Anisotropy of the High-Field Conductivity in n-Type Germanium

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(Received 8 February 1971)

The anisotropy between the drift velocities in the [100], [110], and [111] directions in n-type germanium has been calculated using the Monte Carlo approach with several variance-reducing methods included. The calculations include the effect of the ⟨100⟩ valleys. The theoretical curves are compared with experimental results. Qualitative agreement is obtained.

I. INTRODUCTION

In n-type germanium, in general, the electric current and field are not parallel at high fields. In the [100], [110], and [111] crystallographic directions this directional anisotropy disappears. An anisotropy still remains, however, in that at equal fields, the currents are different[1]:

$$(J[100])_E \geq (J[110])_E \geq (J[111])_E \,. \tag{1}$$

The amount of anisotropy between these three directions has been the subject of a number of experimental investigations.[1-6] Unfortunately, the results are not very consistent. The most recent and probably most exact measurements have been reported by Smith.[1] He obtained a [110] velocity 9% below and a [111] velocity 14% below the [100] velocity at a field of 3×10^5 V/m and a temperature of 300 °K.

Recently, a realistic model of the band structure and scattering mechanisms in n-type germanium, including higher-energy minima, has been used by Paige[7] to explain the bulk negative differential conductivity in this material. This paper is devoted to a study of this model, trying to reproduce the experimental curves obtained by Smith with a suitable choice of various scattering parameters. This transport problem is solved by a Monte Carlo method similar to the one used by a number of authors,[7-10] except for a few modifications that decrease the statistical error significantly.

II. BAND STRUCTURE AND SCATTERING MECHANISMS

In the conduction band of germanium there are three sets of nonequivalent minima with assumed physical parameters according to Table I, which was obtained from Ref. 7. In the following calculations the ⟨000⟩ minimum will be neglected. The mobility in this minimum may be quite high but the density-of-states factor is so small that its contribution to the total mobility is negligible. The remaining energy minima have constant energy surfaces that are ellipsoids of revolution. In the model they are transformed to spherical energy surfaces in the usual manner.[11] Furthermore, the ⟨100⟩ minima are replaced by one suitably averaged minimum. This follows from the strong intervalley scattering rate that will make the anisotropy between ⟨100⟩ valleys very small. It was recently pointed out by Dumke[12] that the nonparabolicity of the ⟨111⟩ minima might be important in an explanation of the conduction process in n-type germanium. Here, this effect is neglected since it is of importance only for electrons of rather high energy. With the inclusion of ⟨100⟩ valleys and a strong intervalley scattering rate between ⟨100⟩ and ⟨111⟩ minima the distribution function will decrease rapidly above the energy where this scattering process is effective. This effect is well illustrated in the case of GaAs in the paper by Fawcett, Boardman, and Swain.[10] The number of electrons in the energy range where nonparabolic effects are important will thus be smaller when the ⟨100⟩ valleys are included in the model.

A general reference for scattering processes in germanium is Paige.[13] In Table II is given a representative set of physical parameters of relevant scattering processes obtained from Ref. 7. The way in which some of these parameters influence the velocity field characteristic will be discussed below in connection with the presentation of the numerical results. In the model an approximation of the acoustical-deformation-potential scattering is used. The general form of the scattering rate for this process is very complicated. Relaxation times can, however, be determined parallel and at a right angle to the symmetry axes of the energy ellipsoids. In the case of n-type germanium these relaxation rates turn out to be almost equal (see Conwell[14]). Therefore it is quite a good approximation to use a single isotropic and velocity random-

TABLE I. Conduction-band parameters of germanium.

Valley	Number	m_L^*/m	m_T^*/m	Δ (eV)
⟨111⟩	4	1.577	0.0815	•••
⟨000⟩	1	0.037	0.037	0.14
⟨100⟩	6	0.90	0.192	0.18

TABLE II. Electron-phonon scattering processes in germanium.

