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Generalizations of multiple trapping

By D. MONROE and M. A. KASTNER

Department of Physics and Center for Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, U.S.A.

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ABSTRACT

The multiple trapping model may be applicable to a wide variety of time-dependent processes in semiconductors. However, previous simple treatments developed to explain power-law current transients assumed trapping in an exponential density of states with a constant trapping 'cross-section'. We present a more detailed analysis of multiple trapping by examining the trapping and emission rates from traps, as well as their occupation. This shift of emphasis, while retaining and enhancing a simple physical picture of the process, allows us to treat several new situations. We give simple results for the effect of repetitive pulses. The effect of variations in trapping 'cross-section' among traps is also found to be fairly simple. We classify all possible current transients into five basic types, for which different sets of states dominate the dynamical behaviour, and derive the form of the current transient for each type.

§ 1. INTRODUCTION

The multiple trapping (MT) problem was originally formulated to deal with the highly dispersive current transients found in time-of-flight measurements on amorphous semiconductors (Schmidlin 1977, Noolandi 1977). More recently, the model has been applied in a simplified form to other transient phenomena in amorphous materials (Orenstein, Kastner and Vaninov 1982, Vardeny, Strait, Pfost, Tauc and Abeles 1982) and even to luminescence in the band tails of a crystalline semiconductor (Göbel and Graudzus 1982). A rigorous analysis of MT was presented in the pioneering papers of Schmidlin and of Noolandi. Unfortunately, in these papers the generality and rigour was achieved at the cost of a high degree of formality. Specifically, one must perform an inverse Laplace transform in order to interpret experimental results. In contrast, more recent treatments (Tiedje and Rose 1981, Orenstein and Kastner 1981 a, b ; together referred to hereafter as the TROK model) have provided a more simple, physical picture, which leads to an intuitive understanding of the process. It is not clear from the latter discussions, however, how general the simple picture is. In view of its widening scope of application, it appears appropriate to try to provide a rigorous method of generalizing the TROK model.

The purpose of this paper is to show how some of the assumptions made in the TROK model may be relaxed without sacrificing the physical intuition that is possible with a simple argument. Specifically, we wish to treat a non-exponential density of states (DOS), and to allow more freedom in the trap parameters. In order to accomplish these goals, we look at the MT

process in a slightly different light, and try to clarify the nature of the assumptions being made. We cannot anticipate all possibilities, but it is hoped that the approach outlined here will allow a better appreciation of the important issues in generalizing the MT picture to other systems and other phenomena.

As applications of our more general approach, we discuss in detail two specific situations which have not been treated previously. The first is a generalization of the formalism to include variations of ' cross-section ' for the traps. We show that the major effect of such variations is that each state participates in MT only in proportion to its ' cross-section ', so that the effective DOS measured in an experiment is really the product of the true DOS and the ' cross-section '. The other application discussed is that of MT at temperatures higher than the energy spread of an exponential DOS.

§ 2. The multiple trapping problem

The MT problem addresses the dynamics of carriers in transport states interacting with a distribution of traps. The essence of MT is the neglect of transitions directly between traps (the hopping problem). Each trap thus interacts directly only with the mobile carriers. We limit our attention to carriers in a single band (for concreteness, the conduction band) and assume that all the mobile carriers are in equilibrium with one another, so that they represent a single reservoir of carriers, occupying an effective number of states N_c. The zero of energy is taken to be the mobility edge, so the thermal energy E of a trap is negative.

Each of the traps, temporarily labelled by i, can be completely characterized, for our purposes, by two coefficients; the release rate ν_i (in s^{-1}), and the trapping coefficient b_i (in $cm^3 s^{-1}$). These coefficients are defined by the equation for the occupation number f_i of trap i,

$$\frac{df_i}{dt} = b_i n(t)(1-f_i) - \nu_i f_i. \tag{1}$$

Examining this equation for equilibrium occupancies shows that

$$\nu_i = b_i N_c \exp(-|E_i|/kT). \tag{2}$$

This equation states the result of detailed balance that the ratio between the trapping and release coefficients is determined solely by the energy of the trap, and is valid even when the trapping coefficient is not the product of a mean velocity and a cross-section.

