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MONTE-CARLO CALCULATION OF IONIZATION COEFFICIENTS IN SEMICONDUCTORS

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Abstract: The ionisation coefficients in semiconductors are calculated by using Monte-Carlo method on the basis of the following assumptions:
— isotropic effective masses of carriers,
— isotropic scattering,
— constant mean free path.
The results obtained differ slightly from the existing theoretical calculations. The agreement with experimental results is good. The method is also aplicable to the case of anisotropic effective masses.

1. Introduction

The interest for the theoretical investigation of ionisation processes in semiconductors is closely related to the operation of semiconductor devices in high fields. Measurements made by various authors[1, 2, 3, 4] on the p-n junctions at high inverse biases provided the information about the ionisation coefficients α, defined as a number of electron-hole pairs created per unit length by the incident carrier (electron or hole). To explain the experimental data several theories were proposed. Wolf[5] and Čuenkov[6] suppose that the distribution function can be well approximated by (the so-called diffusion approximation)

$$f = f_0 + f_1 \cos\theta, \tag{1}$$

where θ is the angle between the carrier velocity and the field, and f_0 and f_1 depend only on the carrier energy. Their results, however, are in poor agreement with experiments[5, 6]. On the other hand Schockley[7] supposes that the ionisation events are due to those carriers only which, starting from low energies have a chance to avoid collisions until they reach ionisation energy.

The agreement of his theory with experiment is good in very low fields, but it is unsatisfactory in higher fields. Baraff[8] showed that two theories are in fact limiting cases for low and high fields and that, unfortunately, the fields of practical interest are of intermediate intensities. Supposing quasi-free carriers, isotropic collisions and a constant mean free path λ, he derived an integral equation equivalent to the Boltzmann equation, which is suitable for a numerical solution. He gives a family of universal curves $\alpha\lambda$ versus $E_{ion}/e\lambda K$, with E_{op}/E_{ion} as a parameter, where E_{op}, E_{ion}, K are energy of the optical phonon, ionisation energy, and electric field, respectively. Choosing such a mean free path λ to get the best fit, the latter authors[3, 4] obtain a fairly good agreement of the experiment with theory.

The subject of the present paper is the Monte-Carlo calculation of the ionisation coefficients using high speed digital computers. The accidental events are simulated with the help of random numbers uniformly distributed on the segment (0,1). In the two following chapters the main features of the model supposed, the results of the calculations and the discussion on further possibilities of the Monte-Carlo simulation approach to the problem, are given.

2. *Monte-Carlo simulation of the ionisation processes*

In the simulation of the ionisation processes we use the following asumptions (also introduced by Baraff[8]):

a) the effective masses of carriers are isotropic,

b) cross-sections for scattering depend only on the carrier energy, i. e. the scattering is isotropic,

c) the mean free path λ is constant, which is a direct consequence of the dominant phonon scattering. Then the relaxation time is

$$1/\tau = v/\lambda; \tag{2}$$

d) to simplify the calculation, for carrier energy $E < E_{op}$ we take into account only the acoustic phonon scattering, for $E_{ion} > E > E_{op}$ only the optical phonon scattering with the emission of phonon (because at room temperatures optical phonon modes are not practically excited), and for $E > E_{ion}$ only the ionisation, and

e) it is assumed that $E_{ion} = 1.5\,E_g$, which is the threshold for ionisation in the case of equal effective masses of both carrier types; E_g is the energy gap.

It is convenient to introduce the following reduced dimensionless quantities:

— velocity $\tilde{v} = v\sqrt{m/2E_{ion}}$, (3)

— time $\tilde{t} = (t/\lambda)\sqrt{2E_{ion}/m}$, (4)

— energy $\tilde{E} = E/E_{ion} = \tilde{v}^2$, (5)

— electric field $\tilde{K} = eK\lambda/E_{ion}$, (6)

— ionisation coefficient $\tilde{\alpha} = \alpha\lambda$. (7)

If we choose the z axis in the direction of the electric field, we have

$$\tilde{v}_z = \tilde{v}_{z0} + \tilde{K}\tilde{t}/2, \tag{8}$$

$$\tilde{E} = \tilde{v}_{r0}^2 + \tilde{v}_z^2, \tag{9}$$

where $\tilde{v}_{r0}$ and $\tilde{v}_{z0}$ are the reduced velocity components at the instant $\tilde{t} = 0$.