Type	Minimum		Branch	Phonon energy (equiv temp) (°K)	Ξ_{av} (eV)	D (eV/m)
	Initial	Final				
Intravalley	[111]	[111]	acoustic	•••	11.8	
	[111]	[111]	optic	430°	•••	9×10^{10}
	[100]	[100]	acoustic	•••	7.4	•••
	[100]	[100]	optic	430°	•••	forbidden
Equivalent intervalley	[111]	[$\bar{1}$11]	acoustic	320°	•••	1.6×10^{10}
	[100]	[$\bar{1}$00]	optic	430°	•••	1.1×10^{11}
	[100]	[$\bar{1}$00]	acoustic	100°	•••	8.8×10^{9}
	[100]	[010]	acoustic	320°	•••	3.8×10^{10}
Nonequivalent intervalley	[111]	[100]	acoustic	320°	•••	5×10^{10}

izing suitably averaged deformation-potential-scattering process. Furthermore, the energy relaxation due to acoustic phonons is neglected, since it is important only at rather high energies where there are few electrons and the energy relaxation by nonequivalent intervalley scattering is strong.

III. MONTE CARLO METHOD

The Monte Carlo approach has been used by a number of authors[7–10] to study transport phenomena in various semiconductor materials. In this method, the random walk of a single charge carrier through momentum space is simulated on a computer using random numbers. Estimates of various transport variables are obtained as time averages over the path in momentum space of this charge carrier. The random numbers are used to generate the time of flight between collisions, the type of scattering mechanism causing a collision, and the direction of initial velocity after collisions.

The major difficulty in this process is the calculation of the time of free flight since the scattering frequency is a complicated function of energy. This problem is solved through the use of a "self-scattering" mechanism as described by Boardman, Fawcett, and Rees,[9] that is an additional scattering process

$$S(\vec{k}, \vec{k}') = [\Gamma(\vec{k}) - \nu(\vec{k})]\delta(\vec{k} - \vec{k}') , \qquad (2)$$

where $\nu(\vec{k})$ is the total scattering rate of real scattering processes, while $\Gamma(\vec{k})$ is a simple function of $\vec{k}$ and usually chosen to be a constant. In the case of n-type germanium, however, it was found to be more efficient to choose Γ as a piecewise constant function of energy.

With the Monte Carlo method in principle an exact solution of the transport equation can be obtained. In practical cases, however, statistical variances remain in the estimates of various transport variables. These variances are proportional to $1/\sqrt{n}$, where n is the number of collisions. Thus a large number of collisions, at least 10 000, have to be generated and a further increase in precision through an increase in the number of collisions soon becomes uneconomical due to the square-root dependence.

For n-type germanium at 300 °K the estimate of the drift velocity turned out to have a large variance. This is, of course, unacceptable in a study of rather small anisotropy effects. The large variance in the drift velocity has two sources. In each valley the estimate of the drift velocity has a variance of the order of $v_{th}/\sqrt{n}$, where v_{th} is the thermal velocity. In our case v_d, the drift velocity, is much smaller than v_{th}, which results in a large variance in the estimate of v_d in each valley. To obtain the total drift velocity, the contributions from all minima have to be summed weighted by

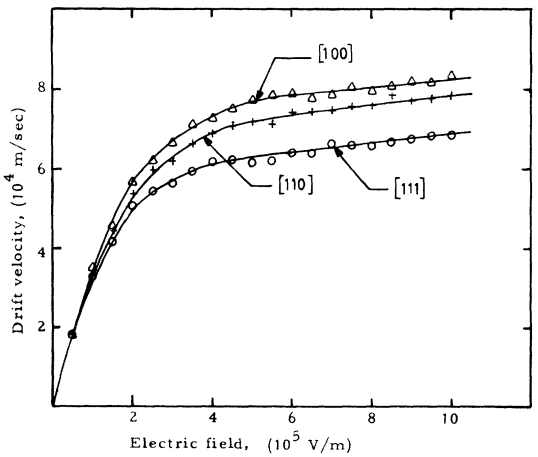

FIG. 1. Drift velocity for three orientations vs electric field at 300 °K.

