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Formation and dissipation of a Schottky barrier in a conducting dielectric*

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The formation of a cathode fall in an insulating material by means of a blocking electrode was studied by von Hippel *et al.* In this paper we consider the formation of the cathode fall, assuming that the material posseses an intrinsic conductivity whose carriers are not blocked by the electrode contacts. It is shown that the contact barrier should gradually dissipate due to charge neutralization, restoring the usual Ohmic behavior. The motion of the shock front and the external current are calculated.

I. INTRODUCTION

The kinetics of a cathode-fall buildup was first considered by von Hippel *et al.*[1] In this picture a cathode fall is formed when negative carriers are pulled by an applied field away from the cathode region, leaving that region with a net positive charge. The presence of a blocking cathode prevents the entrance of negative charges into the crystal, thus allowing a strong potential drop to form at the cathode. It was found that alkali-halide crystals, additively colored with F centers and under white light, provided a good system for demonstrating this process.[1-3]

We know, however, that ionic crystals possess ionic conductivity, and this would tend to neutralize those positive charges responsible for the cathode fall. In this paper we analyse the effect of such a mechanism in the formation of the cathode fall, under the assumption that these carriers responsible for the conductivity are not blocked at the electrode.

Although the approach of von Hippel *et al.* was devised for application in photoconducting crystals, it provides a first insight for the understanding of Schottky-barrier formation in general. The present treatment's generalizing it can be helpful in interpreting more complex situations.

II. THEORY

We shall assume that the material has mobile positive charges, while the compensating fixed matrix is negative. Their space-charge densities will be denoted by $+\rho_0'$ and $-\rho_0'$, respectively. This sign convention is opposite to that used in Ref. 1, and so some of the effects described there will have reverse polarity analogs here, for instance, one should expect an anode (rather than a cathode) fall to be formed. This change, however, is not important, since it is easy to know what happens when the signs of the mobile and fixed charges are interchanged. Also, we shall assume that the crystal has an intrinsic conductivity σ' and that the carriers contributing to it are not blocked by the electrodes.

We thus have two independent routes for conduction within the sample: the first is provided by the conductivity, while the second is due to the motion of the positive charges. The latter are blocked at the anode and thus give rise to the space-charge effects.

Under an applied external voltage V_0 the positive charges will start moving toward the cathode. It is then possible to divide the crystal into the two markedly different regions shown in Fig. 1. Region II $[d'(t')<x'<l]$ is characterized by the absence of excess charge; it extends itself from the shock front [e.g., the position of the last front of positive charge—a time dependent quantity which we will denote by $d'(t')$] to the cathode at l. Region I $[0<x'<d'(t')]$ is the (negatively charged) depleted region bounded on one side by the anode, at $x'=0$, and on the other side by $d'(t')$.

As a result of inclusion of conductivity on the model, one expects that the space-charge density at any point in region I will continuously decay to an asymptotic zero value. This will, in turn, affect the motion of the shock front.

In Sec. II A we set up the basic equations for the position of the shock front as a function of time. In Sec. II B we will then seek the externally measurable quantity, e.g., the total current.

A. Motion of the shock front

We will assume a solution of the Poisson and continuity equation such that (i) in Region I the charge density is $-\rho'(x',t')$ and the conduction current density is given by $\sigma'E'(x',t')$, E' being the electric field and (ii) in Region II the net value of the space charge is zero, while the conduction current density is $\mu\rho_0'E'(d',t')+\sigma'E'(d',t')$. Introducing dimensionless variables through the relations

$$x=\frac{x'}{l}, \quad \sigma=\frac{\sigma' l^2}{\epsilon V_0\mu}, \quad t=\frac{V_0\mu t'}{l^2},$$

$$\rho(x,t) = l^2\rho(x',t')/\epsilon V_0, \quad \rho_0 = \frac{l^2\rho_0'}{\epsilon V_0},$$

$$E(x,t) = \frac{l}{V_0}E'(x',t'), \quad d = \frac{d'}{l},$$

the assumed solution can be written

Region I: charge density $-\rho(x,t)$, conduction current density $\sigma E(x,t)$;

Region II: no net charge density and conduction current density $(\rho_0+\sigma)E(d,t)$.

