calculated exactly in /6/, and from data in T1.

2.2.- The normalizing factor (κ) and the spin degeneracy factor (K)

Using the co-model and κ=2, the asympthotic value of b is found to be equal to G, and for y in (8a) we get

$$y = K = e^{E_d/k_oT - \eta}\ ,\ \therefore\ \eta \equiv \frac{E_F}{k_oT} = \frac{E_d}{k_oT} - ln\ K \text{ for } N>>N_{cd} \qquad (12)$$

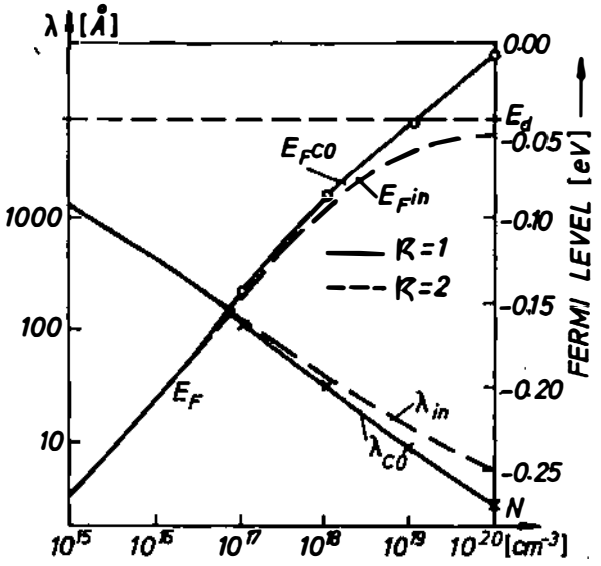

Fig.2. λ and E_F vs. N dependence for κ=2 /7/ and for κ=1.

and for $K=1$ (which was used by us /7/ and many other researchers, e.g. /8/), we find that E_F cannot cross the donor level (E_d), which also lacks physical explanation, and therefore is another reason that κ=2 should be rejected. The asymphtotic limit $E_F \to E_d$ is found by numerical calculations as well (Fig.2). Results for κ=1 are also depicted in Fig.2, and one can see that E_F has no "saturation" here. The third reason is that the number of states is $\int \rho_d dE = \kappa N$, and not $2N$, if we consider the number of electrons that the impurity band can supply. It may be shown that the choice of K_d in (3) is not very critical (both 1 and 1/2 can be used), but, certainly $K_c = 1$.

2.3.- The boundary conditions for eqn.(1)

For small N, i.e. $e^{\eta} \ll 1$, eqn.(1) reduces to

$$N'' \frac{I_{67}(N)\cdot N^{3/4}}{C_5(N')^{11/8}} = N - N'\left(1-2\frac{I_{67}N^{-1/4}}{C_5(N')^{3/8}}\right) \qquad (13)$$

and for $N_{in} = N_c e^{\eta} = N'_{in}$, from (13) $N''_{in} = 2N_{in}$ (!) would follow, instead of $N''=N$. Therefore, it is necessary to introduce a correction /2/ ("in" for initial)

$$N'_{in} = N_{in}(1+\varepsilon_N) \text{ or } \lambda_{in} = \lambda_{nd}\left(1-\frac{\varepsilon_N}{2}\right), \quad \varepsilon_N = \frac{I_{67}}{C_5 N_{in}^{5/8}} \qquad (14)$$

that provides $N''_{in} = N_{in}$. The results for λ_{co} in Fig.2 are actually obtained from (14).

2.4.- Reduction of the incomplete procedure to solving of a differential equation

In this case $\rho \neq F(N)$, which is not physically correct, but if we put ρ', $\partial\rho/\partial\lambda$, $\partial\rho/\partial N = 0$ anyway, it follows from (1) that the expression in brackets $[\ldots]=0$, or simply

$$N' = N - \int f^2 \rho dE, \quad \text{with} \quad N = \int f\rho dE = F(\eta, N, N'). \qquad (14a,b)$$

It is conventional to solve (14a) and (14b) self-consistently, see e.g. /8/,/7/,/1/; (14b) and (14a) cannot be solved as a first order differential equation, because N' appears in an implicite manner. However, if we differentiate (14a) once more, we get, with $\rho' = 0$ and (3a):

$$N'' = N' - 2\int ff'\rho dE = \ldots = 3N' - 2N + 2\int f^3 \rho dE, \qquad (15)$$

where N'' appears explicitely, as in (1), and may be solved numerically (e.g. by Runge-Kutta method). This procedure has an advantage of being more simple than the self-consistent one.

3.- CONCLUSION

We have shown that σ and σ_{eff} starts to decrease with increasing donor density N, if one uses (4a) and (4b), representing a significant principal disadvantage of the model. The normalizing factor in $\int \rho_d dE = \kappa N$ should be $\kappa=1$. If one would take $\kappa=2$, the complete procedure would give $\sigma_{eff}=const$, $E_F \to E_d$ for large values of N. When solving (1), the boundary conditions in the low doping limit cannot be taken as $N_{in}=N_c e^{\eta}=N'_{in}$, because $N''_{in}=2N_{in}$ would follow, and the correction ε_N (14) should be used.

We have also proposed to use solving of a differential equation (15) within the incomplete model, being a more simple procedure than the self-consistent one.

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