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2004 J. Phys.: Condens. Matter 16 5999

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INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **16** (2004) 5999–6015 PII: S0953-8984(04)81849-6

Surface conductivity of insulators: one-dimensional initial value problems and the inviscid Burgers equation

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Received 10 June 2004
Published 13 August 2004
Online at stacks.iop.org/JPhysCM/16/5999
doi:10.1088/0953-8984/16/34/002

Abstract
A generalized derivation of the equations governing surface carrier diffusion in the surface region of an insulator is presented, based on the Mott–Gurney model of ionic diffusion as first proposed in Liesegang *et al* (1995 *J. Appl. Phys.* **77** 5782; 1996 *J. Appl. Phys.* **80** 6336). The resulting non-linear equations are decoupled for the case of one-dimensional diffusion and we show that the decay of the electric field is described by the inviscid Burgers equation. Imposing initial and boundary conditions reflecting the experimental configuration for a Cartesian system as discussed in Liesegang *et al*, a general solution for the carrier density in the surface of an insulating sample is derived for the case of one-dimensional charge motion.

1. Introduction

The electrical resistivity of insulating materials varies over many orders of magnitude, with the polymeric subgroup being among the highest resistivity materials; e.g., the resistivity of fluoropolymer materials is known to be the highest in value.

Common measuring techniques for the resistivity of insulators normally use the application of an electric field and measurement of the resultant current and the potential difference between electrode contacts on the sample. In these experiments, reliable measurement largely depends on obtaining good surface contact with electrodes over contact areas which are usually less than about 1 mm^2. The low conductivity of insulating polymers means there is usually only a small current flow, which is difficult to measure accurately. This in turn suggests that there is not much reliable reported experimental data for surface resistivity, especially for

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highly insulating polymeric materials. Consequently, there have been inconsistencies between descriptions of the nature of the transport process. Some authors [3, 4] suggest ionic conduction as the charge transport mechanism, while others [5] suggest electronic charge transfer. Later literature [6–8] suggests that charge transport mechanisms may involve electrons, holes or ions, or combinations of all three, with the dominant process being determined by the material involved and the details of the experimental situation.

More recent techniques to measure charge dynamics in polymer materials have used a scanning electron microscope, which delivers a non-penetrating electron beam, and a time-resolved current measuring mechanism [9]. These techniques use methods such as pressure wave propagation [10–12], pulsed electro-acoustic methods [13–15] and mirror image methods [16–20]. The effects of charge accumulation are monitored via a measured current as the sample is irradiated (and so charged) until the accumulated charge reaches an asymptotic steady state. These techniques describe measurements rather than a fully developed theoretical description of the charge transport processes which give rise to the measurements.

In an alternative approach to resistivity measurement [1, 2], the sample is first charged and then a portion of its geometry is grounded. The sample is placed in a cylindrical capacitor and charge dissipation is measured via induced charge. This technique is similar to that of [9], but the processes are effectively reversed. In [9], materials were observed as they charged up by trapping electrons in a surface layer, while in [1, 2], materials were observed as they discharged via effective ion carrier diffusion. In [1, 2], a theoretical model was proposed. The model uses a classical rather than quantum mechanical description, appropriate to slowly diffusing large mass ion transport. The model gives non-linear differential equations derived from classical electromagnetic theory and the Mott–Gurney model [21]. The theory gives good reproducible agreement with experimental results for effectively one-dimensional surface charge transport.

In this paper the equations describing the charge carrier diffusion on a sample surface in a coordinate independent form are derived. We show that one-dimensional transport is a special case which reduces to the inviscid Burgers equation [22]. This inviscid Burgers equation can then be solved with appropriate boundary conditions for general initial conditions.

2. Isotropic charge decay model

Following a similar approach as in [1] we begin by deriving a general non-linear carrier diffusion equation for a sample of arbitrary geometry by using an isotropic Ohm's law

$$\mathbf{J} = \sigma \mathbf{E} \tag{2.1}$$

where $\mathbf{J}$ is the current density, $\mathbf{E}$ is the electric field and the time and position dependent conductivity is given by

$$\sigma_v(\mathbf{r}, t) = \frac{q^2 D}{kT} n_v(\mathbf{r}, t). \tag{2.2}$$

This is the Nernst–Einstein equation which can be derived from the Mott–Gurney model of ionic diffusion [21]. We will generally assume that the diffusion coefficient D is a constant scalar, appropriate for an isotropic medium with uniform conductivity. The charge on the diffusing species is q, with number density $n_v(\mathbf{r}, t)$, and T is the absolute temperature in kelvins while k is Boltzmann's constant. The electric field in equation (2.1) may be written in terms of a potential function ϕ as

$$\mathbf{E} = -\nabla \phi. \tag{2.3}$$

We next assume that the ionic flow or carrier diffusion obeys an equation of continuity, so that

$$\nabla \cdot \mathbf{J} = -\frac{\partial \rho}{\partial t} \tag{2.4}$$

where ρ is the charge density; thus

$$\nabla \cdot \mathbf{J} = -q\frac{\partial n_v}{\partial t}. \tag{2.5}$$

Taking the divergence of (2.3) we obtain the Poisson equation for the potential function

$$\nabla^2\phi = -\nabla \cdot \mathbf{E} = -\frac{qn_v}{\varepsilon\varepsilon_0} \tag{2.6}$$

where ε_0 is the permittivity of free space and ε is the dielectric constant of the insulating medium. It is important to note that since this potential function is defined from the electric field governing the carriers by equations (2.1)–(2.3), it is only applicable to the domain where those carriers are defined. Elsewhere it must satisfy Laplace's equation.

It is then simple to derive the result

$$\frac{\partial n_v}{\partial t} = \mu(\nabla\phi \cdot \nabla n_v - \alpha n_v^2) \tag{2.7}$$

where the mobility μ and constant α are given by

$$\mu = \frac{qD}{kT} \qquad \text{and} \qquad \alpha = \frac{q}{\varepsilon\varepsilon_0}. \tag{2.8}$$

The problem is then to solve equation (2.7) and the Poisson equation (2.6) which is coupled to it. Equation (2.7) may be viewed as an evolution equation, which propagates the potential from equation (2.6) forward in time.

