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A Topological Theory of Domain Velocity in Semiconductors

Abstract: A theory is given for the velocity of a free, steadily travelling domain of high electric field in a semiconductor exhibiting a negative differential conductivity. Explicit results are derived for the cases for which the domain behavior is dominated either by the (electric-field dependent) diffusion of electrons, or by the rate of transfer of electrons between states having different mobilities. It is shown that the solution for the electric-field distribution has the required properties only if the system of differential equations involved possesses singular points with special topological properties; this requirement serves to fix the domain velocity. The velocity depends only on the properties of the semiconductor at that high electric field where the effective drift velocity of electrons is equal to that outside the domain.

Introduction

The existence of travelling domains of high electric field in a semiconductor[1,2] requires that the material possess two properties: 1) The current carried in a steady electric field must be a decreasing function of field over a certain range, and 2) during the passage of the domain, the conduction current at a point must not be a single-valued function of electric field. In cases of practical interest, the first property results from the transfer of electrons from high- to low-mobility states as the electric field increases, while the second arises predominantly either from the contribution of diffusion currents, or from the finite rate of transfer between states. From these properties it follows that the differential equation describing domain propagation is a partial one, of at least the second degree, and nonlinear. In general, it can be solved only by computer techniques.[3,4] However, if conditions are such that a domain can be assumed to be travelling *steadily* (that is, with constant shape and velocity, in homogeneous material), the equation can be reduced to an ordinary one of the first degree. The velocity of this steady motion enters the equation as an unknown parameter, whose value is to be determined by satisfying the boundary conditions. This has been done, for the diffusion type of domain, by the use of the "Equal Areas Rule,"[5] which is valid only if the diffusion coefficient is constant.

The boundary conditions are most easily discussed if the electric field in the domain is described, not as a function of position or time, but as a function of its derivative with respect to position or time. In such a phase-plane representation, acceptable solutions appear as closed trajectories, starting from and ending at a given singular point, and encircling a second one. So much has been known for some time[6–8] but it does not seem to have been recognized that the condition that determines the unknown velocity is just the requirement that the trajectory be indeed closed. In this paper we show, by a topological argument, that the requirement that the trajectory be closed determines the nature of the singular point that it encloses. The classical topological theory of nonlinear differential equations gives a necessary condition for the existence of the requisite type of point, in terms of a linear expansion of the equation about that point. Since the domain velocity appears in the expansion as a parameter, it can thus be deduced from the values of the other variables in the problem, *at the point itself.*

Analysis

Let n, μ, D represent the number density, mobility, and diffusion coefficient of electrons in a state. For each of the two kinds of state, which we distinguish by subscripts 1 and 2, these quantities may depend on the electric field E. Also dependent on E are the rates, S_1 and S_2, at which electrons leave each kind of state for the other. If κ is the dielectric constant of the medium, N the net donor density, and e the charge on an electron, we have equations for the total current density $\mathbf{J}$,

$$\mathbf{J} = e\mathbf{E}(\mu_1 n_1 + \mu_2 n_2) - e\nabla(D_1 n_1 + D_2 n_2) + (\kappa/4\pi)\,\partial\mathbf{E}/\partial t, \qquad (1)$$

for the continuity of one of the electron currents,

$$\nabla\cdot(\mathbf{E}\mu_2 n_2 - \nabla D_2 n_2) + \partial n_2/\partial t = S_1 n_1 - S_2 n_2, \qquad (2)$$

