PROCEEDINGS OF THE INTERNATIONAL CONFERENCE ON THE PHYSICS OF SEMICONDUCTORS, KYOTO, 1966
JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN VOL. 21, SUPPLEMENT, 1966

X-6. Monte Carlo Calculation of Hot Electron Problems

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A hot carrier effect in *p*-type germanium is calculated by simulation method. The distribution function of holes in wave number space is found to exhibit strong asymmetry, which rejects the conventional theoretical approach to the problem. Average energy of carriers, drift velocity, and energy distribution function are calculated and in reasonable agreement with experimental data.

§ 1. Introduction

Hot carrier problems are usually studied on the basis of the Boltzmann equation which is an integro-differential equation in wave number space. In several cases, the Boltzmann equation may be reduced to an ordinary differential equation with respect to the energy.[1] In some cases, however, the reduction is not permissible and the Boltzmann equation must be solved in its original form, which is not easy to be treated even with the aid of a high-speed computer.

A different approach is possible. Instead of solving the Boltzmann equation which deals with an ensemble of carriers, we can obtain the same result also by following behavior of one carrier for a long time. This corresponds to substitute the time average for the ensemble average. When the reduction of the Boltzmann equation is possible, the carrier behaves in energy space like a Brownian particle and its statistical behavior is represented by a diffusion equation with respect to the energy.[2] When the reduction is not possible, the simulation of the motion of the carrier by Monte Carlo method is a simple and useful tool for the problem.

As an example of this approach, the "streaming effect"[3~6] found in *p*-type germanium is treated. In a strong electric field above hundreds V/cm, the hole is accelerated rather freely from a low energy up to the energy of the optical phonon $\hbar\omega_{op}$, then emits quickly the optical phonon by the strong interaction between them and again drops to a low energy. In such a case, the k-space distribution function of the hole is strongly asymmetric and the conventional theoretical procedure expanding the distribution function by spherical harmonics does not give a satisfactory result, as pointed out by Pinson and Bray.[4]

The results of the present calculation are satisfactory and show utility of this approach to hot carrier problems.

§ 2. Models and Methods

For simplicity, we assume spherical energy surfaces, the effective masses of which are 0.35 m and 0.043 m, respectively. Thus the problem is axially symmetric. As for scattering frequencies, we adopt values given by Brown and Bray;[7]

$$W_{ac}=1.455\times 10^{8}T\sqrt{E/k}\ \sec^{-1} \qquad (2.1)$$

for acoustical phonon scattering, and

$$W_{op}=1.189\times 10^{11}\left\{n_{op}\sqrt{\frac{E}{k}+\theta}+(n_{op}+1)\sqrt{\frac{E}{k}-\theta}\right\}\sec^{-1} \qquad (2.2)$$

for optical phonon scattering, where E is the energy of the hole, k the Boltzmann constant, and θ is 430°K. For the present, the calculation has been done by neglecting the impurity scattering. The carrier-carrier scattering is also neglected.

The calculation is rather straightforward and carried out by following the recipe as below:

Step 0: Give initial values of E, k_z (the electric field is parallel to the z-axis) and k_ρ $(=\sqrt{k_x^2+k_y^2})$.

Step 1: Generate a random number r, and calculate the following time t, for which the carrier is accelerated freely:

$$-\ln r=\int_0^t\{W_{ac}(E(t'))+W_{op}(E(t'))\}dt', \qquad (2.3)$$

where

$$E(t')=\frac{\hbar^2}{2m^*}\left\{k_\rho^2+\left(k_z+\frac{eF}{\hbar}t'\right)^2\right\}. \qquad (2.4)$$

Step 2: Generate random numbers, and determine the final state (*i.e.*, heavy or light, values of E, k_z, and k_ρ) after the scattering from the prescribed probabilities. Return to the step 1.

On the other hand, the $\boldsymbol{k}$-space is divided into 3000~4000 meshes and visiting time of the hole in each mesh is recorded. The $\boldsymbol{k}$-space distribution function is proportional to the sum of the visiting time in each mesh. Usually the above process is repeated by 20000~25000 cycles.

An error in the distribution function due to statistical fluctuation may be about five times larger for the light hole than for the heavy hole, since the visiting probability of the hole in the light hole band is about 0.04 of that in the heavy one. However, once the heavy hole distribution function is obtained, we can facilitate the calculation of the light hole distribution function by the following procedure. We calculate a probability distribution of the energy which the light hole carries when it comes from the heavy hole band. This probability distribution can be used as a substitute for following the motion of the hole in the heavy hole band, because the hole which left the light hole band comes back to this band carrying an energy given by this distribution.

§ 3. Results and Discussions

Results of the calculation are illustrated in Figs. 1~5. Figure 1 shows an example of the $\boldsymbol{k}$-space distribution function of the heavy hole, which is strongly displaced. In Fig. 2, the distribution function with respect to the energy is plotted in logarithmic scale for several values of F. We see a remarkable kink at $E=\hbar\omega_{op}$. For smaller values of F, curves show a peculiar wavy form of the period $\hbar\omega_{op}$, which is attributed to a partial equilibrium between carriers of E and $E+\hbar\omega_{op}$ through emission and absorption of the opitical phonon.

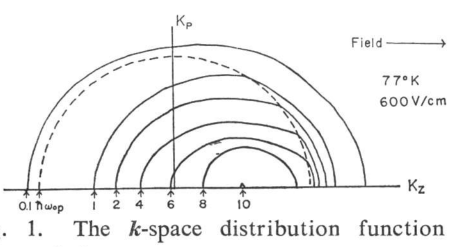

Fig. 1. The k-space distribution function of heavy holes.