Because we may write the carrier density n_v in terms of the divergence of the electric field, we may decouple the equations to obtain

$$\frac{\partial}{\partial t}(\nabla \cdot \mathbf{E}) = -\mu(\mathbf{E} \cdot \nabla(\nabla \cdot \mathbf{E}) + (\nabla \cdot \mathbf{E})^2) = -\mu\nabla \cdot (\mathbf{E}(\nabla \cdot \mathbf{E}))$$

hence

$$\nabla \cdot \left(\frac{\partial}{\partial t}\mathbf{E} + \mu(\mathbf{E}(\nabla \cdot \mathbf{E}))\right) = 0. \tag{2.9}$$

This non-linear equation describes the evolution of the electric field in the sample, during charge decay from the sample.

3. Surface carrier diffusion in Cartesian coordinates

We first analyse this charge transport model by considering a similar model as first proposed in [1]; namely, a finite rectangular sample (typically of sheet material) in which we assume the diffusing carrier density n_v is concentrated mainly in a layer of thickness Δz from the surface of the sample defined to be at $z = 0$. The system of coordinates applied to the sample, as well as an illustration of the residential depth of the carrier density, is depicted in figure 1.

The assumption of a small charge residence depth stems from the physical charging process as outlined in the atmospheric resistivity measurement technique [1, 2]. The sample may be charged via the removal or addition of electrons from its surface. Under the charging conditions outlined in [1] and [2] this effectively leaves a very shallow layer containing the *majority* of positive ionic charge or 'holes' near the surface of the sample ($z = 0$). Even though the grounded strip in [1] and [2] is 'painted' on the surface of the sample, as depicted in figure 1, we assume that since the actual depth of carriers in the surface is very small, the average force acting on carriers in the z-direction is negligible. Therefore there is assumed no overall motion of carriers in the z-direction. From the boundary conditions depicted in figure 1 it is also assumed that the majority of carrier motion is along the x-axis. Taking this

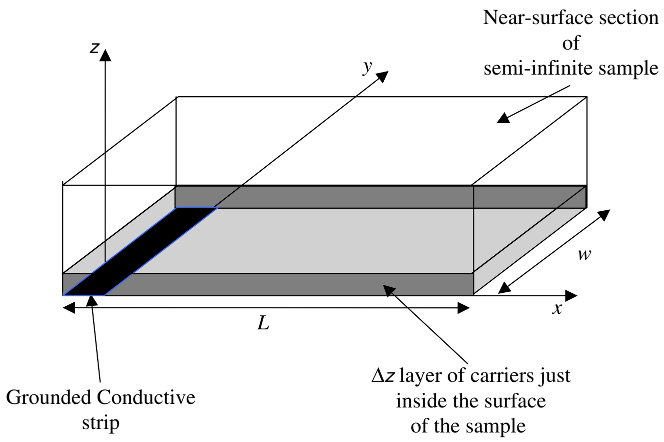

Figure 1. Geometry of carrier transport experiment on an insulator surface, depicting a grounded strip and the carrier density skin depth.

(This figure is in colour only in the electronic version)

into account we simplify the three-dimensional system to that of investigating carrier diffusion in an infinitesimally thin strip Δy along the centre of the sample's surface. As was stated in [1], this approximation provides a means to analyse the important underlying processes of the diffusion mechanism. In doing so we have assumed that the carriers in the entire surface region of the sample follow the description of those that are contained along its centre; we have effectively removed any carrier dependence on z and y and have reduced the system to a study in one dimension.

Equations (2.1)–(2.6) reduced to their one-dimensional equivalent are

$$J(x,t) = q\mu n(x,t)E(x,t) \tag{3.1}$$

$$\frac{\partial^2}{\partial x^2}\phi(x,t) = -\frac{\partial}{\partial x}E(x,t) = -\alpha n(x,t), \tag{3.2}$$

and thus it is easily shown that (2.7) reduces to

$$\frac{\partial}{\partial t}n(x,t) = \mu\left(\frac{\partial}{\partial x}\phi(x,t)\frac{\partial}{\partial x}n(x,t) - \alpha n(x,t)^2\right) \tag{3.3}$$

in agreement with the result from the original derivation in [1].

4. The one-dimensional case

In the one-dimensional case, we envisage an experimental arrangement shown in figure 2.

The insulator sample occupies the region $0 \leqslant x \leqslant L$ with the end at $x = 0$ earthed, so that $\phi(0, t) = 0$. This sample is enclosed in an earthed cage. The cage crosses the x axis at $x = H$, where the potential must also be zero. Charge diffusion is governed by equations (3.2) and (3.3) which are augmented on $L < x \leqslant H$ by

$$\frac{\partial E}{\partial x}(x,t) = 0. \tag{4.1}$$

As was the case for the general three-dimensional derivation, we may decouple equations (3.2) and (3.3) to obtain the one-dimensional equivalent of (2.9); namely

$$\frac{\partial^2 E}{\partial t\,\partial x} + \mu\frac{\partial}{\partial x}\left(E\frac{\partial E}{\partial x}\right) = 0. \tag{4.2}$$

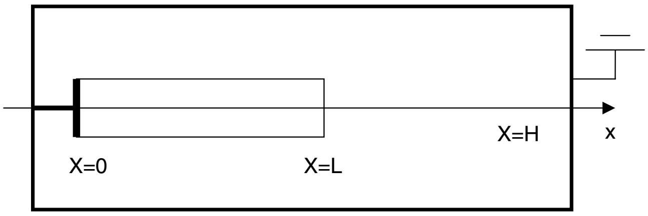

Figure 2. Sketch of experimental arrangement for one-dimensional charge diffusion studies, depicting the sample connected via a grounded strip and chain to a surrounding grounded chamber.

Integrating (4.2) with respect to x we have the quasi-linear evolution equation

$$\frac{\partial E}{\partial t} + \mu E \frac{\partial E}{\partial x} = F(t) \tag{4.3}$$

where $F(t)$ is some function dependent only on t. Equation (4.3) is the non-homogeneous inviscid Burgers equation (sometimes known as a forced inviscid Burgers equation).