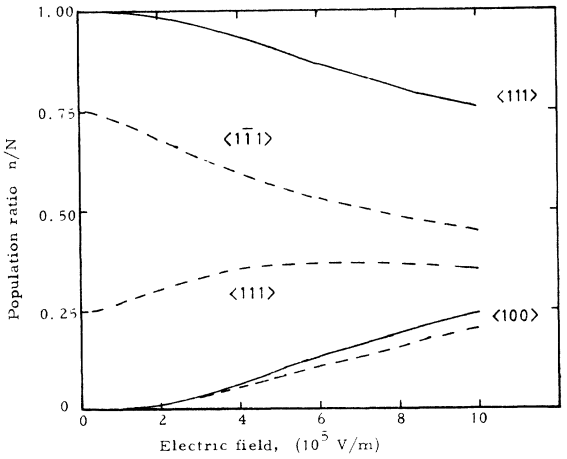

FIG. 2. Fraction of carriers in nonequivalent minima vs electric field for $\vec{E} \parallel [100]$ (full curves) and $\vec{E} \parallel [111]$ (dashed curves).

their respective population ratios. When intervalley scattering is weak, as is the case in n-type germanium below energies for which electrons can be scattered to ⟨100⟩ minima, large variances are obtained in population ratios. This causes a large error in the drift velocity for an electric field in the [110] and [111] directions, when there are large differences between drift velocities in nonequivalent ⟨111⟩ valleys.

The estimate of the drift velocity may be written as

$$v_d = \tfrac{1}{2}\sum (v_f^2 - v_i^2)/\sum (v_f - v_i)$$

$$= \tfrac{1}{2}\langle v_f + v_i \rangle = \tfrac{1}{2}\langle v_f - v_i \rangle + \langle v_i \rangle \,, \qquad (3)$$

where v_f and v_i are initial and final velocities of flight and the summations are over flights in velocity space. In Eq. (3) the last form of v_d is the most revealing. The first term is positive and has a standard deviation of the order of $v_d/\sqrt{n}$. In n-type germanium, where the scattering frequency increases monotonously with energy, the second term is negative with a variance of the order of $v_{th}/\sqrt{n}$. The values of the variances follow from the approximately exponential distribution of the times of flight. The second term in Eq. (3) thus contributes the major part of the variance.

The variance in the drift velocity can be significantly reduced if the conventional Monte Carlo method is suitably modified. These modifications can be most easily explained in terms of the synchronous ensembles introduced by Price.[15] Let f_a be the "after-scattering" distribution function, that is, the distribution obtained if particles are observed only immediately after they are scattered. In the model used here collisions are velocity randomizing. f_a will thus be spherically symmetric in momentum space and a function of energy only.

The random walk generates f_a, that is, how many times the particle starts out from each energy. At the same time, estimates of drift velocities and times of flight are obtained for particles starting out from these energies. Equation (3) can be interpreted as these estimates properly weighted by the estimate of f_a. The way to improve on Eq. (3) is to use a better estimate of the drift velocity at each initial energy. After each collision the particle is split up into two particles starting out with equal energy but oppositely directed initial velocities. The same random number is then used to generate the time of flight of both particles. Finally, one of the particles is chosen at random to continue the random walk. In this way the large error due to the spread in initial velocities is substantially reduced and a total variance more of the order of $v_d/\sqrt{n}$ is obtained.