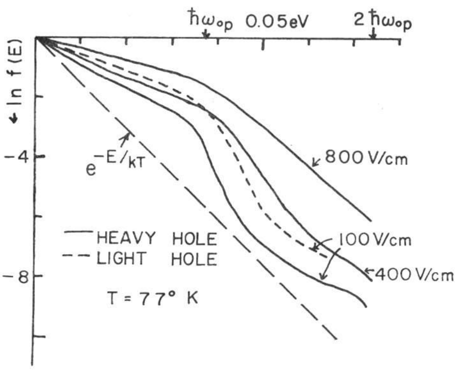

Fig. 2. The distribution function with respect to the energy.

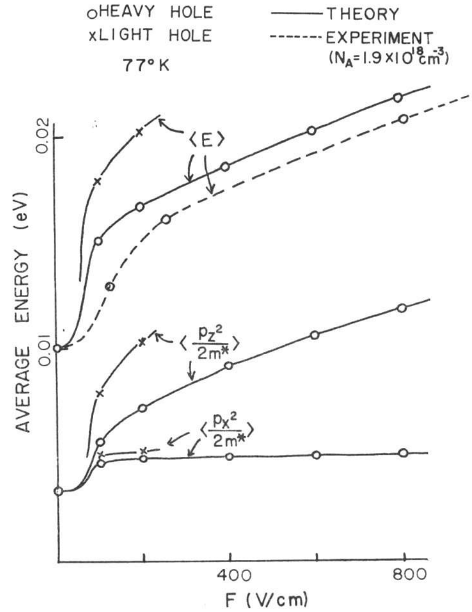

Fig. 3. Field dependence of average carrier energy.

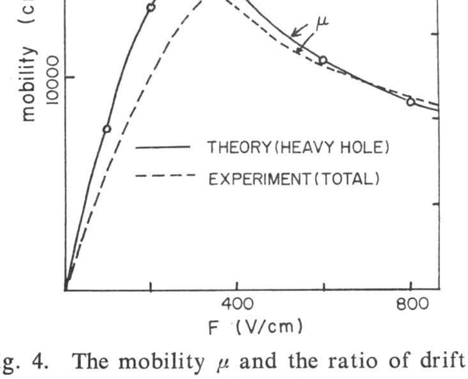

Fig. 4. The mobility μ and the ratio of drift to root-mean-square velocity v_d/v_r.

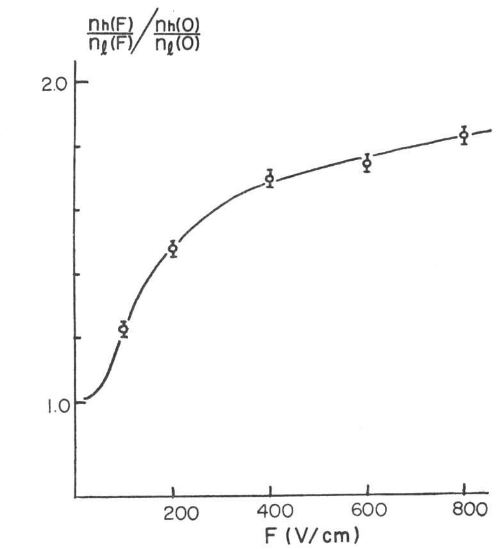

Fig. 5. Depopulation of the light hole band with the field.

The field dependence of average carrier energy is plotted in Fig. 3, where $\langle p_z^2/2m^*\rangle$ is the average kinetic energy along the electric field. Of course, they satisfy the following relation:

$$\langle E\rangle=2\langle p_x^2/2m^*\rangle+\langle p_z^2/2m^*\rangle\,. \qquad (3.1)$$

The dotted line shows experimental results,[4] which were obtained in a crystal of $N_A=1.9\times10^{18}$ cm^{-3}. The agreement between the theory and the experiment is good and also the difference between them is reasonable if we consider that the theory neglects the impurity scattering.

The mobility μ and the ratio of drift to root-mean-square velocity v_d/v_r are shown in Fig. 4. Figure 5 shows a depopulation of the light hole band with increasing field strength, which was suggested by Pinson and Bray.[4]

References

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DISCUSSION

Paige, E. G. S.: Published experimental data (Baynham and Paige: *Proc. Int. Conf. Semiconductor Physics*, Paris (1964) shows two energy ranges characterized by different electron temperatures much as this and the previous speaker predicts. It is interesting to note that above the optical phonon energy both experiment and theory give temperatures close to the lattice temperature for low fields. In the same paper experimental evidence is presented showing that there is no detectable change in light hole population. As mentioned earlier (Paige, review paper) this difference between theory and experiment may be ascribed to hole-hole scattering.

Franz, W.: A change in electron temperature similar to the result of Dr. Kurosawa for *p*-type Germanium has been obtained for *n*-type Germanium by myself in 1963 (Phys. Status Solidi), the effective temperature dropping for electron energy $>\hbar\omega$. This drop then decreases and increases again repeatedly with a period of about $\hbar\omega$, so obviously bumps in the distribution function are transmitted by optical phonons. —My calculations have been done by solving iteratively integro-differential equations somehow similar to the method shown by Dr. Budd, but for the real many-valley problem and different orientations of field, though might be mathematically less accurate.