It is now convenient to introduce scaled functions and variables. We write

$$x = L\xi, \qquad t = \frac{T}{\alpha\mu n_0} \qquad \text{and} \qquad h = \frac{H}{L} \tag{4.4}$$

and scale our carrier density via the transform

$$n(x,t) = n_0 N\left(\frac{x}{L}, \alpha\mu n_0 t\right) \tag{4.5}$$

where the initial carrier density is defined via

$$n(x,0) = n_0 N_0(\xi) \qquad \text{with} \int_0^1 N_0(s)\,\mathrm{d}s = 1. \tag{4.6}$$

We then further write

$$\begin{aligned} &E(x,t) = \alpha n_0 L e(\xi,T), \qquad J(x,t) = q\alpha\mu n_0^2 L j(\xi,T) \\ &\text{and} \qquad \phi(x,t) = \alpha n_0 L^2 \varphi(\xi,T). \end{aligned} \tag{4.7}$$

In terms of these definitions (3.1) and (3.2) become

$$\frac{\partial e}{\partial \xi}(\xi,T) = N(\xi,T) \qquad \text{for } 0 \leqslant \xi \leqslant 1 \quad \text{and} \quad T \geqslant 0 \tag{4.8}$$

and

$$\frac{\partial j}{\partial \xi}(\xi,T) = -\frac{\partial N}{\partial T}(\xi,T) \qquad \text{for } 0 \leqslant \xi \leqslant 1 \quad \text{and} \quad T \geqslant 0. \tag{4.9}$$

These are augmented by (4.1):

$$\frac{\partial e}{\partial \xi}(\xi,T) = 0 \qquad \text{for } 1 < \xi \leqslant h \quad \text{and} \quad T \geqslant 0 \tag{4.10a}$$

where we may write the scaled electric field in terms of a scaled potential function

$$e(\xi,T) = -\frac{\partial \varphi}{\partial \xi}(\xi,T) \tag{4.10b}$$

which must be continuous over the whole domain and satisfy the boundary conditions that reflect the earthed end of the sample and of the external chamber; i.e.,

$$\varphi(0,T) = \varphi(h,T) = 0. \tag{4.11}$$

The inviscid Burgers equation may be written as

$$\frac{\partial e}{\partial T}(\xi, T) + e(\xi, T)\frac{\partial e}{\partial \xi} = \omega''(T). \tag{4.12}$$

We have chosen for later convenience to write the scaled function $\frac{F(t)}{\mu\alpha^2 n_0^2 L}$ via the second derivative of an arbitrary function $\omega(T)$. Equations (4.8) and (4.9) are valid only for the domain of the sample surface; elsewhere the electric potential must satisfy Laplace's equations (4.10*a*), (4.10*b*). Further to this we choose to modify the equation for the electric field in (4.8) in order to obtain the correct behaviour for the current density at the free end of the sample ($\xi = 1$). We do this by introducing a weighted delta function allowing the possibility that as charge diffuses on the surface of the sample, some charge may pile up at the end of the sample at $\xi = 1$. The reason for this will become clear in subsequent sections. Equation (4.8) becomes

$$\frac{\partial e}{\partial \xi}(\xi, T) = N(\xi, T) + \Gamma(T)\delta(\xi - 1) \qquad \text{for } 0 \leqslant \xi \leqslant 1 \quad \text{and} \quad T \geqslant 0$$
$$\text{with } \Gamma(0) = 0. \tag{4.13}$$

The electric field, however, is being described over different media; equation (4.8) is valid on the domain of the sample and thus in a dielectric medium; equations (4.10*a*), (4.10*b*) describes the electric field off the sample in vacuum (in [1] it is actually atmosphere, but we assume vacuum for convenience). Therefore considering the normal component of the displacement field across the boundary of the sample at $\xi = 1$ we have

$$e(1+, T) - \varepsilon e(1-, T) = \Gamma(T) \tag{4.14}$$

where the plus and minus signs indicate the direction to the limit.

Integrating (4.13) we obtain

$$e(\xi, T) = \int_0^{\xi} N(s, T)\,\mathrm{d}s + e(0, T); \tag{4.15}$$

so that by (4.10*a*), (4.10*b*) we have

$$\frac{\partial \varphi}{\partial \xi} = -\int_0^{\xi} N(s, T)\,\mathrm{d}s - e(0, T);$$

and integration again gives

$$\varphi(\xi, T) = -\int_0^{\xi} \mathrm{d}k \int_0^{k} N(s, T)\,\mathrm{d}s - \xi e(0, T)$$

where we have used the fact that the potential is zero at the earthed end $\xi = 0$ for all time T.

Noting that

$$\int_0^{\xi} sN(s, T)\,\mathrm{d}s = \xi \int_0^{\xi} N(s, T)\,\mathrm{d}s - \int_0^{\xi} \mathrm{d}k \int_0^{k} N(s, T)\,\mathrm{d}s$$

via integration by parts, we then have

$$\varphi(\xi, T) = -\xi \int_0^{\xi} N(s, T)\,\mathrm{d}s + \int_0^{\xi} sN(s, T)\,\mathrm{d}s - \xi e(0, T).$$

Hence at the inner limit as we approach the sample's free end

$$\varphi(1-, T) = -\int_0^{1} N(s, T)\,\mathrm{d}s + \int_0^{1} sN(s, T)\,\mathrm{d}s - e(0, T).$$

The fact that the potential must

- be continuous over the entire domain, particularly at $\xi = 1$,
- satisfy (4.10a), (4.10b),
- equal zero at $\xi = h$,

then gives

$$\varphi(\xi, T) = -\frac{h-\xi}{h-1}\left(\int_0^1 N(s,T)\,\mathrm{d}s - \int_0^1 sN(s,T)\,\mathrm{d}s + e(0,T)\right) \qquad \text{on } 1 < \xi \leqslant h. \tag{4.16}$$

Therefore we have

$$e(1+, T) = -\frac{1}{h-1}\left(\int_0^1 N(s,T)\,\mathrm{d}s - \int_0^1 sN(s,T)\,\mathrm{d}s + e(0,T)\right)$$

and hence the discontinuity of the electric field at the end of the sample, given by (4.14) becomes

$$\begin{aligned} e(1+, T) - \varepsilon e(1-, T) = &-\frac{1}{h-1}\left(\int_0^1 N(s,T)\,\mathrm{d}s - \int_0^1 sN(s,T)\,\mathrm{d}s + e(0,T)\right) \\ &- \varepsilon\left(\int_0^\xi N(s,T)\,\mathrm{d}s + e(0,T)\right) = \Gamma(T). \end{aligned}$$

By manipulation one may obtain

$$e(0, T) = -\int_0^1 N(s,T)\,\mathrm{d}s + \frac{1}{\bar{h}}\int_0^1 sN(s,T)\,\mathrm{d}s - \frac{(h-1)}{\bar{h}}\Gamma(T)$$

where $\bar{h} = 1 + \varepsilon(h-1)$.

