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Boltzmann Equation and Wave-Particle Drag in a Shock Strained Semiconductor

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SUMMARY

The theory of the acousto-electric effect is extended to a mechanically shock strained semiconductor by use of the Boltzmann equation with Maxwellian distribution of free electrons. From the linearized equation the explicit expression for the electric field behind the shock front is found in terms of Hermitian polynomials. The result suggests that particularly at low temperatures one may observe an appreciable current behind the shock front.

1. Introduction

It is known [1, 2] that when an acoustic wave travels through a solid medium containing mobile charges, a d.c. electric field appears along the direction of wave propagation. This effect is due to a wave-particle drag when mobile charges lag behind the motion of wave because of a finite time required to reach equilibrium. It is also called "acoustic-electric effect" by Parmenter [1], the first investigator.

Since an infinitely weak shock is an acoustic wave, one will reasonably expect a similar wave-particle drag phenomenon in a shock strained medium with mobile charges. But of course whether this effect for shock wave measurements is significant or not depends upon the magnitude and the relaxation time of unequilibrium free charges during the shock propagation through a sample. Brooks [3] speculated a long relaxation time of excited electrons and recently Graham et al. reported [4] that relaxation times in Germanium might be as long as 10^{-7} sec. This is not small enough to be completely ignored when one recalls the time scale of shock measurements (say 10^{-6} sec) in solids.

Hence it will be interesting to see, theoretically, under what circumstances the preceding effect might be important in shock measurements. This is the first of our attemps in that direction and for simplicity a semiconductor with free electrons of Maxwellian distribution is chosen.

The important difference here between a shock and an acoustic wave is that a shock is discontinuous at its front and a shocked medium will acquire a finite particle velocity with respect to rest co-ordinates. Hence when there exists a d.c. field in moving material co-ordinates attached to a shock strained medium, this field obviously will appear as an apparent current in rest (say laboratory) co-ordinates.

Therefore our object is to determine the magnitude and shape of this current behind the shock front. This is done in what follows by solving a one-dimensional Boltzmann equation with Maxwellian distributions of mobile electrons. In section 2 the equations are set out for an idealized steady state situation, and in section 3 the solution is sought for a linearized version by expanding the distribution function in terms of Hermitian polynomials [5], [6].

2. Electrons in a Shocked Semiconductor and Boltzmann Equation

Let us assume that a steady one-dimensional plane shock is moving from $+\infty$ to $-\infty$ at a speed U (Fig. 1) in a semiconductor. Then there will be a discontinuity in pressure, density, etc. across the shock front, which is assumed to be infinitely thin on the ground that the relaxation time of phonons is much shorter than that of electrons.

In the upstream where the material is undisturbed free electrons are in equilibrium with the lattice and their velocity distribution in one dimension can be given approximately by [7],

$$f_0(v) = n_0(\beta_0/\pi)^{\frac{1}{2}} \exp(-\beta_0 v^2), \tag{1}$$

where β_0 is $m_0/2kT_0$, n_0 is the number of electrons in unit volume, T_0 is temperature, k is Boltzmann constant and m_0 is the electron mass. For an intrinsic semiconductor n_0 is equal to

$$2(2\pi m_0 kT_0/h^2)^{\frac{3}{2}} \exp(-E_g/2kT_0), \tag{2}$$

where h is the Planck constant and E_g is the energy gap.

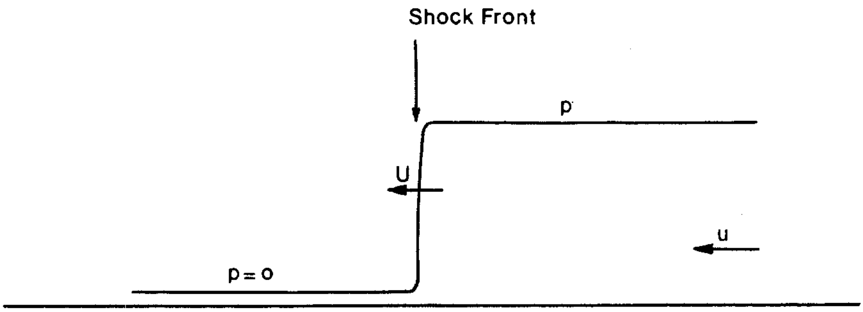

Figure 1. A plane shock.

