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# XII-5. Intervalley Scattering Rate and High-Field Electron Distributions in GaAs

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The Boltzmann equation has been solved for GaAs for a wide range of fields and for several values of the coupling constant $D_{12}$ for scattering between the low- and high-mass valleys. From the resulting distributions the fraction of carriers in the upper valley and the current density have been obtained as functions of field. It can be concluded that $D_{12}>5\times10^7$ eV/cm. If the threshold for Gunn oscillations is around 2300 V/cm, a $D_{12}$ value of about $5\times10^8$ eV/cm appears correct.

It is now widely accepted that the Gunn effect[1] is due to the negative differential resistivity arising from the transfer of electrons in high fields from a low-mass central (000) valley to higher lying large-mass (100) valleys,[2,3] such as exist in the conduction band of GaAs. Calculations of the current-voltage characteristic of *n*-GaAs have been carried out on the assumption that the distribution function is a displaced Maxwellian,[2] or a pair of them, one for each valley.[4] The displaced Maxwellian form was supposed to result from electron-electron collisions being sufficiently frequent so that energy and momentum are shared among the electrons. In fact, for the concentrations and temperatures at which the Gunn effect is usually observed, the effect of electron-electron collisions on the distribution would be negligible.[5] We have solved the Boltzmann equation for a wide range of fields and find that the distributions are quite different from Maxwellian.

For electrons in the lower valley with insufficient energy to make a transition to one of the upper valleys the important scattering is by polar modes.[6] At room temperature the Boltzmann equation for this case is difficult to solve for moderate electric fields because the scattering is quite inelastic, the Debye temperature being 418°, and no relaxation time exists. At high enough fields so that, on the average, the electron energy $\varepsilon\gg h\omega_l$, the optical phonon energy, both of these difficulties are essentially removed. For such fields, the distribution function in the lower valley may be approximated by a spherically symmetric term $f_0(\varepsilon)$ plus a small drift term. The Boltzmann equation may then be put into the form

$$\frac{2e^2E^2}{3mh\omega_l}\frac{1}{(x-x_0)^{1/2}}\frac{d}{dx}\{(x-x_0)^{3/2}\tau f_0'\}+\left(\frac{\partial f_0}{\partial t}\right)_{\text{coll}}=0\,, \tag{1}$$

where $E$ is the electric field intensity, $\tau$ the relaxation time, $m$ the effective mass, $x=\varepsilon/h\omega_l$, and $x_0$ is the distance of the valley minimum, in units of $h\omega_l$, above the zero of our energy scale. This is conveniently taken at the bottom of the central valley. Equation (1) is also a good approximation for the distribution in any one of the (100) valleys for the model we are using.[5] We assume, in addition, that $f_0$ and the drift term are the same for all the (100) valleys. For $f_0$ this should be well justified because: (1) a substantial part of the carrier heating is due to transfer of hot electrons from the (000) valley, for which the distribution is essentially spherically symmetric; (2) scattering among the (100) valleys is expected to be strong by analogy with Si. The drift terms are not expected to be the same for all valleys, but this anisotropy should have small effect. In any case, no dependence of the Gunn effect on orientation has been found experimentally.

In eq. (1) for the lower valley only polar optical and intervalley scattering, for large enough electron energies, were included. The intervalley scattering terms introduce a coupling between the lower valley distribution and the upper valley distribution. For the upper valleys, since the importance of the different scattering processes is difficult to assess *a priori*, we have included polar optical and acoustic intravalley scattering, scattering among the equivalent (100) valleys and between the (100) and (000) valleys.[5] To make the equations tractable, quantities such as $f(x \pm x_{ij})$ were expanded in Taylor's series and terms higher than $f''$ dropped. The resulting pair of coupled equations for $f_1$ and $f_2$ was solved numerically. It is of interest, however, that for the lower valley, for $x$ greater than several $h\omega_l$ but not large enough for intervalley scattering to be possible, an analytic solution to eq. (1) can be obtained.[5]

Almost none of the parameters involved in the theory is known accurately, and the coupling constants $D_{12}$ and $D_{jj'}$ for nonequivalent and equivalent intervalley scattering, respectively, are not known at all. We have carried out calculations for values of $D_{12}$ ranging from $5\times10^7$ eV/cm to $1\times10^9$ eV/cm. The constant $D_{jj'}$ was taken $1\times10^9$ eV/cm, the value obtained for scattering among the (100) valleys in Si.[7] This leads to a low-field mobility of 150 cm$^2$/V sec for the (100) valleys, which appears to be reasonable.[6] Other parameters were chosen to fit the case of the (100) minima located at the edge of the Brillouin zone, but may also be a good approximation for the minima inside.[5] The value of the parameter $E_0$, which is a measure of the strength of coupling to the polar modes, was taken as 5950 V/cm.