However, the individual magnitudes of the trapping and release rates are not determined by this argument. Before discussing the way in which these rates affect the results of MT, we discuss these coefficients in a more physical way. Their magnitudes involve some very complicated and interesting physics which is not well understood, even in crystals. The energies typical of MT are several tenths of an electron-volt, so that the transitions between traps and transport states is likely to involve the emission and absorption of many phonons. Calculating the magnitudes of the transition rates therefore requires a detailed knowledge of the local phonon modes at the trap, as well as the actual wavefunctions of both the trapped and the mobile electron.

One would expect a strong temperature dependence for the coefficients, and presumably different coefficients for different types of trap. Clearly, the question of the magnitude of b_t is a very subtle one, and requires a degree of knowledge that is only rarely available.

In this paper it will be assumed that all of the temperature dependence of the trapping coefficients, as well as the variations in magnitude for different traps, can be described by an activated form,

$$b_t = b_0 \exp(-E_b/kT), \tag{3}$$

where E_b represents the energy barrier which must be overcome for trapping to occur, and may be different for different traps. The prefactor b_0 is taken to be the same for all traps. In spite of its simplicity, this form represents a significant increase in sophistication over the TROK model, in which the barrier energy was taken to be zero. Although our main results will not depend on this form, let us try to justify it in a little more detail. An activated form is exactly what one would expect on the basis of a naïve configurational coordinate model (Mott 1938). More sophisticated quantum-mechanical treatments (Struck and Fonger 1975) of this type of model alter somewhat the activated form. As the temperature is lowered, the trapping coefficient cannot, of course, continue to be activated, but rather must approach a minimum rate as the temperature is lowered, corresponding to transitions induced by the zero-point motion of the phonons. Actually, the quasi-activated behaviour is expected to be valid only for traps in which the electronic states are strongly coupled to phonons. For weakly coupled traps, the rates have a power law (T^n) dependence on temperature, but this weak dependence is not very important for our purposes (for a review, see Stoneham 1981).

Experimentally, several different traps were studied in crystalline III–V semiconductors by Henry and Lang (1977), using DLTS to obtain the temperature dependence and magnitude of the trapping cross-sections. Their observations showed exactly the sort of behaviour described above : at high temperatures, the cross-sections were roughly activated, but for temperatures below about 100 K the cross-sections became constant. The barriers to trapping varied widely, from 0 to roughly 0·5 eV. The room-temperature cross-sections varied by several orders of magnitude, but the extrapolation of the various cross-sections to infinite temperature was quite similar (within a factor of ten or so) for most, but not all, of the traps they studied. This last observation motivates our assumption that the trapping-rate prefactor b_0 is the same for all traps, an assumption that is particularly plausible for states with a similar microscopic nature such as band tail states. It remains to be seen, however, whether the diffusive nature of band transport in amorphous semiconductors affects the trapping processes in a fundamental way.

In fact, the relationship between the time dependence of the current at a particular temperature and the distribution of traps, derived below, does not depend on the assumption of an activated form for b_t. Rather, the effective DOS measured at a given energy will be just the actual DOS, multiplied by the value of b_t at that energy and temperature. However, in order to compare transients observed at different temperatures, some assumption about the temperature dependence of b_t is necessary, and the activated

form seems a reasonable choice. Now that we have discussed the microscopic nature of the coefficients for individual traps, we return to the dynamical behaviour of a system with many different traps.

§ 3. Time-dependent occupation number

The dynamics of the MT process can be understood most easily from an examination of the occupation number at various times. The occupation of each trap at any time can be determined from a knowledge of the number of carriers in transport states, $n(t)$, at all previous times. Since carriers in transport states are responsible for the current, we will refer to $n(t)$ as the current.

