G. Persky
D. J. Bartelink

Negative Differential Mobility in Nonparabolic Bands

Abstract: A strong NDM (negative differential mobility) in n-InSb at low temperatures is predicted from a single non-parabolic band model. Calculations allowing for the anisotropy of the distribution function have been made using (1) a drifted Maxwellian, and (2) a "two-temperature" model. The calculated NDM threshold field of 550 V/cm is in an observable field range in p-n junctions. In bulk samples, where breakdown occurs at $E \approx 200$ V/cm, domain nucleation may take place at high-field inhomogeneities and contribute to the dynamics of the breakdown process and attendant microwave emission.

Introduction

Transfer of electrons into high-mass valleys is a well-known mechanism for the production of NDM (negative differential mobility).[1] Alternatively, within a single band, increase of carrier effective mass with energy can give rise to NDM without intervalley transfer. In particular, several authors have calculated the occurrence of this effect in n-type InSb[2,3] and InAs,[3] but have not given the results much credence. Although "bulk breakdown" is observed in n-InSb[4] at average fields below the NDM threshold, a possible consequence of NDM is the formation of high-field domains that may contribute to the dynamics of the breakdown process and attendant microwave emission.

Single-band NDM[5] may be understood intuitively with the aid of the inset in Fig. 1, wherein for clarity, the simplifications of a dispersionless band and a drifted spherical distribution in crystal momentum, p, space are assumed. The drift velocity contribution v_d of a spherical shell in this distribution at two fields, $E_2 > E_1$, is determined by its radius and the position of the distribution's centroid. Since the electron speed $v = d\epsilon/dp$ in this band is constant, as indicated by the arrows of uniform length, $v_d(E_2)$ may be less than $v_d(E_1)$ although the centroid has moved out. It moves out sufficiently slowly to allow a decrease in v_d because the input power of electrons at all energies is limited to $q\mathbf{v}\cdot\mathbf{E}$ while the scattering loss increases with energy, and at a rate which is enhanced by the nonparabolicity of the band.

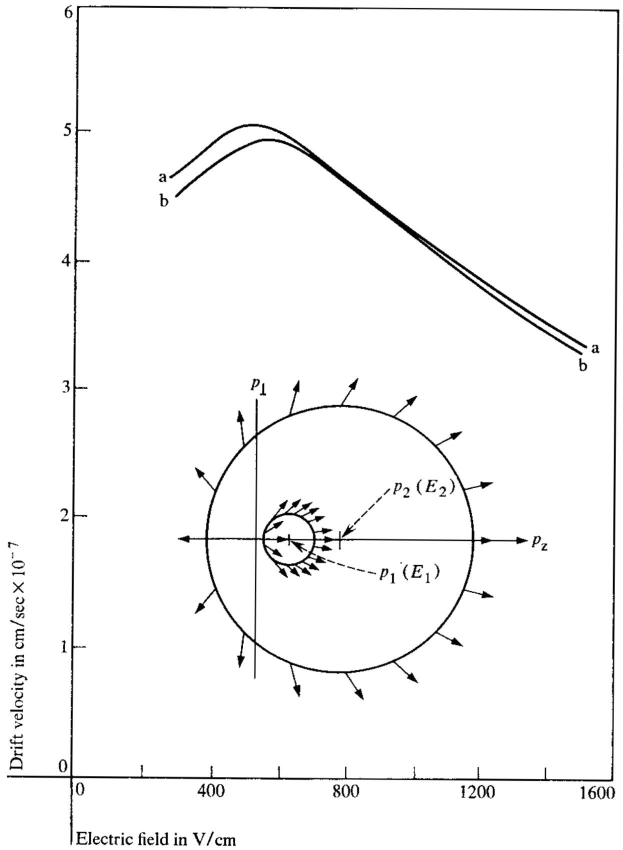

Figure 1 Calculated velocity-field curves for n-InSb at low temperature. (a) Drifted Maxwellian; (b) "Two-Temperature" Model. Inset: Schematic representation of election distribution function in crystal momentum space at two field values.