Hence the electric field (4.15) may now be expressed as

$$e(\xi, T) = \int_0^\xi N(s,T)\,\mathrm{d}s - \int_0^1 N(s,T)\,\mathrm{d}s + \frac{1}{\bar{h}}\int_0^1 sN(s,T)\,\mathrm{d}s - \frac{(h-1)}{\bar{h}}\Gamma(T) \tag{4.17}$$

with initial condition given by

$$e(\xi, 0) = \int_0^\xi N_0(s)\,\mathrm{d}s - 1 + \frac{1}{\bar{h}}\int_0^1 sN_0(s)\,\mathrm{d}s \equiv g(\xi) \tag{4.18}$$

and the boundary condition at the end of the sample as

$$e(1-, T) = \frac{1}{\bar{h}}\int_0^1 sN(s,T)\,\mathrm{d}s - \frac{(h-1)}{\bar{h}}\Gamma(T). \tag{4.19}$$

We now obtain a general solution for the inviscid Burgers equation of (4.12) via the method of characteristics. It should be noted that similar solutions are obtainable via the Hopf–Cole transform [23, 24]; however, the method of characteristics provides a more general approach.

We first make the substitution

$$e(\xi, T) = Q(\xi, T) + \omega'(T), \tag{4.20}$$

which makes no assumptions. The initial condition for Q is given by

$$Q(\xi, 0) = g(\xi) - \omega'(0) \tag{4.21}$$

and we note that by (4.18), $g(\xi)$ is an increasing function of ξ. The inviscid Burgers equation of (4.12) then becomes

$$\frac{\partial Q}{\partial T}(\xi, T) + (Q(\xi, T) + \omega'(T))\frac{\partial Q}{\partial \xi}(\xi, T) = 0. \tag{4.22}$$

The method of characteristics assumes that we can first parametrize any curve in the (ξ, T) plane via a parametric variable, i.e.,

$$\xi = \xi(s) \qquad T = T(s)$$

where s is a measure of the distance along the curve. Considering

$$\frac{\mathrm{d}Q}{\mathrm{d}s}(\xi(s), T(s)) = \frac{\partial Q}{\partial \xi}\frac{\mathrm{d}\xi}{\mathrm{d}s} + \frac{\partial Q}{\partial T}\frac{\mathrm{d}T}{\mathrm{d}s}$$

we note from that for the parametrization to equate to (4.22) we must have

$$\frac{\mathrm{d}Q}{\mathrm{d}s}(\xi(s), T(s)) = 0 \qquad \frac{\mathrm{d}T}{\mathrm{d}s} = 1 \qquad \frac{\mathrm{d}\xi}{\mathrm{d}s} = Q(\xi(s), T(s)) + \omega'(T). \tag{4.23}$$

From this we see that $s = T$, as well as

$$Q(\xi(T), T) = K(\xi(0)) \tag{4.24}$$

where $K(\xi(0)) =$ constant. Additionally from (4.23) we must have

$$\frac{\mathrm{d}\xi(T)}{\mathrm{d}T} = Q(\xi(T), T) + \omega'(T) = K(\xi(0)) + \omega'(T).$$

This implies

$$\xi(T) = KT + \omega(T) - \omega(0) + \xi(0);$$

thus

$$\xi(0) = \xi(T) - KT - \omega(T) + \omega(0). \tag{4.25}$$

Along these characteristic curves, by (4.24), Q is constant, therefore we may express it in terms of the initial condition in (4.21); i.e.,

$$Q(\xi(T), T) = Q(\xi(0), 0) = g(\xi(0)) - \omega'(0) = K. \tag{4.26}$$

Therefore multiplying by T and substituting for KT in (4.25) we obtain

$$\xi(0) = \xi(T) - Tg(\xi(0)) - \Omega(T) \tag{4.27}$$

where

$$\Omega(T) = (\omega(T) - \omega(0) - T\omega'(0))$$

and we note that

$$\Omega(0) = \Omega'(0) = 0. \tag{4.28}$$

Any point in the (ξ, T) plane may be given by a characteristic curve $\xi(T)$ which necessarily has an 'initial' point $\xi(0)$. Thus $\xi(0)$ defines which characteristic curve a point is on, and can be expressed as a function of (ξ, T). We write $\xi(0) = \eta(\xi, T)$ and then have the relation

$$\eta(\xi, T) = \xi - Tg(\eta(\xi, T)) - \Omega(T). \tag{4.29}$$

Therefore (4.26) becomes

$$Q(\xi(T), T) = Q(\xi(0), 0) = g(\eta(\xi, T)) - \omega'(0)$$

and from (4.20) and the definition in (4.28) we then have

$$e(\xi, T) = g(\eta(\xi, T)) + \Omega'(T), \tag{4.30}$$

which is a completely general solution for the original non-homogenous inviscid Burgers equation.

We note that

$$\frac{\partial \eta}{\partial \xi}(\xi, T) = \frac{1}{1 + Tg'(\eta(\xi, T))}$$

where $g'(\eta) = \frac{\mathrm{d}g}{\mathrm{d}\eta}$ and hence

$$\frac{\partial e}{\partial \xi}(\xi, T) = \frac{g'(\eta(\xi, T))}{1 + Tg'(\eta(\xi, T))}, \qquad \frac{\partial e}{\partial T}(\xi, T) = -\frac{g(\eta(\xi, T))g'(\eta(\xi, T))}{1 + Tg'(\eta(\xi, T))}.$$

Thus solutions of (4.30) are only continuous where $1 + Tg'(\eta(\xi, T)) \neq 0$.