In this paper we do not discuss saturation of the traps, i.e. we assume that $f_i \ll 1$ for all times and for all traps important to the dynamics. The question of saturation in MT is closely connected to recombination, as has been discussed elsewhere (Orenstein and Kastner 1981 b, Orenstein, Kastner and Vaninov 1982). By taking $1-f_i=1$, eqn. (1) becomes linear, and can be integrated:

$$f_i(t)=b_i \int_{-\infty}^{t} dt'\, n(t') \exp\left[-\nu_i(t-t')\right]. \tag{4}$$

This expression is easily understood: carriers fall into the trap at a rate $b_i n(t')$, and then leak out at a constant release rate ν_i. We see that the form of this integral depends only on ν_i and the time dependence of the current; b_i enters only as a prefactor.

One interesting limit of eqn. (4) is when the release time ν_i^{-1} is much longer than the time-scale of variations in $n(t)$. For example, in a repetitive pulse experiment, the latter time-scale is the time between pulses t_{rep}. When $\nu_i t_{\mathrm{rep}} \ll 1$, combining eqns. (2) and (4) shows that

$$f_i \cong \exp\left(-E_i/kT\right)\bar{n}/N_c, \quad \nu_i t_{\mathrm{rep}} \ll 1. \tag{5}$$

This time-independent occupation is simply the steady-state Boltzmann distribution corresponding to the *average* number of mobile carriers $\bar{n}$. Thus states which have a release rate slower than the repetition rate of the experiment have a steady-state occupation, and do not contribute to the dynamics. This is clearly also valid for slow states which have become saturated, in which case eqn. (5) must be replaced by the full Fermi distribution. The simple formulation of eqn. (4) shows that very deep traps are unlikely to have significant impact on a repetitive pulse experiment, except to the extent that they alter the steady-state background.

In contrast, states which release carriers more rapidly than the repetitive rate will react significantly to the changing occupancy of the transport states in a transient experiment. We consider the case where a number of carriers is introduced into the transport states at time $t=0$, for example by a light flash. Equation (4) then exhibits two interesting limits, in addition to the slow, steady-state occupancy described above. The limit appropriate for a given state depends on the release time ν_i^{-1}, compared to the time t that has elapsed since the experiment was started.

Shallow states

The current $n(t')$ contributes significantly to the integral in eqn. (4) for a time ν_i^{-1} preceding t. For states with a rapid release rate, $\nu_i t \gg 1$, $n(t')$ will be essentially constant during the entire interval during which the occupancy was determined. The occupancy is therefore given by

$$f_i(t) \cong \frac{n(t)}{N_c} \exp(-E_i/kT), \quad \nu_i t \gg 1. \tag{6}$$

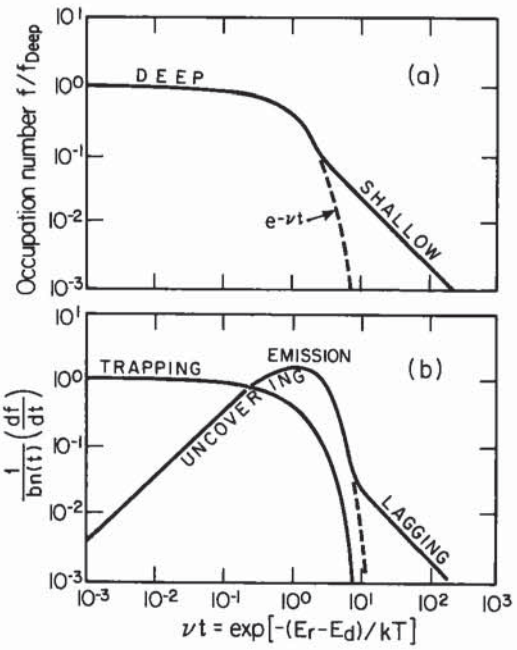
This has the same Boltzmann form as eqn. (5), for the very deep states, except that these shallow, rapidly releasing states have come into equilibrium with the *instantaneous* value of $n(t)$. The carriers in these states form a buffer to changes in the current, since their occupancy must also be changed to change $n(t)$.