The second source of error, the large variances in population ratios, can also be significantly reduced. Expressed in terms of f_a, the solution of the Boltzmann equation may be written as

$$f_{am}(\epsilon) = \sum_n \int_0^\infty T_{mn}(\epsilon, \epsilon') f_{an}(\epsilon')\, d\epsilon' \,, \qquad (4)$$

where the sum is over all valleys and $T_{mn}(\epsilon, \epsilon')$ is the distribution of initial energies ϵ in valley m as a function of the energy ϵ' after the last previous collision. If the energy axis is separated into a number of discrete intervals, $f_{am}(\epsilon)$ becomes a vector, $T_{mn}(\epsilon, \epsilon')$ a matrix, and Eq. (4) a system of linear equations

$$f_a^i = \sum_{j=1}^{k} T^{ij} f_a^i, \quad i = 1, \ldots, k, \qquad (5)$$

where k is the number of intervals in energy. From the random walk an estimate of the matrix T^{ij} can be obtained if at each collision the probabilities of

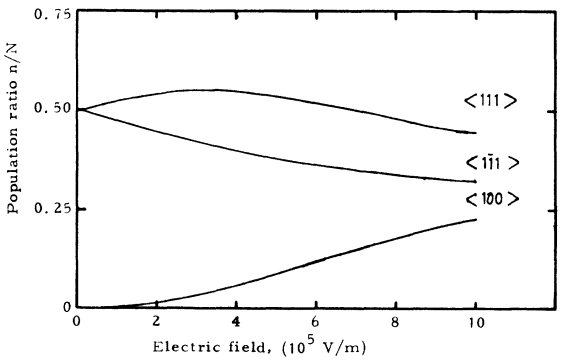

FIG. 3. Fraction of carriers in nonequivalent minima for $\vec{E} \parallel [110]$.

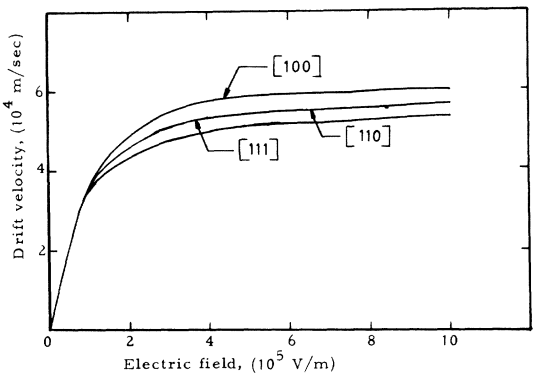

FIG. 4. Experimental drift velocity for three orientations vs electric field (Smith).

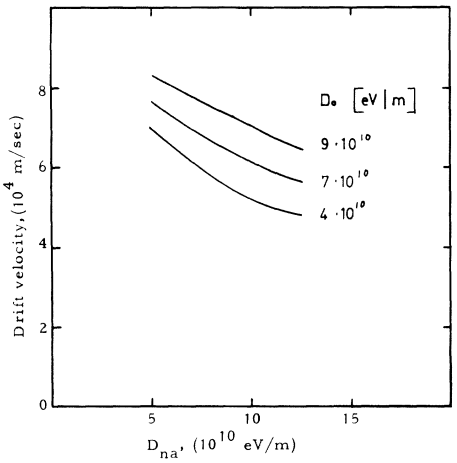

FIG. 6. Drift velocity vs coupling constant for ⟨111⟩-⟨100⟩ intervalley scattering.

transitions to various energy intervals is recorded. Equation (5) can then be solved numerically and since in the estimate of T^{ij} contributions to transition probabilities to other valleys are obtained at each collision, the variances in population ratios will be reduced significantly. It is important to note that in Eq. (5) it is not assumed that f_a is constant within the energy intervals chosen. In the limit of an infinite number of collisions proper averages within the intervals are obtained of all quantities that have to be recorded, like T^{ij} and t_j, the average time of flight of particles with initial energy in interval j. This means that the method does not require a very large number of energy intervals in order to be useful.