We also have

$$\frac{\partial e}{\partial \xi}(\xi, T) = N(\xi, T) = \frac{g'(\eta(\xi, T))}{1 + Tg'(\eta(\xi, T))} \tag{4.31}$$

and further

$$j(\xi, T) = \frac{g'(\eta(\xi, T))}{1 + Tg'(\eta(\xi, T))}(g(\eta(\xi, T)) + \Omega'(T)). \tag{4.32}$$

From (4.13) we see that we have a defined carrier density via

$$\frac{\partial e}{\partial \xi}(\xi, T) = N(\xi, T) + \Gamma(T)\delta(\xi - 1) \equiv \bar{N}(\xi, T).$$

From the continuity condition of (4.9) we have

$$\frac{\partial j}{\partial \xi}(\xi, T) = -\frac{\partial}{\partial T}\bar{N}(\xi, T);$$

integrating over a small neighbourhood near the free end we have

$$j(1 + \varepsilon, T) - j(1 - \varepsilon, T) = -\frac{\mathrm{d}}{\mathrm{d}T}\int_{1-\varepsilon}^{1+\varepsilon} N(s, T) + \Gamma(T)\delta(s - 1)\,\mathrm{d}s.$$

Since we only have carriers defined on $\xi \in [0, 1]$ and strictly no current density beyond the free end of the sample, in any limit, we have

$$\begin{aligned} j(1 - \varepsilon, T) &= \frac{\mathrm{d}}{\mathrm{d}T}\left(\int_{1-\varepsilon}^{1} N(s, T) + \Gamma(T)\delta(s - 1)\,\mathrm{d}s\right) \\ &= \frac{\mathrm{d}}{\mathrm{d}T}(n_T(1, T) - n_T(1 - \varepsilon, T) + \Gamma(T)) \end{aligned}$$

where we have used well known properties of the delta function, and where $n_T(\xi, T)$ represents the total number of carriers which we assume for the time being is continuous on the sample. Allowing $\varepsilon \to 0$ we have

$$j(1-, T) = \frac{\mathrm{d}\Gamma(T)}{\mathrm{d}T},$$

and thus

$$\Gamma(T) = \int_0^T j(1-, \tau)\,\mathrm{d}\tau. \tag{4.33}$$

5. Constant initial carrier density

Assuming as in [1, 2] that the initial carrier distribution in the surface layer of the sample is constant, we take $N_0(\xi) = 1$ and have from (4.18)

$$g(\xi) = \xi - 1 + \frac{1}{2\bar{h}} \tag{5.1}$$

and hence from (4.29)

$$\eta(\xi, T) = \frac{\xi - \Omega(T) + T(1 - \frac{1}{2\bar{h}})}{T + 1}; \tag{5.2}$$

therefore

$$e(\xi, T) = \frac{\xi - \Omega(T) + (1 - \frac{1}{2\bar{h}})}{T+1} + \Omega'(T) \tag{5.3}$$

and we obtain the carrier density and current density as

$$N(\xi, T) = \frac{1}{T+1} \tag{5.4}$$

and

$$j(\xi, T) = \frac{\xi - (1 - \frac{1}{2\bar{h}})}{(T+1)^2} + \frac{\mathrm{d}}{\mathrm{d}T}\left(\frac{\Omega(T)}{T+1}\right) = \frac{\mathrm{d}}{\mathrm{d}T}\left(\frac{\Omega(T) - \xi + \left(1 - \frac{1}{2\bar{h}}\right)}{T+1}\right). \tag{5.5}$$

From (4.33) we have

$$\Gamma(T) = \int_0^T \frac{\mathrm{d}}{\mathrm{d}\tau}\left(\frac{\Omega(\tau) - \frac{1}{2\bar{h}}}{(\tau+1)}\right)\mathrm{d}\tau = \frac{\Omega(T) - \frac{1}{2\bar{h}}}{T+1} + \frac{1}{2\bar{h}} = \frac{\Omega(T) + \frac{T}{2\bar{h}}}{T+1} \tag{5.6}$$

since $\Gamma(0) = 0$.

From the integral representation of the electric field at the free end of the sample in (4.19) we have

$$e(1-, T) = \frac{1}{\bar{h}}\int_0^1 sN(s, T)\,\mathrm{d}s - \frac{(h-1)}{\bar{h}}\Gamma(T) = \frac{1}{2\bar{h}(T+1)} - \frac{(h-1)}{\bar{h}}\Gamma(T),$$

which must equate to the 'propagated' electric field obeying the inviscid Burgers equation, i.e., from (5.3) we have

$$e(1-, T) = \frac{1}{2\bar{h}(T+1)} - \frac{(h-1)}{\bar{h}}\Gamma(T) = g(\eta(\xi, T)) + \Omega'(T) = \frac{\frac{1}{2\bar{h}} - \Omega(T)}{T+1} + \Omega'(T),$$

so that

$$\Omega'(T) - \frac{\Omega(T)}{T+1} + \frac{(h-1)}{\bar{h}}\Gamma(T) = 0.$$

Substituting for the value of $\Gamma(T)$, we obtain

$$\Omega'(T) - \gamma\frac{\Omega(T)}{T+1} = -\frac{(h-1)T}{2\bar{h}^2(T+1)} \tag{5.7}$$

where

$$\gamma \equiv 1 - \frac{(h-1)}{\bar{h}}; \qquad 0 < \gamma < 1.$$

Therefore noting that (5.7) may be written as

$$\frac{\mathrm{d}}{\mathrm{d}T}(\Omega(T)(T+1)^{-\gamma}) = -\frac{(h-1)T}{2\bar{h}^2(T+1)^{\gamma+1}}$$

we may integrate to obtain

$$\Omega(T) = \frac{1}{2\bar{h}\gamma}((T+1)^\gamma - 1 - \gamma T), \tag{5.8}$$

yielding

$$\Gamma(T) = \frac{((T+1)^\gamma - 1)}{2\bar{h}\gamma(T+1)}. \tag{5.9}$$

The current density is therefore given by

$$j(\xi, T) = N(\xi, T)e(\xi, T) = \frac{\xi - (1 - 1/2\bar{h})}{(T+1)^2} - \frac{h-1}{\bar{h}}\frac{\Gamma(T)}{(T+1)}. \tag{5.10}$$

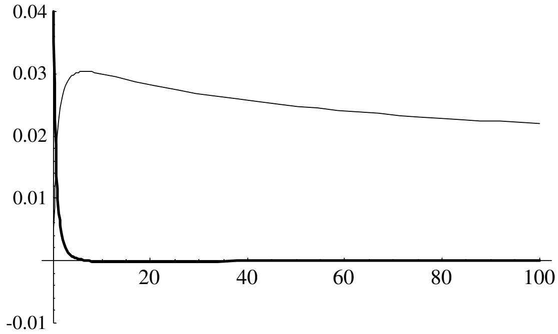

Figure 3. Plot of $j(1-, T)$ (heavy) and $\Gamma(T)$ (fine) for $h = 3$, $\varepsilon = 5$, $\Rightarrow \bar{h} = 11$ and $\gamma \cong 0.818\,182$.