However when a medium is suddenly overtaken by a shock wave, it is very unlikely that all of the free electrons are in thermal equilibrium and obey a Maxwell distribution such as (1). Furthermore at the shock front two lattices, strained and unstrained, have not established an equilibrium contact and they have different electron distributions. But of course they start immediately to redistribute their electrons at the contact in such a way that at equilibrium they have equal Fermi surfaces. Here we assume separate distribution functions across the shock front, the validity of this assumption being further elucidated in section 3.

Then one model which we can use is a double-humped distribution function $f_1(v)$ at the front, when approached from the strained side, i.e.,

$$f_1(v) = f_0(v) + n_1(\beta_1/\pi)^{\frac{1}{2}} \exp\{-\beta_1(v-u)^2\}, \tag{3}$$

where the subscript "1" denotes values in a shocked state and u is the particle velocity. n_0 is also adjusted for density change. It means that the initially existing free electrons are left undisturbed when the lattice is suddenly compressed, but the newly created ones, due to the changes in E_g etc., are in equilibrium with the strained lattice. Since no experiments are available to determine a more realistic form of (3), it is chosen on the basis of simplicity and mathematical manageability. However if one accepts a spherical energy surface and the experimental fact [4] that the intrinsic resistivity of Germanium depends mainly upon E_g under a shock strain, (3) will be a reasonable function as a first approximation.

Downstream, far behind the shock front all the electrons will be in equilibrium in a strained lattice. Hence they should have a velocity distribution given by

$$n(\beta_1/\pi)^{\frac{1}{2}} \exp\{-\beta_1(v-u)^2\}. \tag{4}$$

If there is no sink of electrons and if a sample remains intrinsic, n is given by

$$n = 2(2\pi m_1 kT_1/h^2)^{\frac{3}{2}} \exp(-E_{g,1}/2kT_1). \tag{5}$$

Hence our concern is primarily with the relaxation of $f(v)$ from (3) to (4) and with solving a Boltzmann equation.

The one-dimensional Boltzmann equation for an electron distribution function $f(x, v, t)$ is

$$f_t + vf_x - (eE/m)f_v = (f_t)_{\text{collision}},$$

where the subscripts denote partial differentiations. The electric field E satisfies the Poisson equation,

$$E_x = (4\pi e/\varepsilon)(n^+ - \int_{-\infty}^{\infty} f\,dv)\,,$$

where n^+ is the density of singly ionized lattice atoms per unit volume and is assumed to be equal to n in the shocked lattice. ε is the dielectric constant of a semiconductor.

Since we are assuming a steady state propagation of shock, it is best to treat the problem in the co-ordinate z attached to the shock front (Fig. 2). Then considering the front as the origin

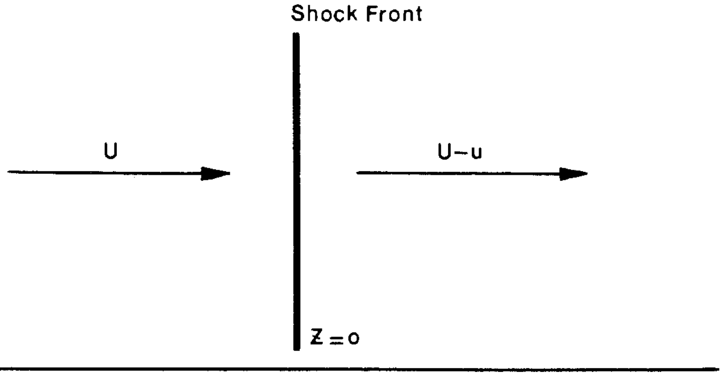

Figure 2. The z co-ordinate and the motion of material.

of the new co-ordinate z one finds a steady state Boltzmann equation in which a simple relaxation model is assumed for the collisional term,

$$(v+U)f_z - (eE/m)f_v = (n\Phi - f)/\tau\,, \tag{6}$$

$$dE/dz = (4\pi e/\varepsilon)(n - \int_{-\infty}^{\infty} f\,dv) \text{ for } z \geqq 0\,, \tag{7}$$

where τ is the relaxation time and Φ is

$$(\beta_1/\pi)^{\frac{1}{2}} \exp\{-\beta_1(v-U+u)^2\}\,. \tag{8}$$

The boundary conditions (3) and (4) are, in the z co-ordinate,

$$f(+0, v) = n_0(\beta_0/\pi)^{\frac{1}{2}} \exp\{-\beta_0(v-U)^2\} + n_1(\beta_1/\pi)^{\frac{1}{2}} \exp\{-\beta_1(v-U+u)^2\}\,, \tag{9}$$

$$f(\infty, v) = n\Phi(v)\,. \tag{10}$$

Hence from (7), (9) and (10) it is found that

$$dE(+0)/dz = dE(\infty)/dz = 0\,. \tag{11}$$

In order to solve the equations (6) and (7) with (9)–(11), we make further simplifications based upon the experiments [4]. They are

$$m_0 = m_1 = m\,, \quad T_0 = T_1 = T\,, \quad \beta_0 = \beta_1 = \beta\,, \text{ and } n_0 \ll n_1\,.$$