Deep states

When $\nu_i \ll 1$, the exponential expression in eqn. (4) is equal to one. Thus

$$f_i(t) \cong b_i \int_0^t dt'\, n(t'), \quad \nu_i t \ll 1. \tag{7}$$

Fig. 1



(*a*) The occupation number of traps as a function of their release rate, at a time delay t, for a steep power law $t^{-0.9}$. The occupancy of deep traps is proportional to b, which is assumed to be constant for this figure. The release and demarcation energies, E_r and E_d, are defined in the text. (*b*) The emission and capture rates of eqn. (8) for the occupancy of (*a*). The magnitudes shown do not depend on a constant value for b. The dashed line indicates the uncovering term of eqn. (9).

These slowly releasing states have only experienced capture events; any carriers that have been captured by them are still trapped. The occupation number is plotted, for constant b, in fig. 1 (a). We have taken $t \ll t_{\text{rep}}$, so eqns. (6) and (7) are the two limits represented.

This description of the occupation number was used in the TROK model as the basis for deriving the form of the current transient. Our approach differs in that we immediately focus instead on the trapping and release from the traps as the driving force behind the dynamics. Clearly, trapping will be the most important process for the deep states, while states intermediate in energy will be changing from deep states into shallow states with time, and will be releasing more than trapping.

The exact trapping/release rate df_i/dt is given by eqns. (1) and (4) for any $n(t)$ and ν_i. In order to understand the dynamics more clearly, we have performed some straightforward algebra on these equations to separate two contributions. The result is

$$\frac{1}{b_i}\frac{df_i}{dt} = \exp(-\nu_i t)n(t) - \nu_i \int_0^t [n(t') - n(t)] \exp[-\nu_i(t-t')]\, dt'. \tag{8}$$

These terms correspond to trapping and release, respectively, and will be discussed in turn. They are plotted in fig. 1 (b).

The trapping term is straightforward: carriers are trapped at a rate $b_i n(t)$. The reason for the exponential cut-off for shallow states is that those states have come into equilibrium with the transport states, so that trapping and release are almost in balance. The separation of terms in eqn. (8) has been performed to exhibit only the unbalanced part of the trapping and release. To avoid confusion, we will use emission rate to refer to the rate per trap, and release rate (ν_i) to the rate per trapped carrier.

The emission term is largest for release rates comparable to the time delay. Clearly, the rate at which a given state can emit any excess carriers is limited by its release rate, so on the slow side of the peak df_i/dt is simply the product of the release rate and the number of carriers in excess of its equilibrium population which the state has captured. On the other hand, states with a rapid release rate have already emitted most of their excess carriers. For $\nu_i \gg 1$, the emission is given by $\nu_i^{-1}\, dn/dt$. This limit is also easy to understand: it represents the inability of the states to follow changes in $n(t)$ immediately. We therefore call this the ' lagging ' emission. The extent to which the occupany lags behind is greater the slower the release rate, and is just sufficient to keep these shallow states almost in equilibrium with the transport states.

It is helpful to derive a lower bound on the emission term. To do this we note that $\exp(\nu_i t')$ is always greater than one, so from eqn. (8)

$$\frac{df}{dt} > \left.\frac{df}{dt}\right|_{\text{uncovering}} \equiv \nu_i \exp(-\nu_i t) \int_0^t [n(t') - n(t)]\, dt'. \tag{9}$$

This expression is also plotted in fig. 1 (b). It is sharply peaked at $\nu_i t = 1$, falling off very rapidly for $\nu_i t > 1$. We refer to the lower limit in eqn. (9) as the ' uncovering ' emission, since it represents the emission of overfilled states as $\nu_i t$ becomes significant.

The relative magnitude of the lagging and uncovering terms depends on the decay of $n(t)$. Specifically, for rapid decays the integral of $n(t')$ becomes more important than the value of $n(t)$ itself, or of its derivative, and the uncovering term therefore becomes more important when $\nu_i t$ is of the order of one or smaller. Figure 1 (*b*) represents a $t^{-0.9}$ decay, which is fast enough to make the uncovering term apparent near the peak, but slow enough for the lagging emission also to be apparent, at faster release rates. For slower decays, the lagging emission merges smoothly into the peak in emission. For decays faster than t^{-1}, the emission is described accurately by the uncovering term throughout the peak region, and the lagging part of the emission is much smaller. The importance of this last feature will become apparent below when we discuss various types of decay.