The authors are with Bell Telephone Laboratories Incorporated, Murray Hill, New Jersey.

Table 1 High field limits of drift velocity vs field for various band dispersion laws.

Dispersion law	*Drift velocity*
$\epsilon = rp^{\gamma}$	$v_d \propto F^{(\gamma-2)/(8-3\gamma)}$
$\epsilon \approx \frac{p^2}{2m}(1 - \alpha p^2)$	$v_d \approx v_s\left(1 - \frac{11}{6}\alpha m l_{op} l_t F^2/\epsilon_0\right)$
$\epsilon = \frac{1}{2}\epsilon_g\left[\left(1 + \frac{2p^2}{m\epsilon_g}\right)^{1/2} - 1\right]$	$v_d \approx \begin{cases} v_s\left(1 - \frac{11}{12}\left(\frac{\epsilon_0}{\epsilon_g}\right)F^2 l_{op} l_t/\epsilon_0^2\right) \\ v_s\left[\frac{\sqrt{3}\cdot\left(\frac{5}{3}\right)^{2/5}\cdot\Gamma\left(\frac{3}{2}\right)}{2\cdot\Gamma\left(\frac{3}{5}\right)}\cdot\left(\frac{\epsilon_g}{\epsilon_0}\right)^{1/10}\cdot(Fl_t/\epsilon_0)^{2/5}\cdot(Fl_{op}/\epsilon_0)^{-3/5}\right. \end{cases}$

A more general dispersion law and isotropic scattering are treated quantitatively in the next section. Numerical results for polar scattering (InSb) are given in the following section and discussed therein.

NDM with nonpolar scattering

For electrons in a spherical nonparabolic band with isotropic elastic acoustic scattering and nonpolar optical phonon emission, the Boltzmann equation takes the form

$$\mathbf{F}\cdot\nabla_p f(\mathbf{p})$$
$$= \int f(\mathbf{p}')[C_{op}\,\delta(\epsilon' - \epsilon - \epsilon_0) + C_a\,\delta(\epsilon' - \epsilon)]\,d^3p'$$
$$- f(\mathbf{p})\int [C_{op}\,\delta(\epsilon' - \epsilon + \epsilon_0) + C_a\,\delta(\epsilon' - \epsilon)]\,d^3p', \qquad (1)$$

where $f(\mathbf{p})$ is the distribution function, $\mathbf{F}$ is the field force, C_{op} and C_a are optical and acoustic deformation potential coupling constants, and ϵ_o is the optical phonon energy. We now make a diffusion truncation, assuming $f(\mathbf{p}) = n_0(p) + n_1(p)\cos\theta$, integrate the right-hand side of (1), and retain only the contributions of lowest order in ϵ_o/ϵ of the resulting difference terms. This yields the following pair of coupled differential equations:

$$\frac{1}{3}F\frac{d}{dp}(p^2 n_1) = \frac{\epsilon_o}{m^2 l_{op}}\frac{d}{dp}\left[\left(\frac{p^2}{v}\right)^2 n_0\right] \qquad (2a)$$

$$F\frac{dn_0}{dp} = -\frac{p^2}{m^2 l_t v}n_1. \qquad (2b)$$

In these equations $v = d\epsilon/dp$ is the group velocity, m is the effective mass at the bottom of the band, $l_{op} = 1/4\pi m^2 C_{op}$, and $l_t = 1/4\pi m^2(C_{op} + C_a)$. In a parabolic band l_{op} and l_t would be the mean free path for optical phonon emission and the net path length for optical and acoustic scattering combined. The collision frequency, which appears implicitly in (2b), is given by

$$\nu = \frac{1}{m^2 l_t}\frac{p^2}{v} = \frac{1}{m^2 l_t}p^2\frac{dp}{d\epsilon}. \qquad (3)$$

