BAND TAILING IN STRONGLY DOPED SEMICONDUCTORS

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The problem of the density of states of deep fluctuation levels in a semiconductor doped by fine donors and acceptors is considered with allowance for Debye screening. The dependence is found of the leading term of the logarithm of the density of states and of the electron localization radius $1/\alpha$ on ionization energy E, for different values of parameter $\delta = N_d r_0^4 / a_B$, where N_d is the donor population, r_0 is the screening radius, and a_B is the Bohr radius of an isolated doping-material atom. It is clarified that the form of the distribution of doping-material electrons in an optimal fluctuation, the potential energy of an electron in an optimal well, and consequently, also the density of states of deep fluctuation levels are highly dependent on the screening radius r_0.

The question of band tailing in semiconductors doped by fine atom materials was examined by the method of optimum fluctuations [1] by Shklovskii and Efros [2]. Results were obtained for the innermost levels on the assumption that the potentials produced by the individual doping-material ions are not screened. The present paper considers the same problem with allowance for screening, on assumption of Debye screening. It is assumed that the semiconductor has been doped by donor and acceptor materials. For definiteness, we shall consider the inner donor states. As in the paper by Shklovskii and Efros [2], the calculations will be performed within the framework of the effective-mass technique, with reference to levels with ionization energy E, which is significantly smaller than the energy of the forbidden zone E_g. In accordance with the technique of Lifshits [1], the excess density of doping-material atoms at optimum fluctuation $\tilde{\xi}_d(\mathbf{r})$ and $\tilde{\xi}_a(\mathbf{r})$, can be calculated from the formulas:

$$\tilde{\xi}_d(\mathbf{r}) = N_d \left\{ \exp\left[\beta \int |\psi(\mathbf{r}')|^2 v_d(\mathbf{r} - \mathbf{r}')\, d\mathbf{r}' \right] - 1 \right\}, \quad (1)$$

$$\tilde{\xi}_a(\mathbf{r}) = N_a \left\{ \exp\left[\beta \int |\psi(\mathbf{r}')|^2 v_a(\mathbf{r} - \mathbf{r}')\, d\mathbf{r}' \right] - 1 \right\}. \quad (2)$$

Here subscripts d and a pertain to donors and acceptors, respectively: N_d and N_a are the donor and acceptor populations, β is an indeterminate Lagrangian factor, introduced by Lifshits [1], $\psi(\mathbf{r})$ is the wave function of an electron in the primary state of an optimal potential well; $v_{da}(\mathbf{r}-\mathbf{r}')$ is the potential energy of an electron in the field of an individual charged donor or acceptor.

Wave function $\psi(\mathbf{r})$ is defined approximately by a variational method, similarly to the manner in which this is done by the present author in [3]. The exact

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wave function $\psi(\mathbf{r})$ should realize the extremum of the functional

$$J'[\psi] = S\{\tilde{\xi}_d[\psi],\ \tilde{\xi}_a[\psi]\} + \beta \int \psi^*(\mathbf{r})\,\hat{H}[\psi]\,\psi(\mathbf{r})\,d\mathbf{r} =$$
$$= \int \left\{(N_d + \tilde{\xi}_d[\psi]) \ln \frac{N_d}{N_d + \tilde{\xi}_d[\psi]} + \tilde{\xi}_d[\psi]\right\} d\mathbf{r} + \tag{3}$$
$$+ \int \left\{(N_a + \tilde{\xi}_a[\psi]) \ln \frac{N_a}{N_a + \tilde{\xi}_a[\psi]} + \tilde{\xi}_a[\psi]\right\} d\mathbf{r} + \beta \int \psi^*(\mathbf{r})\,\hat{H}[\psi]\,\psi(\mathbf{r})\,d\mathbf{r}$$

at the additional conditions

$$\int |\psi(\mathbf{r})|^2 d\mathbf{r} = 1,$$
$$E = \int \psi^*(\mathbf{r})\,\hat{H}[\psi]\,\psi(\mathbf{r})\,d\mathbf{r}. \tag{4}$$

Here

$$\hat{H}[\psi] = -\frac{\hbar_2}{2m}\Delta + \int [\tilde{\xi}_d(\mathbf{r}')\,v_d(\mathbf{r}-\mathbf{r}') + \tilde{\xi}_a(\mathbf{r}')\,v_a(\mathbf{r}-\mathbf{r}')]\,d\mathbf{r}',$$

whereas $\tilde{\xi}_d[\psi]$ and $\tilde{\xi}_a[\psi]$ are defined by Eqs. (1) and (2).

Let us assume that wave function $\psi(\mathbf{r})$ has the simple hydrogen-like form:

$$\psi(r) = \sqrt{\frac{\alpha^3}{\pi}}\, e^{-\alpha r}, \tag{5}$$

where α is the varied parameter.