Two important points should be noted here. The first is that the trapping coefficient enters as a simple factor, and therefore the contribution of each state to the trapping and release depends only on its release rate, except for a prefactor of b_i. The second is that several of the contributions to the trapping and release rate depend on this history of $n(t)$ only in a very simple way. For example, trapping is proportional to $n(t)$, the lagging emission is proportional to dn/dt, and the uncovering depends on $n(t)$ and $\int n(t')\,dt'$. If one of these processes dominates the decay, then we can hope to construct a simple differential equation for $n(t)$. In fact we construct such equations below, but in order to do so we must first discuss the role of the distribution of traps.

§ 4. Density of states (DOS)

So far we have treated the current $n(t)$ as an independent variable which determines both the occupation and the rate of trapping and emission for any given trap. In reality, of course, the observed $n(t)$ is a result of the sum of the trapping and emission from all the traps, and therefore depends on how many traps there are of each type.

The occupation number and its rate of change depend principally on the release rate ν_i. In this section, however, we express our results in terms of a closely related quantity—the energy required to remove a carrier from the trap. To this end, we replace the trap index i with the energy E. We assume that all traps at a given energy have the same barrier to trapping $E_b(E)$. Combining eqns. (2) and (3) gives

$$\begin{aligned}\nu(E) &= b_0 N_c \exp\left[-(|E| + E_b(E))/kT\right] \\ &= \nu_0 \exp\left(-E_r/kT\right), \quad \nu_0 = b_0 N_c,\end{aligned} \tag{10}$$

and

$$E_r = |E| + E_b(E) \tag{11}$$

is the ' release energy ' for a state of energy E. This release energy is positive, and in the absence of a barrier is simply the depth of the trap. We demonstrate below that if the DOS is expressed in terms of release energy, the simple relationship between the time dependence of $n(t)$ and the energy dependence of $g(E)$, derived in the TROK model, can still be obtained. The difference is that the quantity measured is not $g(E)$, but $\tilde{g}(E_r)b(E_r)$, an effective DOS reflecting the degree to which the states participate in the MT process.

In our discussion of the occupation number of the traps, we distinguished two limiting cases on the basis of release rate. By using eqn. (10), we can also make this distinction on the basis of release energy. The cross-over, at which $\nu(E)t=1$, occurs when the release energy is equal to a demarcation energy, E_d, given by

$$E_d \equiv kT \ln(\nu_0 t). \tag{12}$$

It is this separation of states in energy which led to the names shallow and deep for the two types of occupation. E_d moves to larger release energies logarithmically in time.

In order to determine the dynamics, we need to define a density of release rates. We do this in terms of a density of release energies, E_r. We denote the density of states in release energy $\tilde{g}(E_r)$ to distinguish it from the true DOS $g(E)$. The two quantities are related by

$$\tilde{g}(E_r) \equiv g(E)\left(\frac{\partial E_r}{\partial |E|}\right)^{-1} = g(E)\left(1+\frac{\partial E_b}{\partial |E|}\right)^{-1}, \tag{13}$$

which is well defined as long as $\partial E_b/\partial|E| > -1$ everywhere. Normally the two densities of states will be of the same order of magnitude, and the energy dependence of their ratio will be insignificant compared to the frequently observed exponential changes in the DOS as a function of energy, and generally we will not mention it.