In a parabolic band $p \propto \epsilon^{\frac{1}{2}}$, and therefore $\nu \propto \epsilon^{\frac{1}{2}}$. When p increases more rapidly than $\epsilon^{\frac{1}{2}}$, ν will also go up more rapidly with energy, depopulating the high-energy states more effectively. At the same time, because of the increasing effective mass the field does not as readily populate these states. The result is a non-Maxwellian distribution which falls off rapidly at high energies. Equations (2a) and (2b) are easily solved for the isotropic portion of this distribution. One finds that

$$n_0(p) = \exp\left[-3\epsilon_0\int_0^p\frac{p^4}{v^3}\,dp/F^2 l_{op} l_t m^4\right], \qquad (4)$$

which reveals that as the field is raised, there is progressively less heating of the distribution than for a parabolic band.

From (4) v_d is calculated with the power balance formula

$$v_d = \epsilon_0\int_0^\infty \nu_{op} n_0(p) p^2\,dp/F\int_0^\infty n_0(p)p^2\,dp \qquad (5)$$

in which ν_{op} is the optical phonon collision frequency. A few examples of high-field limiting forms of v_d for band-dispersion relations permitting an analytic solution are given in Table 1. They uniformly indicate the occurrence of NDM whenever the effective mass increases with energy. The third example, a hyperbolic band, is treated as a slightly perturbed parabolic band for moderately high fields and as dispersionless for extremely high fields.

NDM in indium antimonide

Although the conduction band of InSb is known to be close to hyperbolic,[6] the occurrence of NDM in this material might seem unlikely because of the focusing effect[7] of the polar optical phonon scattering. Nevertheless, Hammar and Weissglas[2] have computed a velocity-field curve for InSb at 77°K showing an NDM threshold at about 550 V/cm, while Matz[3] obtained weak NDM at room temperature. Matz employed a diffusion truncated Boltzmann equation, and Hammar and Weissglas used the moment balance technique in conjunction with a drifted Maxwellian that was, in effect, also diffusion truncated. Both methods leave some question about the model dependence of the results. We have confirmed the low temperature findings of Hammar and Weissglas by (a) repeating their calculation without truncating, in order to better permit streaming motion, and (b) calculating the drift velocity with a "two-temperature" model of the energy distribution. The drifted Maxwellian calculation is standard in most respects and need not be described here. The two-temperature model, which requires the use of special balance equations, has been previously applied by us to the nonpolar problem of p-Ge.[8] In this model the isotropic part of the distribution function, i.e., the energy distribution, is characterized by two distinct Maxwellians intersecting at the optical phonon energy, but no a priori functional dependence of the angular form of the distribution is assumed; streaming motion is thus fully permitted. We let

$$n_0(\epsilon) = \begin{cases} Ne^{-\epsilon_0/kT_\beta}e^{(\epsilon_0-\epsilon)/kT_\alpha} & \epsilon < \epsilon_0 \\ Ne^{-\epsilon/kT_\beta} & \epsilon > \epsilon_0, \end{cases} \tag{6}$$

where the values of the temperature parameters T_α and T_β are determined by simultaneous solution of the pair of balance equations

$$F^2 \int_0^\infty n_0 p^2\, dp - \int_0^\infty (\hat{S}_0 n_0)\left[\int_0^p (S_1^\dagger p)\, dp\right] p^2\, dp = 0 \tag{7a}$$

and

$$\begin{aligned} &F^2 \int_0^\infty (\hat{S}_0 n_0) p^4\, dp + \frac{1}{2} F^2 \int_0^\infty (\hat{S}_2 n_0) p^4\, dp \\ &+ \frac{3}{2} F^2 \int_0^\infty n_0 \int_0^p \frac{1}{p} (\hat{S}_2^\dagger p^2)\, dp\, p^2\, dp \\ &- \frac{3}{2} \int_0^\infty (\hat{S}_0 n_0) \int_0^p \left[\hat{S}_1^\dagger p \int_0^p \frac{1}{p} (\hat{S}_2^\dagger p^2)\, dp\right] dp\, p^2\, dp \\ &= 0, \end{aligned} \tag{7b}$$