Plotting (5.9) and (5.10) we have the following (figure 3) for the current density and the weight of the delta function at the free end of the sample, i.e., for $\xi = 1$.

We see that the current at $\xi = 1$ is initially positive, with carriers feeding into the delta function, and initially decreases sharply, becoming negative at

$$T = -1 + \left(\frac{1}{1-\gamma}\right)^{1/\gamma},$$

after which it remains negative, slowly increasing towards zero.

From the current density given in (5.10) we note that if we were to consider a carrier density with no charge defined on the free end of the sample, that is we set $\Gamma(T) = 0$ and note that all boundary and initial conditions derived in section 4 still apply, then we obtain

$$j(\xi, T) = \frac{\xi - (1 - 1/2\bar{h})}{(T+1)^2}. \tag{5.11}$$

Thus at the free end of the sample we have

$$j(1-, T) = \frac{1}{2\bar{h}(T+1)^2} > 0$$

and hence we have a description of carriers flowing off the sample. This of course is not physically acceptable and we now see that the inclusion of the delta function in the description of the carrier density over the sample is necessary in order for the current density to adhere to the physical bounds of the sample. This also shows that the function $F(t)$ arising from integration of (4.2) (i.e., as shown in (4.3)) is determined by the boundary condition at the free end of the sample. We note that if we did not have a boundary condition for E at the free end of the sample, $F(t)$ would remain undetermined and the problem, while being solvable, would not be well-posed (or have a unique solution). This is most easily seen by noting the fact that $F(t)$ may be 'removed' via the Orlowski–Sobczyk transform [25]—whereupon it remains arbitrary in the final result, until determined via boundary conditions. This fact justifies the inclusion of the weighted delta function in the carrier distribution as this forces a boundary condition at the free end of the sample, thus determining $F(t)$ uniquely such that the physical description is self-consistent.

Inverting the transforms for the carrier density in (5.4) we obtain

$$n(r, t) = \frac{n_0}{\mu\alpha n_0 t + 1}, \tag{5.12}$$

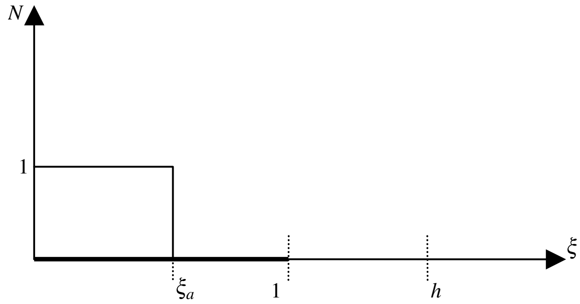

Figure 4. Schematic diagram depicting the initial discontinuous carrier distribution.

which is the same equation obtained in [1] and which was referred to as an asymptotic approximation for small time $t \ll 1$. The reason for this solution being referred to as an approximation for $t \ll 1$ stems from analysing (3.3), namely,

$$\frac{\partial n}{\partial t}(x,t) = \mu\left(\frac{\partial n}{\partial x}(x,t)\frac{\partial \phi}{\partial x}(x,t) - \alpha n^2(x,t)\right).$$

In [1] it was argued that initially for $t \sim 0$ the carrier distribution varies little from its true initial state being that of a constant over x. For this reason the authors assumed that in this time domain

$$\frac{\partial n}{\partial x} \sim 0,$$

and hence the resulting equation for such times is

$$\frac{\partial n}{\partial t}(x,t) = -\mu\alpha n^2(x,t).$$

Solving this and applying an initial condition of constant carrier density n_0 we obtain the same equation as (5.12); however, the previous analysis of this paper shows that the original assumption in [1] of (5.12) being an approximate solution for small times t, while first appearing physically intuitive, is not precise. It has been shown that (5.12) is the exact solution satisfying the initial and boundary conditions specified for all time t.

6. Discontinuous constant initial carrier distribution on the sample

We now illustrate two other cases of interest where much of the exact solution may be derived:

$$\text{(i)} \qquad N(\xi,0) = \begin{cases} 1 & 0 \leqslant \xi \leqslant \xi_a \\ 0 & \xi_a < \xi \leqslant h \end{cases} \qquad \xi_a < 1 \tag{6.1}$$

and

$$\text{(ii)} \qquad N(\xi,0) = \begin{cases} 0 & 0 \leqslant \xi < \xi_a \\ 1 & \xi_a \leqslant \xi \leqslant 1 \\ 0 & 1 < \xi \leqslant h \end{cases} \qquad \xi_a < 1. \tag{6.2}$$

See figures 4 and 5.