We denote by $b(E_r)=b_0 \exp(-E_b(E_r)/kT)$ the trapping coefficient for the release energy in question. We can then write

$$\frac{dn}{dt} = \int dE_r\, \tilde{g}(E_r) b(E_r) \left|\frac{1}{b}\frac{df}{dt}\right|_{\nu=\nu_0 \exp(-E_r/kT,} \tag{14}$$

where the quantity $|(1/b)(df/dt)|$ is given by eqn. (8). It should be noted that each state is reflected in our general dynamical equation, eqn. (14), in proportion to its trapping coefficient, as first stated by Orenstein and Kastner (1981 a). This weighting of states by their trapping coefficients is still valid, it should be emphasized, even if the coefficients are not correctly described by an activated form. This simple multiplicative effect of variations in the trapping coefficient is one of the principal results of this paper, but it appears in the present treatment in a very straightforward way. Of course, in the presence of saturation this result would no longer be correct.

We have described our results in terms of a release energy, a quantity which is meaningful only if the trapping coefficient has an activated form. However, the results for the time dependence at a fixed temperature actually depend only on the release rate; the release energy was introduced to give a more physical picture. Thus, in principle, we could define an effective release energy as $E_r \equiv kT \ln(\nu_0/\nu)$, at any temperature. This is the true release energy if the trapping coefficient is activated. Moreover, if the density of states is defined in terms of this quantity, the results obtained below relating the DOS to the current will be valid. The physical meaning of the release energy so defined is not at all clear, however. This 'release energy' also depends on temperature (for a non-activated trapping coefficient), rather than being a fixed quantity for a given trap. In any event, the MT process is not very sensitive to changes in the magnitude of $b(E)$, since that

quantity enters only logarithmically into the release energy. It can therefore be hoped that the description in terms of an activated barrier to trapping (and the resultant description in terms of release energy) is close enough to the true physical situation for meaningful results to be obtained.

§ 5. Types of decay

In this section we discuss several types of decay within the framework of the various contributions to trapping and emission depicted in fig. 1 (*b*). For simplicity of notation, we express our results assuming a constant trapping coefficient of b_0 for all traps. The more general statement of the results can be determined by interpreting $g(E)$ as $\tilde{g}(E_r)b(E_r)/b_0$, as described in the preceding section.

Before going further, it is convenient to introduce the logarithmic derivative of the DOS, which we define as

$$\beta_0(E) \equiv \frac{\partial \ln g(E)}{\partial E}. \tag{15}$$

This quantity is positive for a DOS which is larger near the mobility edge, e.g. the DOS for a band tail. It should be stressed that β_0 need not have the same magnitude—or even the same sign—at all energies, as it would for an exponential DOS. If the DOS *is* exponential, then $\beta_0 = 1/kT_0$, in the notation of Orenstein and Kastner (1981 a). Rather, the form of the current transient at a given time will depend on the value of β_0 (actually $\beta_0 kT$) at the demarcation energy corresponding to that time, as will be shown below. It should be clear (for example, by examining fig. 1) that the resolution of the measurement is usually of the order of kT, so that only very closely spaced discrete levels could escape detection, and the logarithmic derivative in eqn. (15) is to be interpreted as an average over a region of width kT.

We now describe the results of a transient current measurement, although features of the distribution relevant to other experiments may easily be deduced. As time progresses after the initial excitation, the carrier distribution evolves towards the steady-state distribution, for which there is no net trapping or release. The attainment of this distribution is delayed by the trapping of carriers into some traps at occupations greater than their steady-state occupation. The approach to the steady state is then limited by the release rate from those states.

At any given time the dynamics of $n(t)$ depend on which states dominate the emission and which states dominate the trapping. The behaviour of $n(t)$, in turn, determines the occupancy, release and trapping rates for all traps. In order to determine which states dominate, we assume that the general features of the DOS are known. The dominant states for trapping (emission) are found by multiplying the DOS at each energy by the trapping (emission) rate from eqn. (8), and determining the energy at which the product is a maximum. This is most easily done graphically: if $1/g(E)$ is plotted logarithmically on fig. 1 (*b*), then the height of the trapping (emission) curve above the $1/g(E)$ curve represents the logarithm of the product $g(E)\,df/dt$. The maximum product is then easily determined. Since several parts of the curves on fig. 1 (*b*) are exponential with an energy width of kT, it is clear

that the magnitude of $\beta_0 kT$ will have an important effect on which states dominate. Now let us use this procedure to distinguish different types of decay.