Substituting Eq. (5) into (1) and (2), and assuming that

$$v_{d,a}(\mathbf{r}-\mathbf{r}') = \mp \frac{z_{d,a}e^2}{\varepsilon|\mathbf{r}-\mathbf{r}'|} \exp\left(-\frac{|\mathbf{r}-\mathbf{r}'|}{r_0}\right), \tag{6}$$

we obtain

$$\tilde{\xi}_d(\mathbf{x}) = N_d \left\{\exp \frac{t'}{x}\left[e^{-x/\alpha'} - \left(1 + x\left(1 - \frac{1}{4(\alpha')^2}\right)\right)e^{-2x}\right] - 1\right\}, \tag{7}$$

$$\tilde{\xi}_a(\mathbf{x}) = N_a \left\{\exp\left(-\frac{t' z_a}{x z_d}\left[e^{-x/\alpha'} - \left(1 + x\left(1 - \frac{1}{4(\alpha')^2}\right)\right)e^{-2x}\right]\right) - 1\right\}, \tag{8}$$

where

$$\alpha' \equiv \alpha r_0,\ \mathbf{x} \equiv \alpha r,\ t' \equiv -16\beta z_d e^2 \alpha^5 \varepsilon^{-1}\left[4\alpha^2 - \frac{1}{r_0^2}\right]^{-2}. \tag{9}$$

With reference to deep donor levels with ionization energy $|E| \gg W_B$, we assume that the optimal fluctuation is such that condition $\tilde{\xi}_d \gg N_d$ is satisfied in its center. As follows from Eqs. (7) and (8) this also means that $t' \gg 1$, $\tilde{\xi}_a \ll N_a$, and, consequently, also $\tilde{\xi}_a \ll \tilde{\xi}_d (N_a \lesssim N_d)$.

Similarly to [3], we replace in the subsequent calculations Eqs. (7) and (8) by their simplified equivalents:

$$\tilde{\xi}_d(\mathbf{x}) \approx N_d \exp[t(1 - ax)],$$
$$\tilde{\xi}_a(\mathbf{x}) \approx 0, \tag{10}$$

where

$$t \equiv t'(A - 0{,}5B); \quad a = -B(A - 0{,}5B)^{-1};$$

$$A = \frac{1}{x_0}\left[e^{-x_0/\alpha'} - e^{-2x_0}\left[1 + x_0\left(1 - \frac{1}{4(\alpha')^2}\right)\right]\right];$$

$$B = \frac{1}{x_0^2}\left[-\left(1 + \frac{x_0}{\alpha'}\right)e^{-x_0/\alpha'} + e^{-2x_0}\left[(x_0+1)^2 + x_0^2\left(1 - \frac{1}{2(\alpha')^2}\right)\right]\right].$$

A and B are coefficients of the Taylor-series expansion of the argument of exponent (7) at point $x_0 = 0.5$. It can be shown that the relative error Δ, arising subsequently in calculating energy E and "entropy" $S\{\tilde{\xi}\}$ when using approximate expressions (10), can be estimated from the formula:

$$\Delta \sim \alpha' t' (at)^2 \exp\left[-\left(\frac{3}{\alpha'} + t\right)\right],$$

here $0{,}3 < a < 0{,}5$.

Substituting Eqs. (5), (6) and (10) into equation $\delta J'[\psi] = 0$ with consideration of Eqs. (3) and (9), we obtain, similarly to [3], an expression for α':

$$(1 + 2\alpha')^3\left\{(\alpha')^3 + \frac{32\pi e^t}{(at)^3}\delta\left[\frac{6(at)^2 + 8(at) + 4}{(at+2)^4}\right]\right\} = \frac{32\pi e^t}{(at)^3}\delta(\alpha')^2(2\alpha' + 3), \qquad (11)$$

where $\delta \equiv \frac{N_d r_0^4}{a_B}$.

Then from Eq. (4) we find for ionization energy E:

$$-\eta \equiv \frac{E}{\hbar/2mr_0^2} = (\alpha')^2 - \frac{64\pi e^t}{(at)^3}\delta\left[\frac{1}{(1+2\alpha')^2} - \frac{2(at+1)}{(at+2)^3(\alpha')^2}\right]. \qquad (12)$$

Using Eqs. (7) and (10), we obtain for S

$$S\frac{r_0}{a_B} = -\frac{4\pi e^t}{(\alpha')^3}\delta\left\{t'\left[\frac{1}{(at + 1/\alpha')^2} - \frac{at+4}{(at+2)^3}\right] - \frac{2}{(at)^3}\right\}. \qquad (13)$$

Equations (11)-(13) make it possible to determine the nondimensional localization radius of the electron $1/\alpha r_0 = 1/\alpha'$ and the quantity S (and thus also the density of states $\rho(E)$ with exponential accuracy of $\rho(E) \sim \exp[S(E)]$). The applicable graphs are given in Figs. 1 and 2.

