

APPLICATION OF IRREVERSIBLE THERMODYNAMICS IN THE THEORY OF RECOMBINATION IN SEMICONDUCTORS

By

G. PATAKI

RESEARCH INSTITUTE FOR TECHNICAL PHYSICS OF THE HUNGARIAN ACADEMY OF SCIENCES,
BUDAPEST

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The exact statistical theory of the recombination via traps has been elaborated by W. SHOCKLEY and W. T. READ [1]. They defined the coefficients A_{ik} appearing in the "capture currents", near the equilibrium by

$$U_{cn} = A_{nn} \delta n + A_{np} \delta p, \quad (1)$$

$$U_{cp} = A_{pn} \delta n + A_{pp} \delta p$$

and gave the expressions

$$U_{cn} = \frac{f_{pt} n_0 C_n}{k} \frac{F_n - F_t}{T}, \quad (2)$$

$$U_{cp} = \frac{f_t p_0 C_p}{k} \frac{F_t - F_p}{T},$$

i. e. the relation between the "capture currents" and the quasi Fermi-levels (in the following we use the notations of paper [1]). On the basis of the above equations the theory of recombination can be formulated in terms of irreversible thermodynamics.¹ For the examination of the time dependence of the recombination we write down the equation of motion of thermodynamics in the form given by I. FÉNYÉS [2] and relating to homogeneous systems near the equilibrium. The equation of conduction (with the usual notations) is as follows:

$$I = LX, \quad (3)$$

where X means the general force and is defined by the equation

$$X = -g a \quad (4)$$

(a being the column vector formed from the extensive quantities: here from δn and δp ,

$$g_{ik} = - \frac{\partial^2 S(a_i, a_k)}{\partial a_i \partial a_k},$$

the symmetrical matrix formed from the entropy).

¹ Note added in proof. From the point of view of fluctuations K. M. VAN VLIET deals with a similar problem. Phys. Rev., **110**, 1, 1958.

Thus we have on the basis of the equations (3) and (4):

$$I = -Lg a .$$

On the other hand the relation between a and I holds as well (assuming homogeneity):

$$\dot{a} \equiv I ,$$

i. e.

$$\dot{X} = -gLX; \quad \dot{a} = -Lg a; \quad \dot{I} = -Lg I .$$

Let us now introduce the following correspondence, i. e. notation:

$$U_{ci} = -I_{ri}; \quad X_n = -\frac{F_n - F_l}{T} , \quad X_p = -\frac{F_l - F_p}{T} ; \quad (Lg)_{ik} = A_{ik} ,$$

while the conduction matrix becomes diagonal on the basis of the equation (2) and its diagonal elements are $L_{nn} = f_{pl} n_0 C_n/k$, $L_{pp} = f_l p_0 C_p/k$. Matrices $A = L.g$ and L are then known. From these g can be determined by simple calculations and according to expectation this appears as a symmetrical matrix. According to the above, the equation of motion of the recombination will be as follows:

$$\dot{X} = -AX, \quad \dot{a} = -A a, \quad \dot{I}_r = -A I_r .$$

These matrix equations mean for the components a differential equation of the second order (e. g. for a_i -s):

$$\ddot{a}_i + T(A) \dot{a}_i + D(A) a_i = 0 \quad (i = n, p) ,$$

where $T(A)$, resp. $D(A)$ mean the trace, resp. the determinant of the matrix A . Obviously, the form of the solution is

$$a_i(t) = C_{i1} e^{\lambda_r t} + C_{i2} e^{\lambda_l t} \quad (i = u, p) , \quad (5)$$

where λ_r and λ_l are the two roots of the characteristic equation

$$\lambda_r = \frac{-T(A) \left[1 - \sqrt{1 - \frac{4D(A)}{T(A)^2}} \right]}{2} ; \quad \lambda_l = \frac{-T(A) \left[1 + \sqrt{1 - \frac{4D(A)}{T(A)^2}} \right]}{2} .$$

The equations (5) and (6) describe the time dependence of the recombination

and the quantities $\tau_r = -\frac{1}{\lambda_r}$ resp. $\tau_l = -\frac{1}{\lambda_l}$ give the lifetimes. It is easy to see that expanded in a series in $\frac{4D(A)}{T(A)^2}$ we get in first approximation

$$\tau_r = -\frac{1}{\lambda_r} \doteq -\frac{T(A)}{D(A)} =$$

$$= \frac{\tau_{p0} \left[(n_0 + n_1) + N_l \left(1 + \frac{p_1}{p_0} \right)^{-1} \right] + \tau_{n0} \left[(p_0 + p_1) + N_l \left(1 + \frac{p_0}{p_1} \right)^{-1} \right]}{(n_0 + p_0) + N_l \left(1 + \frac{p_2}{p_0} \right)^{-1} \left(1 + \frac{p_0}{p_1} \right)^{-1}}, \quad (7)$$

i. e. the stationary lifetime given in paper [1].

For the lifetime τ_l we get in a similar approximation:

$$\tau_l = -\frac{1}{\lambda_r} \doteq -\frac{1}{T(A)} =$$

$$= \frac{\tau_{p0} \tau_{n0} N_l}{\tau_{p0} \left[\left(1 + \frac{p_1}{p_0} \right)^{-1} N_l + (n_0 + n_1) \right] + \tau_{n0} \left[\left(1 + \frac{n_1}{n_0} \right)^{-1} N_l + (p_0 + p_1) \right]}, \quad (8)$$

which describes a considerably quicker relaxation process than τ_r and corresponds to the filling of the traps.

Summing up what has been said, on the basis of the equations (1) and (2) the irreversible thermodynamic formulation of the recombination is given. From the point of view of irreversible thermodynamics the interesting case occurs where Onsager's cross effect does not appear (L -diagonal), nevertheless, because of the matrix g being off-diagonal, the cross effect found in paper [2] may appear (A off-diagonal).

The non-stationary lifetime τ_r is given and it renders in first approximation the stationary lifetime given in [1]. We have pointed out the mechanism of recombination, giving the relaxation time of the time dependence of the filling of the traps. This relaxation time was given first by D. SANDIFORD [3]. This term may possibly play a part in the time dependence of luminescent phenomena.

REFERENCES

1. W. SHOCKLEY and W. T. READ, Phys. Rev., **87**, 5, 1952.
2. I. FÉNYES, Acta Phys. Hung., **11**, 131, 1960.
3. D. SANDIFORD, Phys. Rev., **105**, 2, 1957.