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and Poisson's equation,

$$\nabla \cdot \mathbf{E} = (4\pi e/\kappa)(n_1 + n_2 - N). \tag{3}$$

Assuming that $\mathbf{J}$ is constant, and that the domain is travelling steadily in the x-direction with velocity c, we have $\partial/\partial y = \partial/\partial z = 0$, $\partial/\partial t = -c\partial/\partial x = -cd/du$, where u is the moving coordinate $x - ct$. Then, by eliminating n_1 and n_2, Eqs. (1), (2) and (3) can be reduced to an ordinary differential equation of the second order under either one of two simplifying assumptions. If it is assumed that S_1 and S_2 are much larger than the highest frequencies involved in the problem, Eq. (2) reads approximately

$$S_1 n_1 = S_2 n_2; \tag{4}$$

that is, the populations of the two valleys are always in dynamic equilibrium and the domain is controlled by diffusion. In this case, the resulting differential equation is

$$D\frac{d^2E}{du^2} + D^{(1)}\left(\frac{dE}{du}\right)^2 + \left(c - \mu E + \frac{4\pi e N}{\kappa} D^{(1)}\right)\frac{dE}{du} - \frac{4\pi e N}{\kappa}\mu E + \frac{4\pi}{\kappa} J = 0, \tag{5a}$$

where we have written μ for the mean mobility $(S_2\mu_1 + S_1\mu_2)/(S_1 + S_2)$, D for the mean diffusion coefficient $(S_2D_1 + S_1D_2)/(S_1 + S_2)$, and $D^{(1)}$ for dD/dE. Alternatively, if it is assumed that the diffusion coefficients D_1 and D_2 are sufficiently small, the terms involving them can be neglected, and the domain is controlled by the rate of transfer between states. Then, after eliminating n_1 from Eqs. (1) and (2), dividing the resulting equation by $E(\mu_1 - \mu_2) \neq 0$, substituting the resulting value of n_2 in Eq. (3), and dividing by $S_1 + S_2$, we obtain

$$-\frac{v_1 v_2}{(S_1 + S_2)}\frac{d^2E}{du^2} + \frac{G}{(S_1 + S_2)}\left(\frac{dE}{du}\right)^2 + \left\{c - \mu E + \frac{4\pi e N}{\kappa}\frac{H}{(S_1 + S_2)}\right\}\frac{dE}{du} - \frac{4\pi e N}{\kappa}\mu E + \frac{4\pi J}{\kappa} = 0, \tag{5b}$$

where we have written

$$v_1 = \mu_1 E - c,$$

$$v_2 = \mu_2 E - c,$$

$$\mu = (\mu_1 S_2 + \mu_2 S_1)/(S_1 + S_2),$$

$$G = (\mu_1' v_2^2 - \mu_2' v_1^2)/(v_1 - v_2),$$

$$H = \{\mu_2' v_1 (J/eN - \mu_1 E) - \mu_1' v_2 (J/eN - \mu_2 E)\}/(v_1 - v_2),$$

$$\mu_1' = \frac{d}{dE}(\mu_1 E), \quad \text{and}$$

$$\mu_2' = \frac{d}{dE}(\mu_2 E).$$

It will be seen that both Eq. (5a) and Eq. (5b) can be written in the form

$$F_1(E)\frac{d^2E}{du^2} + F_2(E)\left(\frac{dE}{du}\right)^2 + F_3(E)\frac{dE}{du} + F_4(E) = 0 \tag{6}$$

where F_1, F_2, F_3, F_4 are all continuous functions of E. By means of the substitutions $dE/du = p$, $d^2E/du^2 = dp/du$, Eq. (6) can be replaced by the system of equations

$$\frac{dp}{du} = -\frac{F_2}{F_1}p^2 - \frac{F_3}{F_1}p - \frac{F_4}{F_1}, \qquad \frac{dE}{du} = p. \tag{7}$$

The nature of the solutions of this system, in the (E, p) plane, can be discussed using the classical topological theory[9] of nonlinear differential equations.

