Mechanism for nonlinear impurity diffusion in semiconductors

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A simple model is proposed to explain the concentration dependence of the diffusion coefficient of ionized impurity atoms in semiconductors.

As we know, at high impurity concentrations N in a semiconductor the impurity diffusion is nonlinear; i.e., the diffusion coefficient depends on the concentration: $D = D(N)$. When silicon is doped with phosphorus to $N = 10^{21}$ cm^{-3}, for example, D increases by about an order of magnitude from the value (D_0) corresponding to a low concentration.[1] Attempts have been made to explain the increase in the diffusion coefficient in terms of an effect of an internal accelerating field.[2] It becomes important to take this field into account when N exceeds the carrier density in the intrinsic semiconductor, n_i, at the diffusion temperature. That mechanism, however, explains only a doubling of the diffusion coefficient at $N \gg n_i$. A large number of models have now been proposed to explain the behavior[1] $D(N)$. All have been based on particular features of defect formation during the diffusion of some suitable impurity in a given semiconductor.

In this letter we propose a simple model which makes it possible to calculate the concentration dependence of the diffusion coefficient. A decisive aspect of this model is the incorporation of carrier degeneracy at $N > N_{c,v}$, where $N_{c,v}$ are the state densities in the c and v bands; this degeneracy has been ignored in the previous papers on this topic of which we are aware.

For definiteness we consider the diffusion of a donor impurity, under the assumption of strong degeneracy,

$$N \gg N_c , \qquad (1)$$

or, equivalently, a condition on the Fermi energy: $\epsilon_F \gg kT$. If the length scale Δx of the region in which the impurity is distributed is large in comparison with the Debye length,

$$\Delta x \gg L_g \sim (\epsilon \hbar^2 / e^2 m N^{1/3})^{1/2} , \qquad (2)$$

we have quasineutrality; i.e., the electron density satisfies $n \approx N$. An equilibrium is rapidly established in the electron subsystem, and from the condition that the chemical potential remain constant,

$$M = (3/8\pi)^{2/3} (2\pi\hbar)^2 \frac{N^{2/3}}{2m} - e\varphi = \text{const} , \qquad (3)$$

we can easily find an expression for the internal electric field $\mathbf{E} = -\Delta\varphi$. This field

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causes a drift of ionized impurity atoms. Using the Einstein relation between the mobility and the diffusion coefficient, we can write the drift flux density as follows

$$\mathbf{j}_{dr} = -(\pi/6)^{1/3}(N/N_c)^{2/3}D_0\nabla N. \tag{4}$$

Under inequality (1), j_{dr} exceeds the ordinary diffusion flux $j_{diff} = -D_0\nabla N$. It has thus been shown that incorporating degeneracy makes it possible to explain the pronounced nonlinearity of the diffusion on the basis of an internal electric field. We find $D(N) \propto N^{2/3}$. Here we are essentially talking about an ambipolar diffusion in a quasineutral plasma under conditions such that the higher-mobility component is degenerate. For a classical plasma in the corresponding situation, the ambipolar diffusion coefficient is $D = 2D_0$.

These estimates show that the nonlinearity mechanism proposed here must be taken into consideration in calculations of concentration profiles for the characteristic doping levels used in semiconductor-device manufacture (e.g., in heavily doped emitters in bipolar transistors). This nonlinearity should be manifested most clearly in GaAs, for which we would have $N_{c,v} \sim 10^{18}$ cm^{-3} at characteristic diffusion-annealing temperatures; the diffusion coefficient can increase by two orders of magnitude. In a quantitative comparison with experimental data, of course, one must not rule out the possibility of a simultaneous manifestation of other known nonlinearity mechanisms, particularly at high temperatures. The diffusion equation which corresponds to current (4) can be solved exactly for the problem of diffusion from an infinitesimally thin source.[3]

[1]S. M. Sze (editor), *Technology of Very-Large-Scale Integrated Circuits*, (Russ. Transl. Mir, Moscow, 1986).
[2]S. Zaromb, IBM J. Res. Dev. **1**, 57 (1957).
[3]Ya. B. Zel'dovich and A. S. Kompaneets, *Collection Celebrating the Seventieth Birthday of Academician A. F. Ioffe*, Izd. Akad. Nauk SSSR, Moscow, 1950.

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