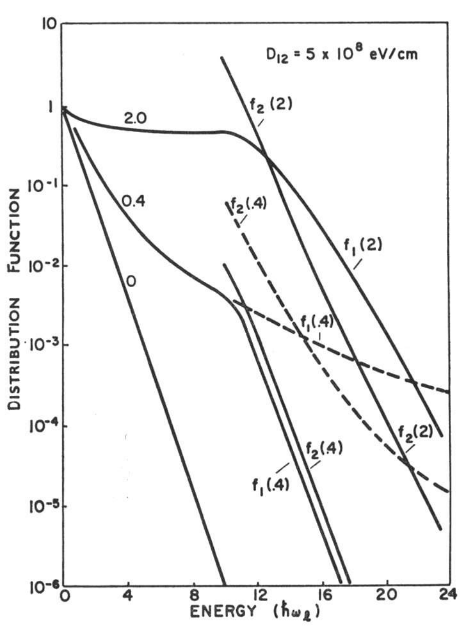


Fig. 1. Calculated distribution functions of electrons in the conduction band of GaAs at 300°K plotted as a function of $x = \varepsilon/h\omega_l$ for fields of 0.4 and 2.0 $E_0$, ($E_0 = 5.95\times10^3$ V/cm). For those shown with solid lines $D_{12} = 5\times10^8$ eV/cm, for those with dashed lines $D_{12} = 5\times10^7$ eV/cm. The line labelled 0 is the Maxwell-Boltzmann distribution for zero field.

Some typical solutions, obtained for $D_{12}$ values of $5\times10^7$ eV/cm and $5\times10^8$ eV/cm, are shown in Fig. 1 for fields of 0.4 $E_0$ and $2E_0$, where the approximations made should be good. These two values of coupling constant correspond to two different extremes of behavior in that, over the energy range shown, for the large $D_{12}$ intervalley scattering is the dominant process, while for the smaller, intervalley scattering is relatively ineffective and the polar scattering remains dominant.[5] Thus for $5\times10^7$ eV/cm it is seen that the behavior of $f_1$ above $x=10$, where the upper valley begins, constitutes a simple continuation of its behavior below $x=10$, whereas for $5\times10^8$ eV/cm the behavior of $f_1$ changes rather abruptly at $x=10$. In the latter case, for $E=0.4E_0$, because of the much stronger scattering above 10 the light-mass electrons are no longer substantially heated by the field and $f_1$ drops at about the same rate as the Maxwell-Boltzmann distribution for $E=0$. Heating of the light mass electrons is seen to occur for the higher $D_{12}$ at $E=2E_0$. So far as $f_2$ is concerned, it is easily verified that, for the range of fields shown here, $\tau$ is too small for any direct heating of the electrons by the field, *i.e.*, the terms involving $E$ in eq. (1) for the upper valley are small. If the effect of the $f_1$ terms could also be neglected, eq. (1) for the upper valley would state essentially $(\partial f_2/\partial t)_{coll} = 0$. The solution of this equation must, of course, be the Maxwell-Boltzmann distribution at the lattice temperature. Comparing $f_2(0.4)$ for the two $D_{12}$ values, we see that for $5\times10^8$, where $f_1 \simeq f_2$, $f_2$ is a Max-

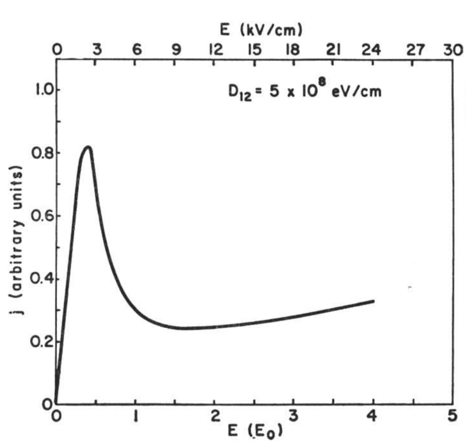


Fig. 2. Calculated $j$ vs. $E$ in units of $E_0$ for GaAs at 300°K with $D_{12} = 5\times10^8$ eV/cm, $D_{jj'} = 1\times10^9$ eV/cm, $E_0 = 5.95\times10^3$ V/cm.