For case (i), we essentially retain all previous analysis for the system of a constant initial carrier distribution over the entire sample. The difference for this system is that as yet there is no carrier at the end of the sample and we may discard the $\Gamma(T)$ function. We also must

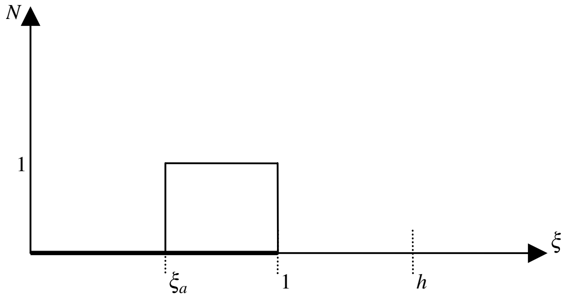

Figure 5. Schematic diagram depicting the initial discontinuous carrier distribution.

account for a different boundary condition at the edge of the defined carrier distribution. That is, equation (4.9) becomes

$$e(\xi_a(T), T) = \frac{1}{\bar{h}} \int_0^{\xi_a} sN(s, T)\,\mathrm{d}s. \tag{6.3}$$

The initial condition of $e(\xi, 0)$ varies slightly from (5.1) due to the new initial carrier distribution (6.1) and we have

$$g(\xi) = \xi - 1 + \frac{\xi_a^2}{2\bar{h}} = \xi - \beta \qquad \text{where } \beta \equiv 1 - \frac{\xi_a^2}{2\bar{h}}, \tag{6.4}$$

where we have normalized the total number of carriers; i.e., $\int_0^{\xi_a} N(s, 0)\,\mathrm{d}s = 1$.

We therefore obtain

$$\eta = \frac{\xi + \beta T - \Omega(T)}{T + 1} \tag{6.5}$$

and the solution of

$$e(\xi, T) = \frac{\xi - \Omega(T) - \beta}{(T + 1)} + \Omega'(T), \tag{6.6}$$

from which we obtain

$$N(\xi, T) = \frac{1}{T + 1}. \tag{6.7}$$

As for the previous system we apply the boundary condition at the edge of the charged area and obtain a differential equation for $\Omega(T)$ as

$$\Omega'(T) - \frac{\Omega(T)}{(T + 1)} = \frac{\xi_a^2 - 2\bar{h}(\xi_a - \beta)}{2\bar{h}(T + 1)}.$$

Substituting for β the right-hand side of the equation evaluates to zero, and we then obtain

$$\Omega'(T) - \frac{\Omega(T)}{(T + 1)} = \frac{1 - \xi_a}{T + 1}. \tag{6.8}$$

From the definition of (4.28) we see that $\Omega(0) = 0$, and the only solution of (6.8) which satisfies this condition is

$$\Omega(T) = T(1 - \xi_a) \tag{6.9}$$

and we have

$$e(\xi, T) = \frac{\xi - \beta + 1 - \xi_a}{(T + 1)}. \tag{6.10}$$

We note that while $\Omega(T)$ is not zero, its second derivative is, and hence the function $F(t)$ originating from integrating (4.2) is, for this system, also zero. Accordingly, we see that this is due to no boundary condition being necessary at the free end of the sample (since there are no carriers present there).

We may now write (6.5) as

$$\eta(\xi, T) = \xi(0) = \frac{\xi(T) + \beta T - T(1 - \xi_a)}{T + 1}. \tag{6.11}$$

Since (6.11) parameterizes points in the plane such that (6.10) satisfies the inhomogeneous Burgers equation, we may use (6.11) to study the time evolution of particular points of interest on the carrier distribution, namely the boundary. We observe that the evolution of the boundary of the carrier distribution is given by

$$\xi_a = \xi(T) + T(\beta - 1) \tag{6.12}$$

and now ask as to which direction this carrier distribution boundary is moving by studying points either side of the initial boundary point; i.e., $\xi(T) = \xi_a \pm \Delta\xi$ and thus

$$\xi_a = \frac{\xi_a \pm \Delta\xi + \beta T}{T + 1}$$

yielding

$$T = \pm\Delta\xi \frac{\xi_a^2}{2\bar{h}} \qquad \text{where } \frac{\xi_a^2}{2\bar{h}} > 0,$$

which implies that the carrier distribution boundary is moving to the right, as points left of this boundary result in negative time indicating the boundary's previous position. The carrier profile may only diffuse as far as the end of the sample, hence from (6.12) we may determine the time at which this occurs via

$$\xi_a = 1 + T_c(\beta - 1)$$

and solve for T_c to obtain

$$T_c = \frac{2\bar{h}(1 - \xi_a)}{\xi_a^2}, \tag{6.13}$$

where the subscript merely indicates that, at this time, the system changes to that of one with a constant carrier distribution over the entire sample. At that particular point in time, carriers exist at the end of the sample and the $\Gamma(T)$ function must, after that time, be positive to account for the correct behaviour of current density at the free end. All previous results now apply for the behaviour of the charge diffusion on the sample, except that initially the carrier density is now given by

$$n(\xi, T_c) = \frac{n_0 \xi_a^2}{2\bar{h}(1 - \xi_a) + \xi_a^2} \leqslant n_0 \tag{6.14}$$

and we see that, as expected, the previous system begins with an initial carrier density less than that which was initially defined. Note also that the total charge at the cut-over, in untransformed coordinates, is

$$q(x, t_c) = q_0 \frac{A}{2\bar{h}(1 - A/L) + 1},$$

where A is the initial boundary point of the carrier distribution on the x-coordinate system. We see that the total charge at the cut-over is not simply reduced by a ratio of the initial length of distribution over the final length of the entire sample—which would be the case if the carriers were *not* diffusing off the sample at the grounded end; hence, as one would expect, the carriers are diffusing off the sample *while* the boundary of the charge distribution moves towards the free end.

In the second case (ii) we have a similar approach as the first except that we must include the extra complication of the $\Gamma(T)$ function. From the initial carrier distribution we have

$$g(\xi) = \xi - 1 + \kappa \qquad \text{where } \kappa \equiv \frac{(1-\xi_a^2)}{2\bar{h}}, \tag{6.15}$$

which leads to

$$\eta = \frac{\xi + T(1-\kappa) - \Omega(T)}{(T+1)} \tag{6.16}$$

and the solution of

$$e(\xi, T) = \frac{\xi - \Omega(T) + \kappa}{(T+1)} + \Omega'(T). \tag{6.17}$$

We can determine the transformed current density as being

$$j(\xi, T) = \frac{\mathrm{d}}{\mathrm{d}T}\left[\frac{\kappa - \xi + \Omega(T)}{(T+1)}\right]. \tag{6.18}$$

Therefore we obtain

$$\Gamma(T) = \int_0^T j(1-, \tau)\,\mathrm{d}\tau = \frac{\kappa - 1 + \Omega(T)}{(T+1)}. \tag{6.19}$$