We note first that the system (7) has singular points at $p = 0$, $F_4(E)/F_1(E) = 0$; that is, in the (E, p) plane, a singular point exists at a point E_i on the E-axis wherever $\mu(E_i)\cdot E_i = J/eN$, provided the appropriate quantity D or $v_1v_2/(S_1 + S_2)$ is not zero. Now, if a solution is to describe a single, steadily travelling domain in the (E, u) plane, as shown in Fig. 1(a), the trajectory T in the (E, p) plane must be a closed curve, emanating from and returning to a *saddle point*, as shown in Fig. 1(b). The closure of T depends on the value of c relative to other quantities in the problem, as we now show. Suppose there exists a closed trajectory* T_0, corresponding to a particular velocity c_0. If we can show that, when the conditions are changed, the new trajectories cross T_0 only in one sense, then it follows that, as we trace out a given one of these, say T_1, more and more trajectories enter the space between T_1 and T_0. Thus, if T_0 is closed, T_1 cannot be, and must diverge farther and farther from T_0. (See Fig. 2.) To show this, in the diffusion-controlled case, we have only to eliminate u between Eqs. (7), by taking their ratio and then differentiating with respect to c. Thus, at any given point (E, p), say on T_0, we have

$$\left[\frac{\partial}{\partial c}\left(\frac{dp}{dE}\right)\right]_{p,E} = -1/D. \tag{8a}$$

Since it will be shown later that other mathematical conditions (not to mention physical considerations) require that D be positive, we see that the trajectories corresponding, e.g., to $c = c_0 + \Delta c$ have, at any point

*This closed trajectory is not a Poincaré limit cycle, as it is not periodic.

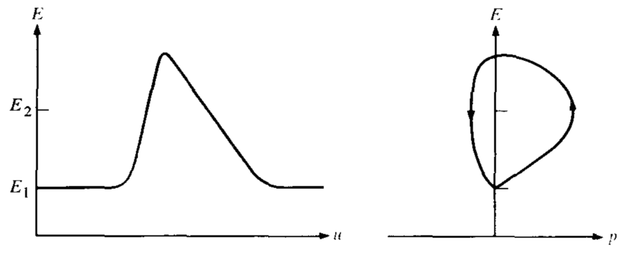

Figure 1 A steadily travelling high-field domain. (a) Electric field E as a function of the moving coordinate u. (b) E as a function of $p = dE/du$.

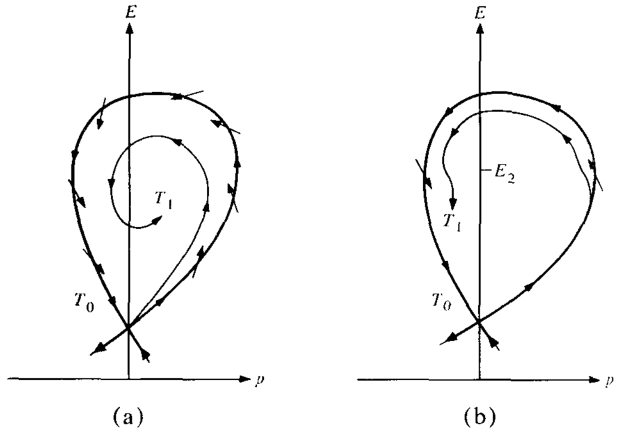

Figure 2 Effect of variation of parameters on trajectories in the (E, p) plane. T_0 is an acceptable closed trajectory, T_1 is a result of incorrect choice of parameters. (a) Diffusion-controlled case: variation of velocity c. (b) Transfer-controlled case: variation of transfer rate S at $E = E_2$.

on T_0, a smaller value of dp/dE than has T_0. Since the change in trajectory shape must be a continuous function of c, this change in dp/dE can amount only to a small change, not a reversal of direction, of the motion of the representative point. Hence almost all trajectories for $c = c_0 + \Delta c$ cross T_0 toward the inside, and therefore spiral inward. Since it cannot cross them, the singular trajectory T_1 which starts from the saddle point must spiral similarly, as shown in Fig. 2(a). Correspondingly, for $c = c_0 - \Delta c$ the trajectories spiral outward.