wellian at the lattice temperature, while for $5\times10^7$, where $f_1$ at high energies is considerably larger than $f_2$, the latter departs from Maxwellian, particularly at high fields. This heating of the upper valley carriers by intervalley transfers can be seen for the larger $D_{12}$'s at higher fields than those shown here.

Integrations have been carried out to obtain the fraction of the electrons in the upper valleys for the different fields and coupling constants. For $E=0.4E_0$, or 2380 V/cm, it was found that for $D_{12}=5\times10^7$ eV/cm 78% of the electrons are in the upper valleys, while for $5\times10^8$ eV/cm only 30% are. It appears intuitively, and was verified by calculations for the other $D_{12}$ values (see Fig. 3, for example), that a transfer as large as 78% should require a field well past the beginning of the negative resistance region. The threshold for Gunn oscillations has been found to lie between 2300 and 4000 V/cm.[8] We conclude therefore that the correct $D_{12}$ is greater than $5\times10^7$ eV/cm.

Current density was calculated as a function of field for $D_{12}$ values in the range $(5/\sqrt{2})\times10^8$ to $1\times10^9$ eV/cm, and the values of the other parameters given above. For this, solutions of the Boltzmann equation were obtained also at low fields, where the approximations made for the polar scattering should not be good. It was found that Ohm's law is obeyed up to close to the maximum current, as is observed experimentally, and the low-field mobility was 6200 $cm^2$/V sec. This is a typical value for a moderately doped GaAs sample, in which there will be some impurity scattering in addition to the polar scattering. Thus our approximations had the useful effect of simulating the presence of impurity scattering in addition to polar scattering. The curves for the different $D_{12}$'s were quite similar. The maximum, *i.e.* the beginning of the negative resistance region, occurs between 2100 and 2300 V/cm. With increasing $D_{12}$ the maximum increases somewhat and shifts to higher fields, the shift being 200 V/cm for a change in $D_{12}$ from $5/\sqrt{2}$ to $5\sqrt{2}\times10^8$ eV/cm. Shown below is the $j-E$ curve for $D_{12}=5\times10^8$ eV/cm. The drift velocity at the maximum is $1.1\times10^7$ cm/sec, which coincides with the lower limit of the range 1.1 to $1.65\times10^7$ cm/sec found experimentally for the drift velocity at threshold.[8] The minimum of the $j-E$ curve lies a little below 10 kV/cm. This is in disagreement with Ridley's[9] idea that the field at the minimum should equal that of the high-field domain, for which values as high as 75 kV/cm have been measured.[10] There is, however, experimental evidence that the negative resistance region ends at about 10 kV/cm.[11,12]

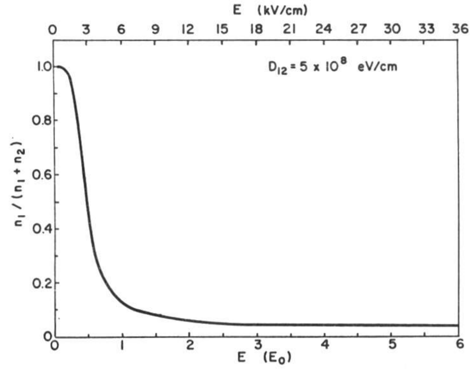


Fig. 3. Calculated fraction of carriers in the lower valley as a function of $E$ for GaAs at 300°K with the same parameters as used for Fig. 2.

A plot of the fraction of carriers in the lower valley vs. $E$ is shown in Fig. 3 for $D_{12}=5\times10^8$ eV/cm. It is seen that once the transfer of carriers into the upper valley has begun it increases very rapidly and is essentially complete before 10 kV/cm. About 20% of the carriers are transferred at the beginning of the negative resistance region. Curves similar to that of Fig. 3 are found for the other $D_{12}$ values, shifted somewhat to lower fields for $D_{12}<5\times10^8$, to higher fields for $D_{12}>5\times10^8$ eV/cm.

