PHYSICAL REVIEW B VOLUME 9, NUMBER 10 15 MAY 1974

Low-temperature limit of screening length in semiconductors

Frank Stern

IBM Thomas J. Watson Research Center, Yorktown Heights, New York 10598

(Received 5 February 1974)

The conventional result for the screening length in a semiconductor with a discrete impurity level vanishes at absolute zero. When level broadening is included in a self-consistent way, a finite value is obtained. Results for the screening length and the root-mean-square potential fluctuation at absolute zero are given as functions of the degree of compensation.

The screening length enters in many semiconductor problems including band bending near surfaces and junctions, scattering by Coulomb centers, and broadening of energy levels. We consider screening at low temperatures in a semiconductor in which the Fermi energy E_F lies near a discrete impurity level, here chosen to be an acceptor, taking level broadening into account self-consistently.

At temperatures low enough that few electrons are excited across the gap, the conventional screening length L is[1,2]

$$L=\{\epsilon KTN_A/e^2[N_Ap+(N_D+p)(N_A-N_D-p)]\}^{1/2}, \qquad (1)$$

where p is the hole concentration, $\epsilon=\kappa\epsilon_0$ is the dielectric permittivity, K is Boltzmann's constant, T is the absolute temperature, and N_A and N_D are the acceptor and donor concentrations, respectively, with $N_A>N_D$.

When all impurities are ionized, i.e., $p=N_A-N_D$, the screening length equals the conventional result $(\epsilon KT/e^2p)^{1/2}$. At low temperatures, where $p\sim 0$,

$$L=[\epsilon KTN_A/e^2N_D(N_A-N_D)]^{1/2}, \qquad (2)$$

which is perhaps less familiar. Note that the screening in the low-temperature limit is produced by changes in the occupation of the majority impurity center.

The screening length in Eq. (1) is derived with the assumption of a sharp acceptor level. But the Coulomb potentials associated with the ionized impurities lead to potential fluctuations whose root-mean-square value when the impurities are randomly spaced is[3]

$$\sigma=(e^2/\epsilon)[(N_D^+ + N_A^-)L/8\pi]^{1/2}, \qquad (3)$$

where N_D^+ and N_A^- are the concentrations of ionized donors and acceptors, respectively. Thus the acceptor level will be broadened into a band with a density of hole states given approximately by[3]

$$\rho_h(E)=[N_A/\sigma(2\pi)^{1/2}]\,e^{-(E-E_A)^2/2\sigma^2}, \qquad (4)$$

where E_A is the center of the broadened acceptor level. Note that odd moments of the distribution of levels vanish at very low temperatures because $N_D^+=N_D=N_A^-$ and $n=p=0$.

When $\sigma>KT$, the assumption of a sharp acceptor level used in deriving Eq. (1) is no longer valid and the screening length is given by

$$L=\left(\frac{e^2}{\epsilon}\int_{-\infty}^{\infty}\rho_h(E)\frac{df_h}{dE}\,dE\right)^{-1/2}, \qquad (5)$$

where $f_h(E)=\{1+\exp[(E_F-E)/KT]\}^{-1}$ is the probability that a state of energy E be occupied by a hole. This relation also applies when the level broadening is so large that the impurity level has merged with the adjacent band edge, a case that has been widely studied.[4,5] The considerations of the present paper apply only when the level broadening is small compared to the energy separation of the majority impurity level and the adjacent band edge. We also ignore the energy levels associated with placing a second hole on an acceptor.[6]

Equations (3)–(5) must be solved self-consistently for L and σ, with the subsidiary condition

$$N_A-N_D=\int_{-\infty}^{\infty}\rho_h(E)f_h(E)\,dE \qquad (6)$$

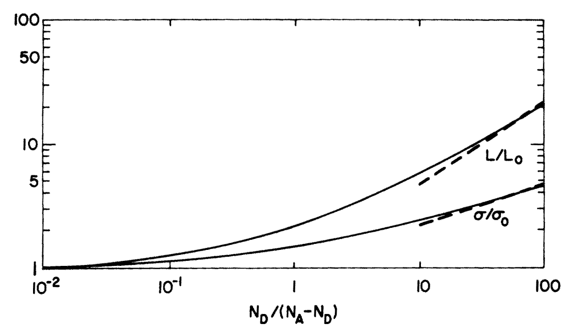

FIG. 1. Self-consistent screening length L and root-mean-square level broadening σ at absolute zero for a p-type semiconductor. See Table I for definitions and for the approximate expressions which give the dashed lines in the figure. Small values of the abscissa correspond to weak compensation and large values to strong compensation.