In the case of the transfer-controlled domain, it is not possible to prove such a simple result, because c appears in F_1 and F_2, as well as in F_3. However, the conclusion that the relative value of c determines the closure of the trajectory can be reached in a more roundabout way. Thus for comparison with T_0 we take a new situation in which, with one exception, all parameters (including c) have the same values. The exception is that, in the immediate neighborhood of the field E_2 corresponding to the upper singular point, S_1 and S_2 have been changed while their ratio has been kept constant. This leaves $\mu(E)$ unchanged, while varying $S = S_1(E_2) + S_2(E_2)$ from its value S_0 on T_0. On eliminating u as before from Eq. (7), and differentiating with respect to S, we obtain

$$\left[\frac{\partial}{\partial c}\left(\frac{dp}{dE}\right)\right]_{p,E_2} = [(\mu E - c_0)/v_1 v_2]_{E_2}. \qquad (8b)$$

The term in F_4/F_1 does not appear because $F_4(E_2) = 0$, by definition. The right-hand side of Eq. (8b) has the same, as yet unknown, sign on both sides of the E-axis. Thus new trajectories cross T_0, e.g., inward on *both* sides near E_2, and T_1 again fails to close in the same way [Fig. (2b)]. Inwardly or outwardly spiralling behavior again results, depending now on the departure of S from S_0. If we can show (as we shall do) that the value of S_0 depends on c_0, and that $c_0 \neq (\mu E)_{E_2}$, then it follows that a departure of c from c_0, at fixed S, leads to inward or outward spiralling for the transfer-controlled case also. This change from inward to outward spiralling as c passes through c_0 shows that, for $c = c_0$, the trajectories immediately inside T_0 must be closed curves, both in the transfer- and diffusion-controlled cases. Because all the functions entering the problem are continuous, no limit cycle can exist inside T_0 under these conditions. The nest of closed curves must therefore continue inward to enclose a singular point, which is thus seen to be a *center* when $c = c_0$. Note that the proof that the singular point inside T_0 is a center, on which the rest of this paper depends, is purely topological in nature, and does not depend on the usual analytical expansion procedure. This procedure is used in the next section to obtain a condition on c_0.

We are now in a position to state a topological condition for the existence of an isolated, steadily-travelling high-field domain: There must be at least two singular points, of which the lowest $(E_1, 0)$ is a saddle and the next lowest $(E_2, 0)$ is a center. The nature of a singular point can be determined by making an expansion to first order in $(E - E_i)$ and p in its neighborhood:

$$\frac{dp}{du} \approx \frac{F_3}{F_1} p - \frac{1}{F_1}\left(F_4^{(1)} - \frac{F_4 F_1^{(1)}}{F_1}\right)(E - E_i);$$

$$\frac{d(E - E_i)}{du} = p. \qquad (9)$$

Then the characteristic equation for Eq. (9) is

$$\begin{vmatrix} -\dfrac{F_3}{F_1} - \lambda & -\dfrac{1}{F_1}\left(F_4^{(1)} - \dfrac{F_4 F_1^{(1)}}{F_1}\right) \\ 1 & -\lambda \end{vmatrix} = 0. \qquad (10)$$

A necessary condition for a center is that the roots λ_1 and λ_2 of Eq. (10) be purely imaginary, whereas the

* Strictly speaking, this singularity might be an outwardly stable or unstable limit cycle, but these do not in fact exist in this problem.

condition for a saddle is that they be real but of opposite signs. Thus the required conditions are found to be

$$F_1(E_2)F_4^{(1)}(E_2) > \tfrac{1}{4}F_3^2(E_2) = 0;$$
$$F_1(E_1)F_4^{(1)}(E_1) < 0, \quad (11)$$

where we have made use of the conditions $F_4(E_2) = F_4(E_1) = 0$ defining the singular points.