We conclude that if the threshold field for the Gunn effect is in the neighborhood of 2300 V/cm, the lower limit of the range found experimentally, the foregoing theory gives good agreement with experiment for $D_{12}\simeq5\times10^8$ eV/cm and the other parameters chosen as specified. A threshold field much higher than 2300 V/cm would suggest that some of the other parameters used in the calculation, such as $E_0$ or the energy separation between valleys, are incorrect.

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## COMMENT BY THE AUTHORS

Since the time this paper was written, experimental evidence, such as that given by Gunn in his conference paper, has accumulated for a Gunn effect threshold in the neighborhood of 3800 $cm^2/V \cdot sec$. It cannot be concluded, therefore, from our calculations that the value $5 \times 10^8$ eV/cm is correct for $D_{12}$. From considerations based on hole generation at low fields in GaAs, Copeland [Appl. Phys. Letters, Aug. 15, 1966] suggests that $D_{12}$ is of the order of $1 \times 10^8$eV/cm.

The fact that the threshold obtained in our calculations is considerably lower than the measured values may be due to the presence in actual samples of an additional scattering mechanism. Such a mechanism has been suggested by L. Weisberg (*Proc. Int. Conf. Semiconductor Physics*, Prague). Incorporation of this mechanism in our calculations has led to a value of threshold in much better agreement with experiment.

## DISCUSSION

**Paul, W.:** I should like to comment on the values of some of the band parameters used. The value of 0.36 eV for (100)–(000) band separation was deduced originally from an analysis of Hall effect vs. temperature and resistivity vs. pressure. We now know that the variation of resistivity with pressure, done on the purest GaAs then available, is in fact dependent on the type and number of defects. The implication is that a new data analysis is necessary which may yield new energy gap separations. It is already clear from Bell Laboratories' work and work at STL in England that one must take account of impurity levels connected with the (100) minima. Perhaps one should also take account of such levels in Gunn effect analysis, since it appears that even the high purity GaAs used in Gunn effect studies shows the effect of such additional levels.

The position of the (111) minima should not be forgotten. It is probably very close to that of the (100); the effect of such minima may not show up in stress or alloying experiments, but this does not eliminate their effect under ordinary conditions.

These remarks about impurity levels are also pertinent to analysis of the Gunn effect in CdTe and InAs; they may even apply to materials whose upper band minima are so high that pair production would prevent Gunn oscillations.

Finally I should like to add the suggestion that in such impurity levels may lie the source of mobility reduction often noticed for example in GaAs and GaSb.

**Conwell, E. M.:** It seems to me that the effect bound impurity states below the (100) valleys would have on the Gunn effect would be a lowering of the threshold. Since the threshold we calculate for GaAs is too low, I am not inclined to think this effect is important for the usual GaAs sample. It may be so for CdTe, InAs, etc..

The (111) minima undoubtedly have an effect on $V_d$ vs. $E$ and should, if possible, be incorporated into our calculations· Presumably the density of states in these minima is smaller than that of the (100) minima.

**McCumber, D. E.:** Do your calculations support Copeland's theory of low-field hole generation? Specifically, do some of the central-valley electrons become very hot for fields of the order of 5 kV/cm?

**Conwell, E. M.:** Whether or not a substantial number of light electrons is hot enough to generate holes, *i.e.* has $\varepsilon > 1.6$ eV, depends, according to our calculations, on the value of $D_{12}$. As can be seen from Fig. 1 of our paper, for large $D_{12}$ this would not be the case because $f_1$ decreases very rapidly with $\varepsilon$. The value of $D_{12}$ that Copeland suggests to make hole generation competitive with scattering to the (100) valleys is $1 \times 10^8$ eV/cm. For fields of about 5 kV/cm, $f_1$ for this value of $D_{12}$ would be something like that shown in Fig. 1 for 2.4 kV/cm and $D_{12}=5 \times 10^7$ eV/cm, *i.e.* it would have a long tail to high energy. In addition, it must be remembered that, because of non-parabolicity, the density of states in the central valley will be considerably larger at $\varepsilon \gtrsim 1.6$ eV. Thus it is quite plausible that there would be a substantial number of electrons hot enough to ionize at fields of about 5 kV/cm. Quantitative calculations would, of course, be necessary to substantiate this. Such calculations should include the effect of the (111) minima.