Since for a shock of 44 kb in Germanium, $(T_1 - T_0)/T_0 \leqq 0.02$ and $(E_{g,0} - E_{g,1})/E_{g,0} = 0.33$, they can be justified as a first approximation.

3. A Linear Isothermal Solution

Since $n_0 \ll n_1$, it is assumed $f(z, v)$ can be put in the form

$$f(z, v) = n_1\Phi + F(z, v)\,, \tag{12}$$

where $n_1\,\Phi \gg F$.

Then ignoring F in the second term of (6) one finds

$$(v+U)F_z-(n_1 eE/m)\Phi_v=(n_0\Phi-F)/\tau\,. \tag{13}$$

$$dE/dz=(4\pi e/\varepsilon)\left(n_0-\int_{-\infty}^{\infty} F\,dv\right). \tag{14}$$

In order to solve (13) and (14) we expand F in Hermitian polynomials.
This expansion enables us to integrate (14) first.
Let

$$F=\sum_{n=0}^{\infty} g_n(z)H_n(y)\exp(-y^2)\,,$$

where $y=(v-U)\beta^{\frac{1}{2}}$.
This choice of y is based on the condition (compare (9) and (12))

$$F(+0,v)=n_0(\beta/\pi)\exp\{-\beta\ (v-U)^2\}\,. \tag{15}$$

The orthogonality relation of the Hermitian polynomials is given by

$$\int_{-\infty}^{\infty} H_n(y)H_m(y)\exp(-y^2)dy=2^n n!\,\pi^{\frac{1}{2}}\delta_{n,m}\,. \tag{16}$$

Then the boundary conditions for $g_n(z)$ can be found as follows:
Since

$$F(+0,v)=n_0(\beta/\pi)^{\frac{1}{2}}\exp(-y^2)=\sum_0^{\infty} g_n(0)H_n(y)\exp(-y^2)\,,$$

$$F(\infty,v)=n_0(\beta/\pi)^{\frac{1}{2}}\exp\{-(y+\sqrt{\beta}u)^2\}=\sum_0^{\infty} g_n(\infty)H_n(y)\exp(-y^2)\,,$$

the coefficients $g_n(0)$ are

$$g_0(0)=n_0(\beta/\pi)^{\frac{1}{2}}\,,\qquad g_n(0)=0\ \text{ for }\ n\neq 0\,, \tag{17}$$

and it is found that

$$g_n(\infty)=\{n_0(\beta/\pi)^{\frac{1}{2}}/2^n n!\}\int_{-\infty}^{\infty}\pi^{-\frac{1}{2}}H_n(y)\exp\{-(y+\beta^{\frac{1}{2}}u)^2\}\,dy\,.$$

This integral can be evaluated by the formula

$$q_n=\int_{-\infty}^{\infty}\pi^{-\frac{1}{2}}y^n\exp\{-(y+\beta^{\frac{1}{2}}u)\}^2\,dy\,,$$

$$=\sum_{i=0}^{[n/2]}(-\beta^{\frac{1}{2}}u)^{n-2i}n!/2^{2i}i!(n-2i)!\,.$$

For example we have

$$q_0=1\,,\quad q_1=-\beta^{\frac{1}{2}}u\,,$$

and

$$g_0(\infty)=n_0(\beta/\pi)^{\frac{1}{2}}\,, \tag{18}$$

$$g_1(\infty)=-n_0\beta u/\pi^{\frac{1}{2}}\,. \tag{19}$$

Since the reference point of $E(z)$ can be taken anywhere and $E(0)$ is so chosen, (14) can be integrated as

$$E(z)=(4\pi e/\varepsilon)\left\{n_0 z-\beta^{-\frac{1}{2}}\sum_0^{\infty}\left[\int_0^z g_n(z)dz\right]\left[\int_{-\infty}^{\infty}H_n(y)\exp(-y^2)dy\right]\right\}.$$