If now we interpret conditions (11) in terms of Eqs. (5a) and (5b) for the diffusion and transfer-controlled domains, respectively, we obtain, after some rearrangement,

$$c_0 = \frac{J}{eN} - \frac{4\pi eN}{\kappa} D^{(1)}(E_2),$$
$$D(E_2)\mu'(E_2) < 0 < D(E_1)\mu'(E_1), \quad (12a)$$

and

$$c_0 = \frac{J}{eN}\left(\frac{1-\omega_r^{**}/S}{1+\omega_r^{*}/S}\right)_{E_2},$$
$$v_1(E_2)v_2(E_2)\mu'(E_2) > 0 > v_1(E_1)v_2(E_1)\mu'(E_1). \quad (12b)$$

Here we have written $S = S_1 + S_2$, $\mu' = d(\mu E)/dE$,

$\omega_r^* = (4\pi eN/\kappa)(S_1\mu_2' + S_2\mu_1')/S$, and

$\omega_r^{**} = (4\pi eN/\kappa)(S_1\mu_1\mu_2' + S_2\mu_2\mu_1')/(S_1\mu_2 + S_2\mu_1)$.

The quantity μ' is simply the macroscopic differential mobility. Both ω_r^{**} and ω_r^* have the form of a dielectric relaxation frequency. In addition, the latter has a simple physical significance; it is the value that would be measured at high frequencies, where only the drift velocities of the carriers can follow a changing applied field, and n_1 and n_2 remain constant at the appropriate average value. It will be seen that the required dependence of c_0 on S has now been deduced, so that our previous conclusion about the effect of c on the trajectories is justified as long as N and S are finite.

A striking feature of Eqs. (12) is that, given J, the domain velocity is independent of the properties of the semiconductor, except for those at a single high value E_2 of electric field. This field is, of course, that at which the electron velocity returns again to the value J/eN, which it must have outside the domain in order to carry the current density J under constant-field conditions. As long as they do not introduce additional singular points, the properties at other fields are irrelevant.

Discussion

In spite of its simplicity, Eq. (12a) for the velocity of a diffusion-controlled domain appears to be novel. Butcher[10] and Lampert[11] have previously obtained a result, which in our notation can be written as

$$c_0 = \frac{J}{eN} - \frac{4\pi eN}{\kappa} \times \oint (pD^{(1)}/D)\, dE \Big/ \oint [1/D(p + 4\pi eN/\kappa)]\, dE, \quad (13)$$

which gives the domain velocity in terms of integrals around the closed trajectory in the (E, p) plane. This result, however, cannot be evaluated until the exact shape of the trajectory is known, whereas (12a) requires only a knowledge of $\mu(E)$ and $D(E)$. The two results appear qualitatively consistent, both depending on $D^{(1)}$ in a similar way. The biggest contribution to (13) comes from the region where the trajectory is widest, that is, near E_2. Presumably, it should be possible to show that the two results are equivalent, but we have not been successful in this. The conditions on the sign of $D\mu'$, given in (12a), contain nothing surprising. For $D > 0$, they merely require that the differential mobility μ' be positive at E_1 and negative at E_2. We now see that the other assertion made in the introduction to this paper (that a steadily-travelling domain cannot exist unless $D \neq 0$ or $(S_1 + S_2)^{-1} \neq 0$) can be proved from the condition $F_1 \neq 0$, which is required in order that the points $p = 0$, $F_4(E) = 0$ be singular points. It may also be noted that the condition $\mu'(E_2)D(E_2) < 0$ precludes the existence of domains due to a field-dependent D (the diffusion instability[12]) alone, as long as D and μ' remain positive.

For the transfer-controlled domain, Eq. (12b) shows that, if μ_1, μ_2, μ_1', μ_2' are non-negative, as is normally the case, the velocity of the domain is less than J/eN, that of the electrons outside the domain. In the important case for which the transfer is between the conduction band and traps, for which, e.g., $\mu_2 = \mu_2' = 0$, the velocity is given by

$$c_0 = \frac{J}{eN}\left\{1 + \frac{4\pi eN}{\kappa}\frac{\mu_1' S_2}{(S_1 + S_2)^2}\right\}^{-1}, \quad (14)$$

where the field-dependent quantities are, of course, to be evaluated at E_2. This equation can be compared with a result of Kalashnikov and Bonch-Bruevich[13] which, under certain approximations, gives a similar equation, but in which the field-dependent quantities are to be evaluated, not at E_2, but at the somewhat higher field existing at the peak of the domain.

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