With the help of the step function, here defined as

$$\Theta(d-x) = \begin{cases} 1 & \text{for } 0<x<d \\ 0 & \text{for } d<x<1 \end{cases},$$

we can write for the charge density $\bar{\rho}(x,t)$ and conduction current density $i(x,t)$ the following expressions valid for regions I and II:

$$\bar{\rho}(x,t) = -\rho(x,t)\Theta(d-x),$$

$$\bar{i}(x,t) = \sigma E(x,t) + \rho_0 E(x,t)\Theta(x-d).$$

We try to satisfy the Poisson and continuity equations,

$$\frac{\partial E}{\partial x} = \bar{\rho} \tag{1}$$

and

$$\frac{\partial\bar{\rho}}{\partial t} + \frac{\partial\bar{i}}{\partial x} = 0. \tag{2}$$

For this we find

$$\frac{\partial\bar{\rho}}{\partial t} = -\frac{\partial\rho}{\partial t}\Theta(d-x) - \rho\delta(d-x)\dot{d},$$

$$\frac{\partial\bar{i}}{\partial x} = -\sigma\rho\Theta(d-x) + \rho_0 E\delta(x-d),$$

or, using (2)

$$-\frac{\partial\rho}{\partial t}\Theta(d-x) - \rho\delta(d-x)\dot{d} = \sigma\rho\Theta(d-x) - \rho_0 E\delta(x-d). \tag{2a}$$

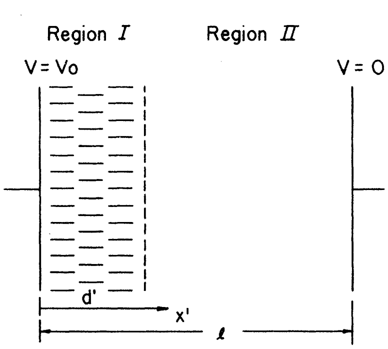

FIG. 1. Situation during the motion of shock front.

For $0<x<d$, we find

$$-\frac{\partial\rho}{\partial t} = \sigma\rho. \tag{3}$$

Integrating around $x=d$, (2a) becomes

$$\rho(d,t)\dot{d} = \rho_0 E(d,t).$$

Since the shock front moves with the velocity $\dot{d} = E(d,t)$, we conclude that the modulus of the negative charge density just after the front has passed is ρ_0. But this conclusion is just what we should expect from the model.

Calling $t(x)$ the time when the front passed the plane at x, we write, as the solution of Eq. (3),

$$\rho(x,t) = \rho_0 e^{-\sigma[t-t(x)]}.$$

The function $t(x)$ can be found as long as we know d as a function of t, because inverting $d=d(t)$ as $t=t(d)$ and substituting d for x, we have $t(x)$. We proceed to find $d(t)$. For this, we will use the condition

$$\int_0^1 E\,dx = 1. \tag{4}$$

Calling E_0 the field just in front of the anode $(x=0)$, we have

$$0<x<d, \quad E(x,t) = E_0(t) - \rho_0 e^{-\sigma t}\int_0^x e^{\sigma t(x')}dx', \tag{5}$$

$$d<x<1, \quad E(d,t) = E_0(t) - \rho_0 e^{-\sigma t}\int_0^d e^{\sigma t(x')}dx'. \tag{6}$$

Using (4), and performing a convenient integration by parts, we find

$$1 = E_0(t) - \rho_0 e^{-\sigma t}\left(\int_0^d e^{\sigma t(x')}dx' - \int_0^d x' e^{\sigma t(x')}dx'\right).$$

Since $\dot{d} = E(d,t)$, we write, taking account of Eq. (6),

$$\dot{d} = 1 - \rho_0 e^{-\sigma t}\int_0^d x' e^{\sigma t(x')}dx'.$$

Multiplying through by $e^{\sigma t}$ and differentiating once, we find

$$\ddot{d} + \dot{d}(\sigma + \rho_0 d) = \sigma. \tag{7}$$

Integrating Eq. (7), we have, with C a constant

$$\dot{d} + \sigma d = \sigma t - \tfrac{1}{2}\rho_0 d^2 + C. \tag{8}$$

At $t=0$, $\dot{d}=1$, $d=0$, and so C is found to be 1.