Following the procedure of Kurosawa[9], with modifications necessary to our problem we arrive at the following simulation scheme:

1. Immediately after a collision the carrier has the velocity components $\tilde{v}_{r0}$ and $\tilde{v}_{z0}$. (At the beginning of the calculation we set $\tilde{v}_{r0} = \tilde{v}_{z0} = 0$.) Generating random number R_t we calculate the time between two successive collisions as a solution of the equation

$$-\ln R_t = \int_0^{\tilde{t}} \tilde{v}\,\mathrm{d}\tilde{t} = \int_0^{\tilde{t}} (\tilde{v}_{r0}^2 + \tilde{v}_z^2)^{1/2}\,\mathrm{d}\tilde{t}, \tag{10}$$

which, by solving the integral, can be reduced to the transcendental equation for velocity component $\tilde{v}_z$. Finding $\tilde{v}_z$ we get the energy immediately before the collision using (9) and we calculate the velocity after a collision as:

a) $\tilde{v} = \tilde{E}^{1/2}$, if $\tilde{E} < \tilde{E}_{op}$;

b) $\tilde{v} = (\tilde{E} - \tilde{E}_{op})^{1/2}$, if $\tilde{E}_{ion} > \tilde{E} > \tilde{E}_{op}$;

one optical phonon collision is recorded;

c) if $\tilde{E} > 1$, ionisation is recorded and we start from the step 1., with $\tilde{v}_{r0} = \tilde{v}_{z0} = 0$. (The calculation was also performed with the energy after ionising collision $\tilde{E}_1 = (1/3)(\tilde{E} - 2/3)$ and the velocity $\tilde{v} = \tilde{E}_1^{1/2}$, which is the

consequence of the conservation laws with the assumption of equal effective masses for both carrier types. As should be expected, it turned out that the assumption $\tilde{v}_{r0} = \tilde{v}_{z0} = 0$ after ionising collision introduces insignificant error).

2. Knowing the moduls of the velocity $\tilde{v}$ immediately after a collision, we obtain the velocity components generating the second random number R_v

$$\begin{aligned} \tilde{v}_{z0} &= \tilde{v} \cos\theta, \\ \tilde{v}_{r0} &= \tilde{v} \sin\theta, \\ \cos\theta &= 2R_v - 1, \end{aligned} \tag{11}$$

and proceed further returning to the step 1.

After a great number of ionisations, depending on desired accuracy, we calculate ionisation coefficient $\tilde{\alpha}$ as:

$$\tilde{\alpha} = \alpha\lambda = \tilde{K}/(1 + \tilde{E}_{op} N_{op}/N_{ion}), \tag{12}$$

where N_{ion} is the number of ionisations, and N_{op} the total number of collisions with optical phonons.

3. *Results of calculation and discussion*

It is well known that the relative error in Monte-Carlo calculations is proportional to $N^{1/2}/N$, where N is the number of trials. This is a direct consequence of Gaussian distribution of errors for a given number of trials. Using this fact it is easy to calculate the necessary number of trials for a required accuracy. We chose 300 ionisation, as giving satisfactory accuracy of 10% with the probability greater than 0.9.

The final calculation was performed on the IBM 360 model 44 computer. The results are represented on Figs. 1a and 1b. We see that the results of Monte-Carlo calculation deviate from that of Baraff (Fig. 1b), but that the agreement of the experimental results is equally good in both cases, Monte-Carlo calculation giving slightly lower values for the mean free path λ (compare Fig. 1a with Fig. 1 in[3]) and Fig. 13 in[4]). The most probable reason for the discrepancy between the Monte-Carlo and Baraff's calculation lies in some mathematical approximations introduced to find analytical expression for the kernel of Baraff's integral equation. Because of the latter approximations the Monte-Carlo calculation is probably more accurate.