which already incorporate the kinetic content of the Boltzmann equation, and are valid for nonparabolic bands and arbitrary scattering mechanisms.[9] In (7a) and (7b), the various $\hat{S}_i$ and $\hat{S}_i^\dagger$ are respectively Legendre polynomial expansion components of the scattering operator $\hat{S}$ and $\hat{S}^\dagger$ wherein $\hat{S}f \equiv (\partial f/\partial t)_{col}$. Satisfying (7a) equalizes the rate of gain of crystal momentum from the field to the loss rate to the scattering system. For a parabolic band (7b) would be equivalent to the power-balance relation.

We solved (7) numerically for T_α and T_β for the hyperbolic band and polar scattering in InSb, and computed the drift velocity with a power balance formula similar to (5). The results are displayed in Fig. 1, along with those obtained from the drifted Maxwellian. Only emission of the polar optical phonons was taken into account, so accuracy is not expected at low fields. Both curves confirm the result of Hammar and Weissglas by showing a pronounced NDM threshold below 600 V/cm. Their good agreement, despite the great dissimilarity in the models, lends strong theoretical support to the existence of the effect. The abrupt onset of the NDM may be understood as follows. At lower fields the mobility remains especially high because strong streaming motion results from the random nature of the phonon emission process ("lucky electron" effect)[10] as well as from polar focusing. However, in the field range in which NDM sets in the average electron energy is larger than ϵ_o. The lucky electron mechanism thus loses its importance, while at the same time, because the ratio ϵ_g/ϵ_o is only about 10 in InSb, the band hyperbolicity sets in quickly ($m \approx 1.7\, m_0$ at $\epsilon = \epsilon_o$). The latter prevents polar runaway, while defocusing of the streaming distribution, necessary for the NDM, is accomplished by the finite angle contribution to the polar scattering of electrons which can now remain at high energies after multiple collisions.

Neither of the parameterized models gives evidence of a vanishing or positive differential mobility in the high-field limit, but this may be due to deficiencies of the calculation at higher energies. We assumed the scattering probability to be inversely proportional to the square of the scattered phonon wave vector. A more refined treatment of the scattering matrix elements, as used by Matz,[3] would reduce the collision cross-section at high energies and should raise the mobility. Since Matz still obtained a negative differential mobility, we believe this improvement would diminish the theoretical low-temperature NDM but not eliminate it. It might, however, alter the threshold or cause an eventual rise in v_d. The effect of impact ionization on the distribution function has also been neglected in this calculation, but this is likely to reduce the drift velocity at high fields.

Although it is well known that in InSb p-n junctions at 77°K fields can greatly exceed the theoretical NDM threshold without appreciable impact ionization, in bulk samples where there is sufficient carrier density for domain formation such effects may be difficult to observe directly because breakdown occurs at fields not much over 200 V/cm.[4] However, it is an attractive possibility that domains resulting from the NDM contribute to the dynamics of breakdown in the bulk and the microwave emission that accompanies it. It has been shown for GaAs that field inhomogeneities can lead to nucleation sites for domains.[11] The same idea may be carried over to InSb. With an average applied field of 200 V/cm there can be inhomogeneous regions in which the field locally exceeds the 550 V/cm NDM threshold. From the theoretical velocity-field curve we estimate a critical doping-length product $\sim 10^{10}$ cm^{-2}. Therefore, for $n \sim 10^{14}$ cm^{-3}, only a few microns of high-field region are needed to nucleate a domain which is then capable of being sustained by the much lower field outside. Strong ionization will take place within the domain where the high peak field (in excess of 550 V/cm) increases the ionization coefficient several orders of magnitude, thus greatly enhancing the normal statistical fluctuations of the breakdown process. Random nucleation of such domains would be accompanied by incoherent microwave noise. It also suggests itself that a high-field region associated with a suitable contact can lead to domain nucleation, propagation, and subsequent extinction. Such domain dynamics may be responsible for microwave emission at fields below bulk breakdown.

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