The boundary condition for the transformed electric field at the free end of the sample must satisfy equation (4.19), hence we have

$$e(1-, T) = \frac{\kappa}{(T+1)} - \frac{(h-1)}{\bar{h}}\Gamma(T), \tag{6.20}$$

which must equate to the propagated solution satisfying the inviscid Burgers equation; hence

$$\frac{1 - \Omega(T) + \kappa}{(T+1)} + \Omega'(T) = \frac{\kappa}{(T+1)} - \frac{(h-1)}{\bar{h}}\Gamma(T). \tag{6.21}$$

Substituting for $\Gamma(T)$ from (6.19) and rearranging we obtain

$$\Omega'(T) - \gamma\frac{\Omega(T)}{(T+1)} = \frac{\chi}{\bar{h}(T+1)} \qquad \text{where } \chi \equiv (h-1)(\kappa-1) + \bar{h}. \tag{6.22}$$

Solving (6.22) we have

$$\Omega(T) = \frac{\chi}{\bar{h}\gamma}[(T+1)^{\gamma} - 1]. \tag{6.23}$$

This results in

$$\eta(\xi, T) = \frac{\xi + T(1-\kappa)}{(T+1)} - \frac{\chi}{\bar{h}\gamma}[(T+1)^{\gamma-1} - (T+1)^{-1}]. \tag{6.24}$$

From this we may again determine in which direction the boundary of the charge distribution moves. Setting $\eta(\xi, T) = \xi_a$ in (6.24) and rearranging, we obtain

$$\xi(T) - \xi_a = (\xi_a + \kappa - 1)T + \frac{\chi}{\bar{h}\gamma}((T+1)^{\gamma} - 1). \tag{6.25}$$

We cannot solve (6.25) explicitly for T; however, we may approach the problem by considering the coefficients of T.

We note that

$$\xi_a + \kappa - 1 = \frac{\xi_a(2\bar{h} - \xi_a) - (2\bar{h} - 1)}{2\bar{h}} \tag{6.26}$$

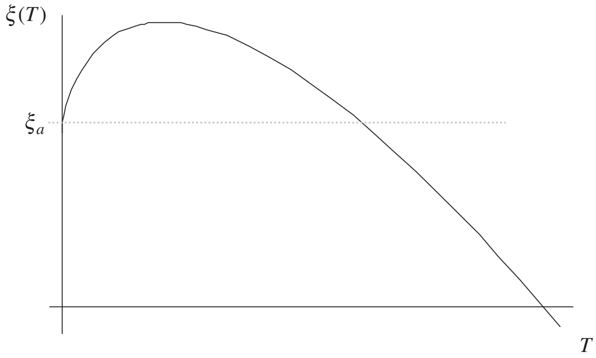

Figure 6. Schematic plot of the trajectory of the discontinuity in the charge distribution on the sample. We observe that the discontinuity passes back through the initial point towards the origin.

and since $0 \leqslant \xi_a \leqslant 1$ and $\bar{h} > 1$ by definition we obtain the bounds

$$-\frac{(2\bar{h}-1)}{2\bar{h}} \leqslant \xi_a + \kappa - 1 \leqslant 0; \tag{6.27}$$

hence the leading coefficient of the linear term in (6.25) is negative. The coefficient of the second term equates to

$$\frac{\chi}{\bar{h}\gamma} = \frac{1}{\gamma}\left(1 - \frac{\xi_a^2(h-1)}{2\bar{h}^2}\right) \tag{6.28}$$

and

$$\frac{\xi_a^2(h-1)}{2\bar{h}^2} = \frac{\xi_a^2(h-1)}{2(1+\varepsilon(h-1))^2} < 1 \tag{6.29}$$

since we take the dielectric constant of the material to be greater than unity, implying that $\frac{\chi}{\bar{h}\gamma} > 0$; however, we also note that $0 < \gamma < 1$ and hence the second term will always eventually be dominated by the first, and thus for some time T_i we obtain

$$\xi(T_i) - \xi_a = (\xi_a + \kappa - 1)T_i + \frac{\chi}{\bar{h}\gamma}((T_i+1)^\gamma - 1) < 0$$

after which it remains so for all $T > T_i$. The sign of $\xi(T) - \xi_a$ is relative to the initial point ξ_a with negative values corresponding to points left of ξ_a, and positive to the right of ξ_a. We have therefore shown that the discontinuity may at first approach the free end of the sample, after which there exists a time T_i when the boundary has returned to ξ_a and then progresses past this initial point towards the origin (see figure 6). Once the boundary reaches the grounded end of the sample (the origin) the carrier density is then a constant over the entire surface of the sample, and we again return to the first system studied previously in section 5.

We note that the discontinuity in the carrier distribution as it returns to its initial point continues through to the origin and does not oscillate. As the boundary initially travels towards the free end of the sample, charge feeds into the weight of the delta function, until such time as enough charge has accumulated and forces the boundary to move back towards the origin. When the boundary returns to its initial position, and due to the slow decay of carriers from the weight of the delta function (as seen in figure 3), there is still enough charge to force the boundary past its initial position towards the origin. This provides a quantitative explanation as to why we do not see the boundary oscillate.

7. Conclusion

Starting from assumptions similar to those proposed in [1] we have re-derived the general equations governing surface carrier diffusion in the surface of an insulator. We have shown that for the special case of one-dimensional carrier diffusion the equations for the electric field reduce to that of the inhomogeneous inviscid Burgers equation. A general solution for an initial value problem of this equation was derived via the method of characteristics. Using this solution in conjunction with boundary conditions pertaining to a system similar to that in [1], solutions have been derived for three particular initial values of carrier distribution. It has been shown that in order to obtain a physically consistent description of carrier diffusion for this one-dimensional system, the carrier density needed to be off-set by a weighted delta function of charge at the free end of the sample. This provided insight into the function $F(t)$ originating from integrating (4.2), and it was seen that this function is uniquely determined via boundary conditions on the sample. For the system of an initial constant carrier distribution over the entire sample, the same form of carrier density was obtained as in [1]. It is argued in [1] that this solution is an approximation valid for $t \ll 1$; however, it has been shown that this solution is indeed exact for all time t. It will be shown in a later paper that the hyperbolic solutions of the carrier density provide an adequate fit to experimental observations and allow for the determination of a sample's resistivity that is in excellent agreement with literature.

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