But using the orthogonality relation (16), one finds

$$E(z) = (4\pi e/\varepsilon)\left\{n_0 z - (\pi/\beta)^{\frac{1}{2}} \int_0^z g_0(z)\,dz\right\}. \tag{20}$$

Then from (13) and (20), it is found that

$$\tau(v+U)\sum_0^\infty g_n'(z) H_n \exp(-y^2) + \sum_0^\infty g_n H_n \exp(-y^2) - n_0 \Phi,$$

$$-(4\pi\tau n_1 e^2/m\varepsilon)\left\{n_0 z - (\pi/\beta)^{\frac{1}{2}} \int_0^z g_0(z)\,dz\right\}\Phi_v = 0\,.$$

By use of (16) and the recurrence relation

$$H_{n+1} = 2yH_n - 2nH_{n-1}\,,$$

we get an infinite set of second order equations with constant coefficients;

$$G_n'' + (1/2\tau U)G_n' + Q_n \pi^{\frac{1}{2}} G_0 + (1/2U\beta^{\frac{1}{2}})\{(n+1)G_{n+1}'' + 1/2G_{n-1}''\} = R_n + n_0 z \beta^{\frac{1}{2}} Q_n \qquad \text{for } n = 0, 1, 2, \ldots \tag{21}$$

where

$$G_n = \int_0^z g_n(z)\,dz\,,$$

$$Q_n = (\omega_p^2/2^{n+1} n!\,\pi^{\frac{1}{2}} U)\int_{-\infty}^{\infty} (d\Phi/dy) H_n\,dy\,,$$

$$R_n = (n_0/2^{n+1} n!\,\pi^{\frac{1}{2}} \tau U)\int_{-\infty}^{\infty} H_n \Phi\,dy\,,$$

and

$$\omega_p^2 = 4\pi n_1 e^2/m\varepsilon\,.$$

Unfortunately it is not possible to get the complete solution. But from the point of view of experimental work, one's concern is not with a complete solution of G_n (or g_n) but rather, as mentioned in section 1, with $E(z)$. Then a solution by truncating G_n (n=0, 1, ...) at a finite number, as we shall see shortly, provides an approximation of $E(z)$. It is, however, difficult to assess whether or not the solution thus obtained yields a good approximation to the distribution function $F(z, v)$ for the entire domain of z and v.

(A) *A single term solution*; $F = g_0 H_0 \exp(-y^2)$.
From (21) one finds the differential equation for $g_0(z)$.

$$g_0' + (1/2\tau U) g_0 = n_0 \beta^{\frac{1}{2}}/2\pi^{\frac{1}{2}}\tau\ U\,.$$

Hence it can be shown that the solution which satisfies the boundary conditions (17) and (18) is

$$g_0 = n_0(\beta/\pi)^{\frac{1}{2}}.$$

Then from (20) $E(z)$ becomes zero for all z. In fact if one assumes $F = g_0 H_0 \exp(-y^2)$, this is what we expected from (14). Physically it means that there is no change in the old distribution function.

(B) *Two term solution*; $F = (g_0 H_0 + g_1 H_1)\exp(-y^2)$.
Now one has a set of equations

$$G_0'' + (1/2\tau U)G_0' + (1/2U\beta^{\frac{1}{2}}) g_1' = n_0 \beta^{\frac{1}{2}}/2\pi^{\frac{1}{2}}\tau U\,,$$

$$(1/4U\beta^{\frac{1}{2}})G_0'' - (\omega_p^2 \beta^{\frac{1}{2}}/2U) G_0 + g_1' + (1/2\tau U) g_1 = -n_0 \beta u/2\pi^{\frac{1}{2}}\tau U - n_0 \omega_p^2 \beta z/2\pi^{\frac{1}{2}} U\,,$$

where G_1' is replaced by g_1 for convenience.