Finally, it can be remarked that both procedures outlined above can be extended to cover cases with collisions not velocity randomizing. The second procedure can be used without modifications, while in the first one the two particles starting out from the same energy have to be given unequal weights. It can also be remarked that the second synchronous ensemble used by Price, [15] the "before-scattering" distribution function f_b, can be used to give an estimate of the first few moments of the usual distribution function f. Since

$$f_b = \nu \times f \,, \tag{6}$$

where ν is the scattering frequency, for example, the symmetric part of f can be estimated if in each energy interval the number of collisions is recorded weighted by $1/\nu$.

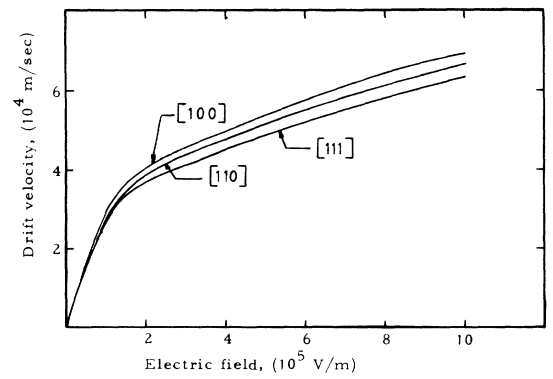

FIG. 5. Drift velocity for three orientations vs electric field with D_0 equal to 4×10^{10} eV/m.

IV. NUMERICAL RESULTS AND DISCUSSION

In Figs. 1–3 are plotted the velocity field characteristic and the population ratios calculated with the parameters given in Table II. The particle generating the random walk was followed through 10 000 collisions. For comparison, experimental curves obtained by Smith[1] are plotted in Fig. 4. The theoretical and experimental results are in qualitative agreement. However, in the theoretical curves the amount of anisotropy is too large and v_s, the velocity of saturation, too high. The anisotropy can be decreased by a slight increase in D_i, the coupling constant of intervalley scattering between ⟨111⟩ valleys. To decrease v_s, however, seems to present more of a problem. In the ⟨111⟩ valleys, the value of D_o, the coupling constant to optical phonons, is not well determined. Values of D_o in the range 4×10^{10}–9×10^{10} eV/m have been reported. [14] In Fig. 5 is plotted the velocity field characteristic for D_o equal to 4×10^{10} eV/m and D_a, the acoustic deformation potential, adjusted to give a low-field mobility of 0.38 m^2/V sec. The drift velocity is decreased although in such a way that the saturation disappears. A higher value of D_o is thus in better agreement with experiments. Another important parameter is D_{na}, the coupling

constant to nonequivalent intervalley scattering. It is of particular importance in connection with the Erlbach instability.[16] The Monte Carlo method described above can be generalized to give differential effects. The results of such computations[17] show that the Erlbach instability can exist in n-type germanium at 77 °K if the value of D_{na} is not too small. It is possible to decrease v_s both by an increase and a decrease of D_{na}. The variation in the drift velocity at a field of 10^6 V/m with an increase in D_{na} is shown in Fig. 6. A strong intervalley scattering rate might explain why avalanche breakdown does not occur until at very high fields. If D_{na} and the mobility in the $\langle 100 \rangle$ valleys are decreased, it is also possible to obtain a velocity of saturation of the correct magnitude. Both alternatives outlined above are not, however, consistent with hydrostatic pressure experiments.[18] It is thus difficult to obtain a correct value of v_s. This might indicate that the nonparabolicity in the band structure is of importance. To check the consistency of the model it would be very valuable if other transport effects could be computed. There are a number of experiments suitable for a comparison, like measurements of the frequency dependence of the conductivity,[19] of the Hall effect,[20] and of the magnetoresistance.[21,22] All these effects can be studied if the Monte Carlo method is suitably generalized. This is possible, but the labor required for the numerical programming would be considerable.

ACKNOWLEDGMENTS

The author would like to thank Dr. H. Kroemer for giving him the impulse to start this work. He is grateful to the National Bureau of Standards and the University of Colorado for their hospitality during the time when a part of this report was prepared.

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