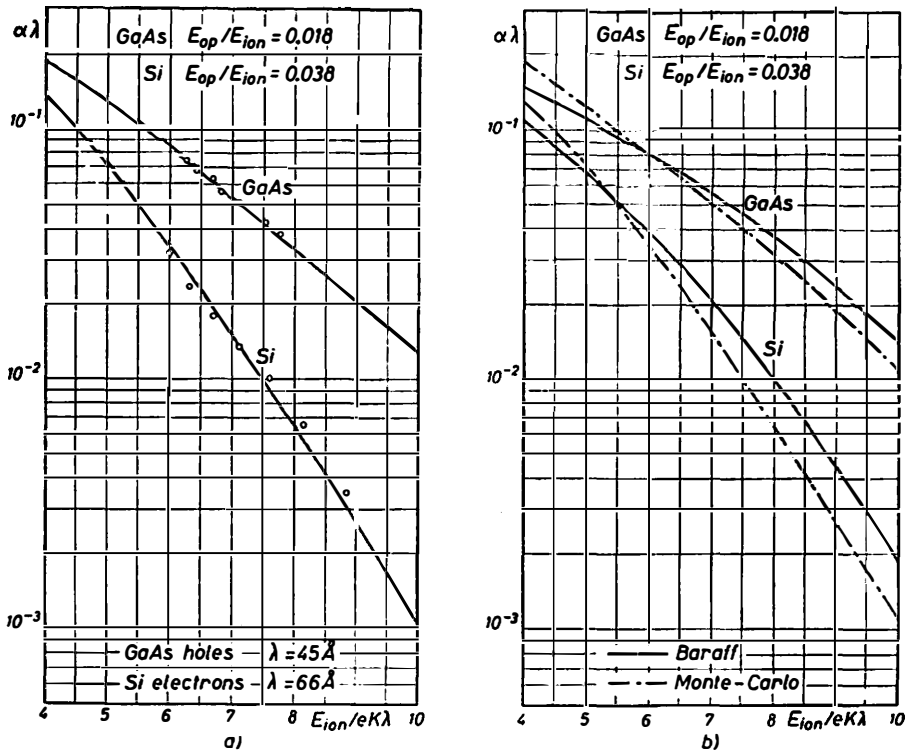

Fig. 1. Comparison of the Monte-Carlo simulation results with
a) experimental data (according to Refs. [3, 4])
b) with Baraff's theory

It is interesting to note that for silicon[4] the slope of the experimental results differs from that predicted by the theory, and that it cannot be fitted with the change of the parameter E_{op}/E_{ion} in addition to λ. This is probably due to the fact that effective masses are highly anisotropic. Baraff's theory is more economic than the Monte-Carlo simulation from the point of view of the computation time, but according to his own opinion it is not applicable to ellipsoidal equi-energy surfaces.

A Monte-Carlo calculation enables a relatively simple incorporation of the anisotropic masses in the calculation. The preliminary results, although raising some questions about the validity of effective mass concept at high energies, promise to give an excellent fit of the experimental results with the introduction of an additional parameter, the ratio of longitudinal and transverse effective mass.

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MONTE-KARLO PRORAČUN KOEFICIJENTA JONIZACIJE U POLUPROVODNICIMA

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Sadržaj

U radu je dat algoritam proračuna koeficijenta jonizacije u poluprovodnicima Monte-Karlo metodom, koja se zasniva na sledećim glavnim pretpostavkama:

— izotropne prividne mase nosilaca;
— izotropno rasejanje;
— konstantan srednji slobodni put.

Proračun je izvršen za GaAs i Si i dobijeni rezultati se nešto razlikuju od ranijih teorijskih proračuna. Slaganje sa eksperimentalnim rezultatima je dobro. Istaknuta je mogućnost primene Monte-Karlo metode i na slučaj anizotropnih prividnih masa.