The solution is straightforward. The characteristic roots λ_i are

$$\lambda_1 = 0$$

$$\lambda_{2,3} = -4\beta U/\tau(8\beta U^2-1) \pm \{(2\beta)^{\frac{1}{2}}\omega_p/(8\beta U^2-1)\}\{(1-8\beta U^2)+(1/\tau^2\omega_p^2\}^{\frac{1}{2}} . \tag{22}$$

Hence if

$$8\beta U^2 < 1 \quad \text{or} \quad 2U < (kT/m)^{\frac{1}{2}} ,$$

there exists an exponentially growing solution. Since the squared average electron velocity $\langle v^2 \rangle^{\frac{1}{2}}$ is $(kT/m)^{\frac{1}{2}}$, this growing solution will set in when the average velocity is twice the shock speed. This may be due to the truncation error but is likely to be from the idealized boundary conditions at $z=0$. Because for the latter if the average electron velocity exceeds the shock velocity a great deal, we are ignoring the majority of electrons outrunning the shock front (see Fig. 3). But our assumption on a contact of shocked and undisturbed lattices is implicitly

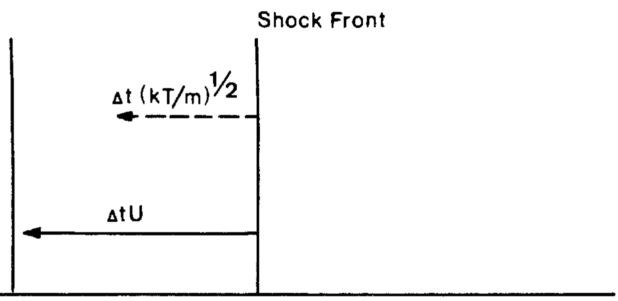

Figure 3. The motions of shock front and average electrons.

stating the condition that U must be greater than the average speed $(kT/m)^{\frac{1}{2}}$. Of course one can always discard the exponentially growing solution on physical grounds, but then it can be shown that the solution G_0 which satisfies its boundary conditions is again $n_0(\beta/\pi)^{\frac{1}{2}} z$.

Therefore for the two term solution, let us assume

$$8\beta U^2 > 1 . \tag{23}$$

Then one has

(i) two negative real roots for $1+1/\tau^2\omega_p^2 > 8\beta U^2 > 1$,

(ii) two conjugate imaginary roots for $8\beta U^2 > 1+1/\tau^2\omega_p^2$.

By way of illustration let us study the first case which in fact corresponds to a temperature not too close to absolute zero. From (22) one can immediately draw the general solutions G_0 and g_1;

$$G_0 = a_1 + a_2 \exp(\lambda_2 z) + a_3 \exp(\lambda_3 z) + n_0 u \beta^{\frac{1}{2}}/\omega_p^2 \tau \pi^{\frac{1}{2}} + n_0 \beta^{\frac{1}{2}} z/\pi^{\frac{1}{2}} , \tag{24}$$

$$g_1 = m_1 a_1 + m_2 a_2 \exp(\lambda_2 z) + m_3 a_3 \exp(\lambda_3 z) , \tag{25}$$

where m_i are given by

$$m_1 = \beta^{\frac{1}{2}}\omega_p^2 \tau ,$$

$$m_2 = -2\beta^{\frac{1}{2}} U(\lambda_2 + 1/2\tau U) ,$$

$$m_3 = -2\beta^{\frac{1}{2}} U(\lambda_3 + 1/2\tau U) ,$$

and where the forms of particular solutions were already chosen to be the best for satisfying the boundary conditions. It should be pointed out that since (24) and (25) are the truncated solutions, they cannot satisfy all of their boundary conditions, unless it happens by accident as in (A). But what we need is $G_0(z)$, so we can put all the errors into $g_1(z)$. If we add a third term in the expansion of F, we can choose the solutions G_0 and g_1 for which all of their boundary conditions are satisfied, but not some of g_2.

Since our interest is in the vicinity of $z=0$ where the two term solution is most valid, one finds, by introducing an error in $g_1(\infty)$, the following values for the coefficients

$$a_1 = -\beta^{\frac{1}{2}} n_0 u/\omega_p^2 \tau \pi^{\frac{1}{2}}(1+\omega_p^2\tau^2),$$
$$a_2 = -\beta^{\frac{1}{2}} n_0 u\tau\lambda_3/\pi^{\frac{1}{2}}(\lambda_3-\lambda_2)(1+\omega_p^2\tau^2),$$
$$a_3 = -\beta^{\frac{1}{2}} n_0 u\tau\lambda_2/\pi^{\frac{1}{2}}(\lambda_3-\lambda_2)(1+\omega_p^2\tau^2).$$

Then from (23) and the Poisson equation (14) it is found that the apparent charge ρ behind the shock front is.

$$\rho(z) = n_0 e\beta^{\frac{1}{2}} u\{\exp(\lambda_3 z)-\exp(\lambda_2 z)\}/2^{\frac{1}{2}}\omega_p\tau\{(1-8\beta U^2)+1/\omega_p^2\tau^2\}, \tag{26}$$

where $\lambda_3 > \lambda_2$ is assumed.