Calling

$$y = \sigma + \rho_0 d, \tag{9a}$$

Eq. (8) becomes

$$\dot{y} + \tfrac{1}{2}y^2 = \sigma\rho_0 t + \rho_0 + \tfrac{1}{2}\sigma^2. \tag{9b}$$

Performing a new change of variable with

$$z = \frac{y}{\sqrt{(2\rho_0)}}, \quad T = \sqrt{(\tfrac{1}{2}\rho_0 t^2)}, \quad \alpha = \sigma\sqrt{(2/\rho_0)}, \text{ and } \beta = \sigma/\rho_0, \tag{10}$$

Eq. (9b) becomes

$$\frac{dz}{dT} + z^2 = 1 + \alpha\left(T + \frac{\alpha}{4}\right). \tag{11}$$

We note that with the use of the dimensionless variables the whole theory is made to depend only on two parameters, either ρ_0 and σ or α and β.

In order to make a connection with the quantities defined in Ref. 1, we note that

$$\alpha = \frac{2l}{d'_\infty}\frac{\tau'}{\mu\rho'_0} = \frac{\sigma'\tau'}{\epsilon} \text{ and } \frac{\beta}{2\alpha} = \frac{d'_\infty}{l}, \tag{12}$$

where τ' is the relaxation time and d'_∞ the cathode-fall length, defined there to be

$$\tau' = (\epsilon l^2/2\rho'_0\mu^2 V_0)^{1/2} \text{ and } d' = (2\epsilon V_0/\rho'_0)^{1/2}.$$

Returning to Eq. (11), the initial value of z and its maximum value (corresponding to $d=1$) are found from Eq. (9a) and (10) to be

$$z(T=0) = \tfrac{1}{2}\alpha, \quad \max z = \tfrac{1}{2}\alpha + \alpha/2\beta. \tag{13}$$

It is possible, by means of a new change of variable, to transform Eq. (9b), which is of Ricatti type, in such a way as to be integrable by series. Instead, we preferred to perform computer integration, chosing convenient values for the parameter α. It is interesting that the equation of motion of the shock front depends only on the parameter α, which, according to Eq. (12), can be appreciable since it depends on the factor $2l/d'_\infty$, which usually is large.

We also see that for small α the solution of Eq. (11) approaches that of Ref. (1), while, for large values of α, the intrinsic conductivity dominates the behavior of the shock front, which now moves with a uniform velocity. This is illustrated in Fig. 2, where a plot of z vs T is shown, for $\alpha = 0$, 0.1, 1, 5, and 10.

It is important to realize that the continuous charge neutralization happening in region I allows the shock front to move till the cathode is reached. There is no rest point for the shock front, as was the case in Ref. 1.

On the other hand, the parameter β only appears as helping to fix the upper limit of z. This is not the case when we look for the total current.

B. Density of total current

The total current density j is constant through the sample. In region II, that is, for $d(t) < x < 1$, it is

$$j = (\rho_0 + \sigma)E(d(t)) + \frac{d}{dt}E(d(t)).$$

But $E(d(t)) = \dot{d}$; so j can be written

$$j = (\rho_0 + \sigma)\dot{d} + \ddot{d}. \tag{14}$$

With the help of Eq. (7) and Eq. (10), this becomes

$$j = (\alpha^2/2\beta^2)\{\beta + [1 - z^2 + \alpha(T + \tfrac{1}{4}\alpha)][1 - (2\beta/\alpha)z + \beta]\}.$$

The initial value of z is $\frac{1}{2}\alpha$, according to Eq. (12). If instead of z we use $S = z - \frac{1}{2}\alpha$, j is

$$j = (\alpha^2/2\beta^2)[\beta + (1 - S^2 - S\alpha + \alpha T)[1 - (2\beta/\alpha)S]]. \tag{15}$$

The term $\alpha^2/2\beta = \sigma$ gives the constant contribution coming from the conductivity. The remaining is related with the motion of the shock front. For $T = 0$, S is also zero, and it gives a contribution for $j(t=0)$, $\alpha^2/2\beta^2 = \rho_0$, as should be expected.