Our results show that the distribution of doping-material atoms in optimal fluctuation with a given energy of the fundamental state depends significantly on r_0. Figure 3 depicts curves of the nondimensional excess density of doping-material atoms $\tilde{\xi}_d(r)/N_d$ and the potential energy of the electron V(r) on the distance from the center of fluctuation r for two optimal fluctuating potential wells. In both cases reference is had to a material with parameters of germanium at $N_d = 10^{18}$ cm^{-3} for the same fundamental-state energy E of -0.063 eV; however, the former curves were calculated for $r_0 = 3.16 \cdot 10^{-7}$ cm, whereas the latter at $r_0 = 7.96 \cdot 10^{-7}$ cm. The probabilities of realization of such fluctuations are substantially different: in the first case S = -19.8 and in the second S = -10, i.e., the corresponding densities of states differ more than by four orders of magnitude. These results allow the assumption that screening must be taken into account in this problem. As was shown by the present author [3], these results are in agreement with those of Shklovskii and Efros [2] in the case of maximum ionization energies. As follows from Eqs. (11), (12) and (7), the limit transition $E \to -\infty$

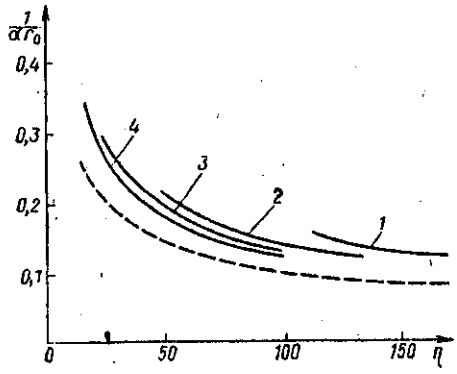

Fig. 1

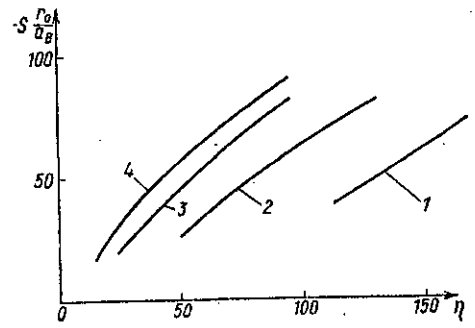

Fig. 2

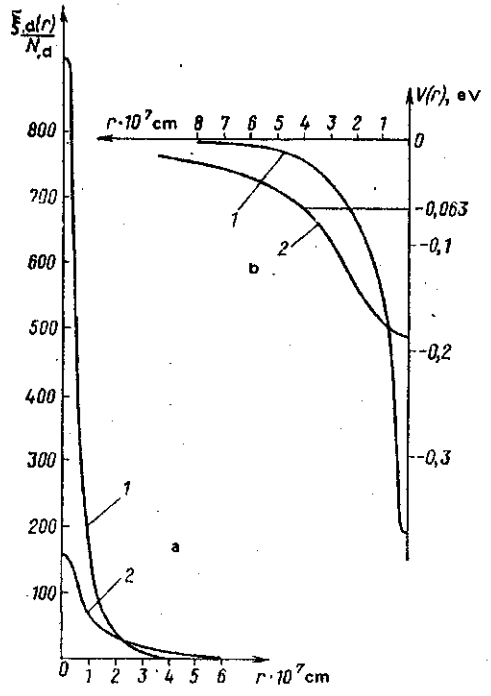

Fig. 3

Fig. 1. Nondimensional electron localization radius $1/ar_0$ vs. energy $-\eta = \frac{E}{\hbar^2/2mr_0^2}$. The dashed curve corresponds to: 1) $1/ar_0 = 1\sqrt{|\eta|}$. $\delta = 10$; 2) 3; 3) 1; 4) 0.5.

Fig. 2. Plot of Sr_0/a_B vs. nondimensional energy $-\eta = \frac{E}{\hbar^2/2mr_0^2}$. For legend see Fig. 1.

Fig. 3. Excess density of donor atoms $\tilde{\xi}_d(r)$ vs. distance r from the center of fluctuations (a). Potential energy of the electron V(r) vs. r (b). 1) $r_0 = 3.16 \cdot 10^{-7}$ cm; 2) $7.96 \cdot 10^{-7}$ cm.

simultaneously means that $t \to \infty$, $t' \to \infty$ and $\tilde{\xi}_d(0) \to \infty$. The value of $\tilde{\xi}_d(\mathbf{r})$ within the framework of our assumptions cannot exceed a magnitude of the order of 10^{22}

cm^{-3} since interatomic repulsion sets on at such concentrations. Estimates based on Eq. (7) show that in the case of $N_d \sim 10^{18}$ cm^{-3} this is equivalent to the constraint that $t < 15$. An even more rigorous constraint follows from the conditions of applicability of the effective-mass technique: in a material with parameters of germanium the limitation on the energy $|E| < 0.1$ eV is equivalent to $t < 8.25$ if $r_0 = 3.16 \cdot 10^{-7}$ cm and $t < 5.5$ if $r_0 = 10^{-6}$ cm. Shlovskii and Efros [2] showed that in the case of maximum energies the optimum cluster has a linear dimension significantly smaller than the electron localization domain. It follows from our results that the linear dimension of the optimal fluctuation can be comparable with the screening radius r_0. The doping-material atoms are not uniformly distributed over the cluster; the shape of the distribution changes smoothly with a rise in the ionization energy. All other conditions being equal, lower energies have corresponded to the more "smeared out" clusters, whereas higher energies have clusters more concentrated in the center. The change in the form of $\xi_d(\mathbf{r})$ with an increase in ionization energy can be followed with Eq. (7) by increasing t'.

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