AN ANALYSIS OF APPLICABILITY OF LINEAR SCREENING THEORY IN DOPED SILICON

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ABSTRACT - Investigation of doped semiconductor characteristics generally uses the linear screening theory of particular scattering centers based on the possibility of the Poisson's equation linearization. This paper checks the correctness of the applicability of this theory to a doped noncompensated Si. It is concluded that the linearization may be applied in the region of light doping while at higher impurity concentration one should take care of the nonlinear screening.

1. INTRODUCTION

The ever increasing requests for an accurate calculation of the relaxation time due to electron and hole scattering on the charged impurity donors and acceptors, as well as the state densities an a doped semiconductor require the corresponding accuracy in the screening length calculation. This is particularly interesting in the case of heavily doped semiconductors. In literature one can encounter the connection between the idea of heavy doping and the fulfilment of inequality $R > r_s$, $na^3 \gg 1$, $nR^3 \gg 1$. (Here, R is the screening length, r_s is the distance between impurity ions, a - Bohr's radius, n - free carrier concentration).

The expressions used to determine this parameter are based on the linearization of the Poisson's equation. However, the particularity of Si is in relatively high electron effective mass that brings into doubt the fulfilment of the linearization condition.

The objective of this paper is in the attempt of more precise calculation of the screening length in a doped noncompensated Si at T=300 K, and impurity concentration in the range from 10^{15} to 10^{20} cm^{-3}. Based on the obtained results an analysis of the applicability of the linear screening theory in a doped Si as well as the correctness of the heavy doping definition through the relation $R>r_s$, $na^3>>1$ and $nR^3>>1$, was done.

2. SCREENING LENGTH CALCULATION

In the noncompensated semiconductor the general expression for the screening length calculation is [1]

$$R^{-2} = \frac{e^2}{\varepsilon\varepsilon_o}\frac{dn}{dE_f}, \tag{1}$$

where E_f is Fermi level energy, e electron charge, ε relative dielectric constant of the material, ε_o dielectric constant of vacuum.

Taking into account that the carrier concentration at T=300 K is defined by equation [2]

$$N \simeq n = \int f\rho(E)dE \tag{2}$$

and $\partial f/\partial E_f = -\partial f/\partial E$, equation (1) under condition that the state density does not depend on the impurity concentration N gives

$$R^{-2} = \frac{e^2}{\varepsilon\varepsilon_o}\int -\frac{\partial f}{\partial E}\rho(E)dE. \tag{3}$$

However, in a heavily doped semiconductor, state density depends not only on the screening energy but on the screening length too, as well as on the impurity concentration. In that case the equation (1) becomes

$$R^{-2} = \frac{e^2}{\varepsilon\varepsilon_o}\left[\int -\frac{\partial f}{\partial E}\rho(E,N,R)dE + \int f\,\frac{\partial\rho(E,N,R)}{\partial E_f}dE\right]. \tag{4}$$

General expression for the screening length given by equation (1) is the consequence of the Poisson's equation linearization which is possible under condition that in all points of the potential well, potential energy is less than Fermy energy, that is

$$E_f >> E_p = \frac{e^2}{4\pi\varepsilon\varepsilon_o R} , \qquad (5)$$

and Fermi energy is calculated like in metals, i.e. upward from the bottom of the conduction band and is of the order of $E_f = \hbar^2 N^{2/3}/m^*$, where m* is an effective electron mass. Only fulfilling this condition inhomogeneity of the state density may be considered to be weak. In noncompensated semiconductors it is generaly considered that this condition is fulfilled. Then its fulfilment in the region of heavy doping is connected with the fulfilment of the conditions $na^3>>1$ and $nR^3>>1$.

The principle consequences of the linear screening theory are:

1) The screening length do not depend on the magnitude of Coulomb's potential and is determined by the concentration of free electrons and their effective mass,

2) The screening of each charged ion is done independently of other ions.

3. NUMERICAL RESULTS AND DISCUSSIONS

Determination of the screening length in doped semiconductors is complicated by the fact that there are four mutually dependent parameters: impurity concentration, Fermi energy, state density and screening length. In paper [3] we worked out a self-consistent model to determine screening length and Fermi energy including equations (2) and (3).