Figures 3(a)–3(d) show $(2\beta^2/\alpha^2)j - \beta$ (the contribution from the motion of shock front) as a function of T for some values of $2\beta/\alpha = d'_\infty/l$ and α [see Eq. (12)]. In all cases the whole plot is significant in the sense that the shock front has not reached the cathode and so Eq. (15) is valid.

We note from expression (14) that when the shock front reaches the cathode the current has only the ohmic component, remaining with this value thereafter. This can be seen, by considering the expression of the density of total current, now of region-I type,

$$j = \sigma E + \frac{\partial E}{\partial t}.$$

Integrating in x, from $x = 0$ to $x = 1$, and taking account of Eq. (4), we get

$$j = \sigma = \alpha^2/2\beta.$$

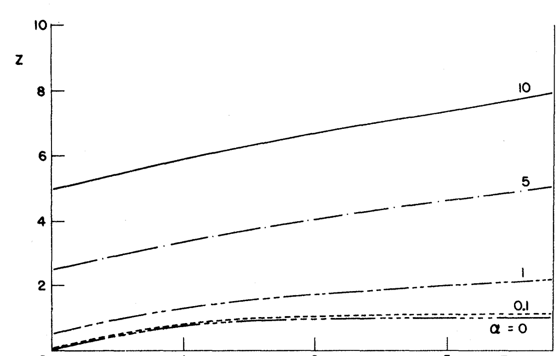

FIG. 2. Motion of the shock front for some values of α. The upper bound value of T depends on the parameter β and is not specified here.