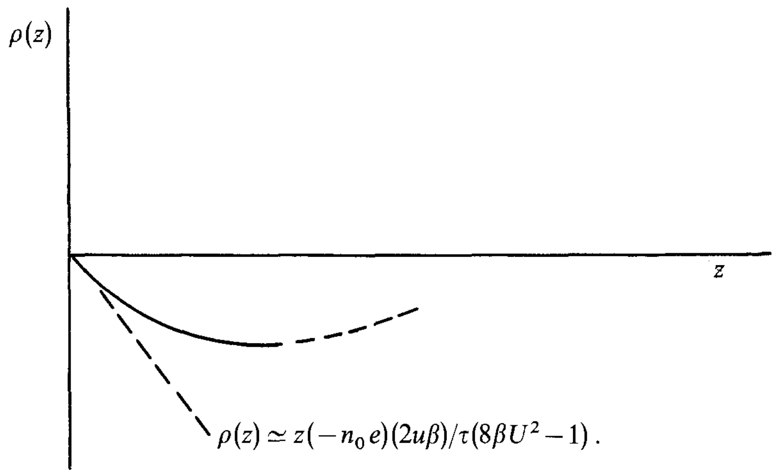

Figure 4. The apparent charge behind the shock front.

$\rho(z)$ is schematically shown in Fig. 4. Because of the nature of H_n, (26) is a good approximation only for a small z. Then expanding the exponential functions, it is found that

$$\rho(z) \simeq z(-n_0 e)(2u\beta)/\tau(8\beta U^2-1). \tag{27}$$

A word about the error in $g_1(\infty)$ is in order. Substituting a_i into $g_1(z)$, we obtain the value $g_1(\infty)$ as

$$g_1(\infty) = -\beta n_0 u/\pi^{\frac{1}{2}}(1+\omega_p^2\tau^2). \tag{28}$$

Hence it is desirous to have the condition

$$\omega_p\tau \ll 1.$$

In contrast, it is interesting to note [8] that the possibility of a plasma oscillation in an ionized medium is $\omega_p\tau \gg 1$.

4. Discussion

Since the z co-ordinate is moving with the speed U, the charge density ρ appears as a current ρU when looked at from laboratory co-ordinates. Whether or not this is easily measurable depends upon condition (23). For example if one substitutes a shock speed of 6 mm/μsec which is quoted [4] as the elastic shock speed in Ge for 44 kb, one obtains the critical temperature of 9°k. This is probably too cold for shock measurements to be carried out.

However if one raises the speed to 1 cm/μsec the temperature is 26°k, and it may not be an impossible temperature. But even then it is obvious from (2) that an intrinsic semiconductor will not serve as a good sample for demonstrating a wave-particle drag unless the energy gap is or becomes very narrow.

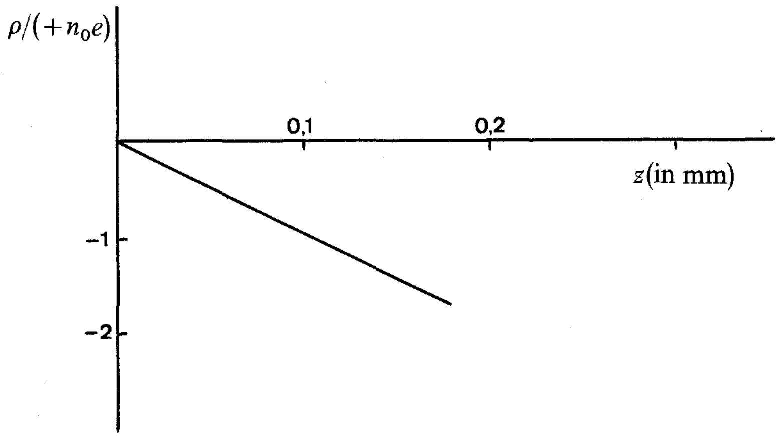

Figure 5. An hypothetical example of $U=10^6$ cm/μsec; $u=10^5$ cm/μsec and $\tau=10^{-8}$ sec.

In Fig. 5 in order to get an idea of the magnitude, an hypothetical case of (27) is demonstrated.

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