Fig. 1 shows the screening length in phosphorus doped Si at T=300 K in function of impurity concentration. For comparison, there were shown the values calculated according to (1) and (3), as well as according to the well-known expressions for metals and nondegenerated semiconductors. Besides, the figure shows Bohr's radius and the distance between impurity ions, r_s. One can also see the errors that might appear using improper expressions. In addition to this the obtained results show that in a heavily doped Si screening length is <u>less</u> and not greater than the distance between impurity ions. At the observed impurity concentration none of the formal conditions of heavy doping is fulfilled, and therefore the correctness of the screening theory

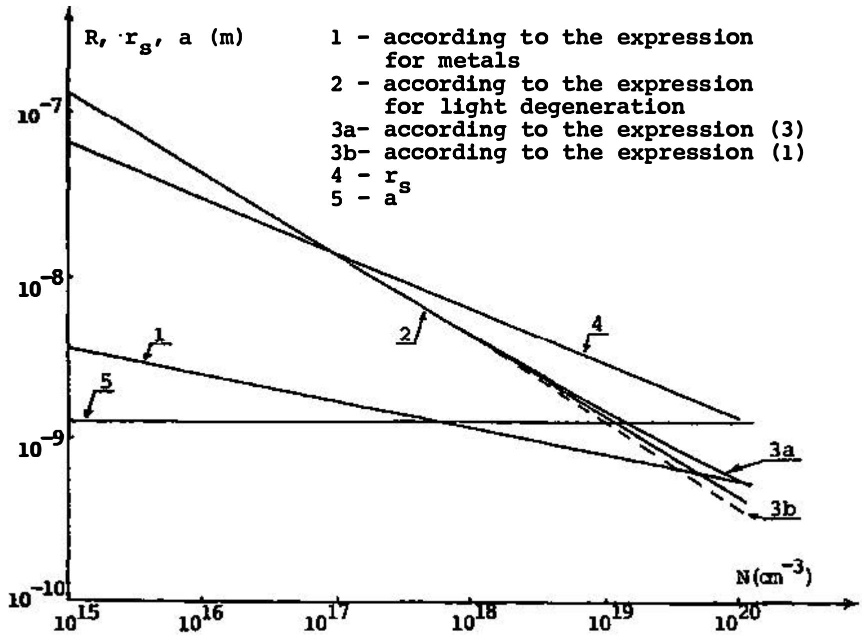

Fig.1 Screening length dependence in function of impurity concentration

applicability under such conditions is doubtful. We checked the fulfilment of the linearization condition given by equation (5). The obtained results showed that this condition is fulfilled only in the regions of light and medium doping up to the concentrations of the order of $10^{18}cm^{-3}$ while higher concentrations disturb the equation (5). Thus, at $N=5\cdot10^{19}cm^{-3}$ the Fermi energy is 25 meV while potential well energy for the same concentration is 505 meV.

To obtain more accurate data on the screening length value we tried to realize the equation to calculate R in a general form (1). Analytic solution of this equation does not exist due to the mutual connection among a number of parameters defining the concentration of free carriers and Fermi energy. The use of the numerical differentiation gave the results which are in a very good agreement with the results obtained using the equation (3). The difference appears above the concentration of the order of 10^{18} cm^{-3} and does not exceed 20 % at $N=10^{20}cm^{-3}$, when one obtains the values less than those obtained with the equation (3). This means that this approach as well leads to a conclusion that linearization condition is not fulfilled. It also makes doubtful the supposition that the screening of each ion is done independently of other ions. In the region where the screening length becomes smaller than the Bohr's radius the ionized impurity atom cannot be observed as a point charge. In addition to this, at such small distances the macroscopic dielectric constant loses its sense. Therefore, the obtained results point to the necessity of using the phenomenon of the impurity ion clusters in heavily doped Si.

The calculations done showed that in a doped Si formal criteria of heavy doping are not fulfilled. However, from the point of view of physical processes this region rather belongs to the region of heavy doping [4]. Besides, in a doped Si it should avoid the use of the expressions based on the fulfilment of formal conditions of heavy doping. So, for example, [5] gives an analysis of impurity band in heavy doped semiconductors including the fulfilment of the condition $R>r_s$ which brings into question the applicability of the given theory to Si.

4. CONCLUSION

The particularity of Si reflected in a relatively high effective mass may bring into doubt some theories and analyses of doped semiconductors based on the fulfilment of the relations $R>r_s$, $na^3>>1$, $nR^3>>1$, because none of them is fulfilled in Si.

The screening length values calculated according to (1) and (3) are in a very good agreement. They bring about the unsatisfaction of the Poisson's equation linearization condition. The obtained results point to the necessity of using the phenomenon of impurity ion clusters in heavily doped Si.

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