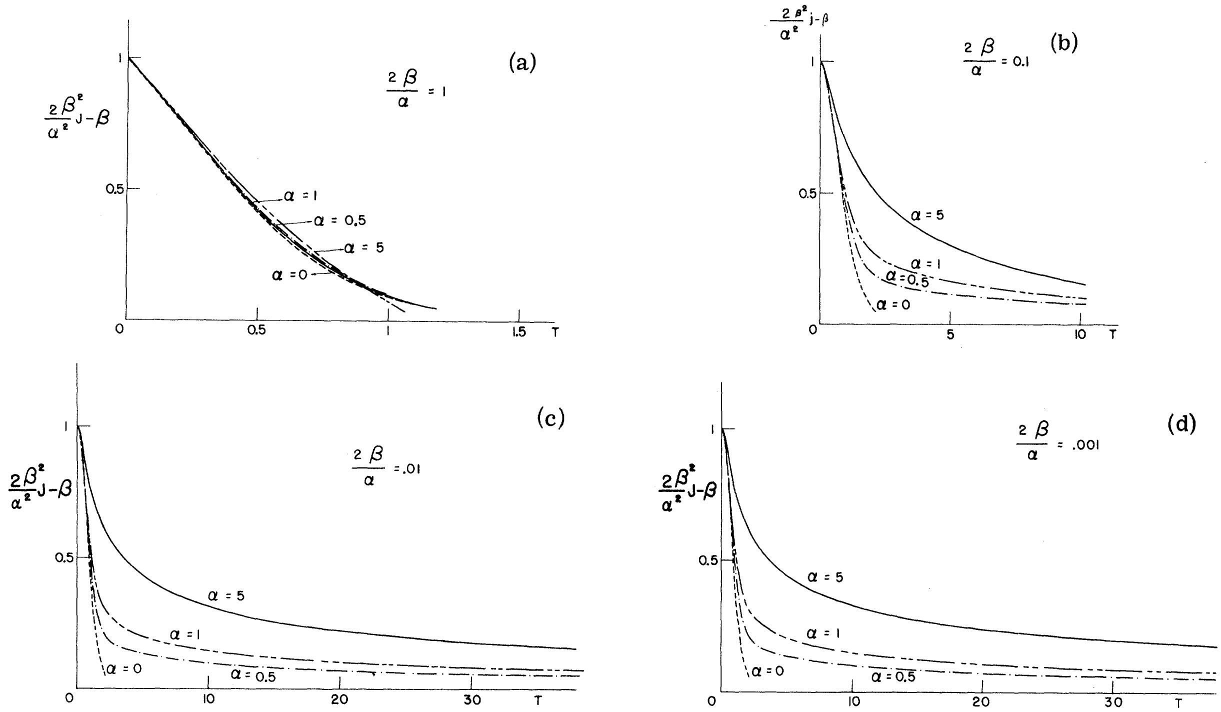

FIG. 3. Contribution to the total current coming from the shock front for specified values of the parameters α and $2\beta/\alpha$.

We see that j is continuous but its derivative with time is not. Besides, if the crystal were short circuited after the shock front had reached the anode, no current would be observed.

Another quantity of interest is the total charge Q per unit area that circulates in the external circuit, while the shock front moves from $d = 0$ to $d = 1$. Using Eq. (14) we easily find

$$Q = \int_0^{t(d=1)} j\,dt = \tfrac{1}{2}\rho_0 + \sigma t(d = 1).$$

The term $\sigma t(d = 1)$ clearly gives the contribution coming from the conductivity. The remaining one corresponds to the product of the charge ρ_0 with the mean distance it travels during the process. It is clear that as long as the shock front reaches the cathode the total charge depends only on the density of moving charges ρ_0' and the electrode distance l.

III. DISCUSSION

Figure 2 shows the motion of the shock front in units of z and T for some values of the parameter α. The $\alpha = 0$ curve reproduces the result of von Hippel *et al.*[1] For $\alpha = 0.01$ the curve practically duplicates that of $\alpha = 0$, at least in the range of T shown. For increasing α, the curve z vs T tends to a straight line, as a result of the increasing influence of the conductivity, which rapidly destroys the space charge just formed behind the shock front. The upper limit of T, corresponding to $z = \frac{1}{2}\alpha + (\alpha/2\beta)(d = 1)$ depends on the parameter β, and so should be found accordingly. [Figure 3 is a plot of $(2\beta^2/\alpha^2)j - \beta$ vs T, or the equivalent $(1/\rho_0)(j - \sigma)$ vs T.] Now, we have chosen the parameters α and $2\beta/\alpha = d'_\infty/l$ to express our results. Increasing values of α and decreasing values of $2\beta/\alpha$ mean decreasing barrier length of the sample.

We see that significant differences between the conducting and the perfect insulator crystals are already present for $2\beta/\alpha = 0.1$ and α of order of a few tenths, stressing again the relative importance of the conductivity for thin barriers. The $\alpha = 0$ curves reproduce, in each instance, the result of von Hippel *et al.*[1] and are only partially shown.

The present results constitute an exact solution for the problem of a fixed negative matrix and a free positive initially compensating space charge in a conducting dielectric, diffusion being neglected. In actual cases, the mobile space charge will not be free and trapping mechanism will come into play. Therefore at most we may expect an approximate resemblance of our results with some observed experimental dielectric polarizations. Among these, the polarization of naphthalene has been attributed in part to the formation of a Schottky barrier,[4] and the time dependence of its polarization is in apparent agreement with our results for small $2\beta/\alpha$ [Figs. 3(c) and 3(d)].

A competitive explanation for the nature of these decaying polarization currents can be found in the field of injection currents (space-charge limited currents).[5] Here a different boundary condition is assumed, e.g., ohmic contact at the injecting electrode, as opposed to our blocking contact for one kind of carrier. As Many and Rakavy[6] have shown, the transient before the establishment of the stationary regime can also show a decreasing current when a great deal of trapping is present and detrapping is almost absent. One of the characteristics of such a process is the dependence of the initial value of the current on V_0^2/l^3, differing markedly from the model studied in this article, which predicts an initial value of the current proportional to V_0/l. Aside from experimental difficulties, the difference just mentioned could, in principle, be used to distinguish both kinds of process.

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