TABLE I. Approximate analytic results for the screening length L and the root-mean-square level broadening σ at absolute zero for a p-type semiconductor with acceptor concentration N_A and donor concentration N_D. The results are given in terms of the quantities $L_0 = (8\pi^2 N_D)^{-1/3}$ and $\sigma_0 = (e^2/4\pi\epsilon)(8\pi)^{1/6} N_D^{1/3}$, where $\epsilon = \kappa\epsilon_0$ is the permittivity; mks units are used.

	L/L_0	σ/σ_0
$N_D \ll N_A$	1	1
$N_D \sim \frac{1}{2} N_A$	$(2\pi N_D/N_A)^{2/3}$	$(2\pi N_D/N_A)^{1/3}$
$N_A - N_D \ll N_A$	$[N_D/(N_A - N_D)]^{2/3}$	$[N_D/(N_A - N_D)]^{1/3}$

to fix the position of the Fermi level. The equations can be easily solved at absolute zero, and lead to the results shown in Fig. 1. Approximate values for the case of low compensation $N_D \ll N_A$, for compensation near 50%, and for the case of high compensation $N_A - N_D \ll N_A$, are given in Table I. We expect a smooth transition from the screening results given here for absolute zero to the conventional result in Eq. (1) in the temperature range $0 < KT < \sigma$. The case of perfect compensation, $N_D = N_A$, cannot be treated with this model, and other screening mechanisms must be sought.[7,8]

Falicov and Cuevas[9] treated the low-temperature screening problem without introduction level broadening explicitly. They obtained a correlation length $[8\pi(N_D - N_A)]^{-1/3}$ for an n-type sample. For the n-Ge sample considered in Figs. 1 and 3 of their paper,[9] with $N_D = 3.9\times10^{15}$ cm^{-3} and $N_A = 2.9\times10^{15}$ cm^{-3}, we find a screening length of 5.2×10^{-6} cm at $T=0$ while their result is 3.4×10^{-6} cm. Our value predicts less screening and therefore a lower mobility, and should give better agreement with the mobility at very low temperatures than their exponential correlation model with the correlation length they use. Our calculated rms fluctuation is $\sigma = 4$ meV at $T=0$ for this example. Thus we expect a transition from the low-temperature screening limit to the conventional value when $KT \sim \sigma$, i.e., near 40 K. This is consistent with Fig. 3 of Falicov and Cuevas, which shows the observed mobility approaching the conventional Brooks-Herring curve near 40 K.

The low-temperature screening problem is also covered in a paper by Morgan,[10] who used a self-consistent theory but introduced an additional length parameter $a = [3/4\pi(N_D + N_A)]^{1/3}$ into the theory. We believe an appropriate screening length is supplied by the self-consistent theory itself, as described here in the low-temperature limit.

A criterion for the validity of a linear screening model is that the number of screening sites within a sphere of radius L be greater than unity.[4] Since the minority carriers are always fully ionized at very low temperatures, we write this criterion in the form $\frac{4}{3}\pi N_A L^3 > 1$. It is marginally satisfied throughout the compensation range in Fig. 1.

We conclude that the screening length and the level broadening at absolute zero are easily obtained from the simple theory of linear screening, applied self-consistently. The model ignores local correlation effects, because the expressions for the screening length and for the potential fluctuations are averaged independently, but the predicted dependence of screening and level broadening at low temperatures on the concentrations of majority and minority impurities is expected to have at least qualitative validity.

I am indebted to P. J. Price for helpful comments.

---

[1] H. Brooks [in *Advances in Electronics and Electron Physics*, edited by L. Marton (Academic, New York, 1955), Vol. VII, p. 158] gives the result for n-type semiconductors.

[2] We use mks units. For cgs units, replace ϵ_0 by $1/4\pi$.

[3] T. N. Morgan, Phys. Rev. 139, A343 (1965).

[4] E. O. Kane, Phys. Rev. 131, 79 (1963).

[5] B. I. Halperin and M. Lax, Phys. Rev. 148, 722 (1966).

[6] See, for example, N. F. Mott and E. A. Davis, *Electronic Processes in Non-crystalline Materials* (Oxford U. P., London, 1971), Chap. 6.

[7] F. Stern, Phys. Rev. B 3, 3559 (1971).

[8] G. Neumark, Phys. Rev. B 5, 408 (1972).

[9] L. M. Falicov and M. Cuevas, Phys. Rev. 164, 1025 (1967).

[10] See Eqs. (27)–(29) of Ref. 3.