Let us first examine the total trapping rate. The rate of trapping, $bn(t)\exp(-\nu t)$, is negligible for states much shallower than $-E_d$, and is approximately $bn(t)$ for deeper states. The total deep trapping rate is therefore given by

$$\left.\frac{dn}{dt}\right|_{\text{trapping}} = n(t)bN_d(t) \equiv n(t)\int_{-\infty}^{\infty} bg(E)\,dE\exp(-\nu t)$$

$$\cong n(t)\int_{-\infty}^{-E_d} bg(E)\,dE. \tag{16}$$

The total number of trapping centres $N_d(t)$ decays with time. However, this decay will be negligible unless the states at $-E_d$ dominate the integral. If deeper states dominate the trapping, then the trapping rate will be roughly independent of time. This latter condition also describes what happens during monomolecular recombination, and the part of a time-of-flight experiment long after the transit time, because, in both these cases as well, the rate of removal of carriers from the transport states is independent of time. Therefore we can distinguish two very difference types of decay, depending on which states dominate the trapping: states at $-E_d$, or deep states.

The form of the decay will also depend on the source for the emitted carriers: shallow states (lagging emission), states near $-E_d$ (uncovering) or deep states. We first discuss the case in which uncovering dominates the emission, then lagging, and finally domination by deep states. For the uncovering and lagging emission, the decay will also depend on the dominant trapping states.

The first case we discuss is that in which the emission is dominated by states near $-E_d$; this has been treated by previous authors (Tiedje and Rose 1981, Orenstein and Kastner 1981 a, b). In order for this situation to occur it is necessary that $\beta_0 kT > 1$, because if this condition were not satisfied then the DOS would grow more rapidly at shallow energies than the excess emission rate of eqn. (8) and fig. 1 (*b*) decays, and emission would be dominated by the shallower states. It is possible, of course, that even if the DOS is growing slowly with increasing energy near $-E_d$ ($\beta_0 kT < 1$), it grows so much faster at even shallower energies that the emission is still dominated by shallow states. This will occur if the DOS at some shallower energy exceeds the DOS at $-E_d$ by more than the corresponding Boltzman factor, a condition which can easily be evaluated using the graphical method described above, for a given DOS.

Now, for uncovering-dominated emission let us first treat the case in which trapping is also dominated by states near $-E_d$. This requires at least that $\beta_0 > 0$, since otherwise deeper states will dominate. Unfortunately this case is rather difficult to treat using the present method. The difficulty arises because the total emission rate near $-E_d$ is not simply a multiple of $n(t)$ or its integral or derivative, but must be calculated from the full form of eqn. (4). This calculation can be done numerically. For an exponential DOS with $0 < \beta_0 kT < 1$, however, the current is given by a power law, a result

which can be derived very simply. We reproduce very briefly the discussion of this case presented for the TROK model, although strengthened somewhat by eqn. (4).

The argument is based on the fact that, for a power-law decay of $n(t)$, the current $n(t')$ at an earlier time t', depends on t'/t in the same way at all times t. Because of this absence of an intrinsic time-scale, the form of the occupation number (eqn. (4)) is simply a function of νt, except for an overall factor. Thus, the occupation number curve does not change shape, but simply moves through the DOS as E_d grows. The overall magnitude of the occupation number is determined by the requirement that the total number of carriers remain constant. The magnitude is thus inversely proportional to the DOS at $-E_d$, $g[-kT \ln(\nu_0 t)] \propto (\nu_0 t)^{-\beta_0 kT}$. Since the Boltzmann factor describing the occupation of shallow states and transport states differs by a factor proportional to $\nu_0 t$ from the occupation number at $-E_d$, and since the total number of carriers is conserved, the power-law exponent is given by $1-\alpha$, where $\alpha \equiv \beta_0 kT$. When this exponent is inserted into eqn. (4) and integrated to give the total number of carriers, we obtain the magnitude of the current as well :

$$n(t) = \frac{\sin(\alpha\pi)}{\alpha\pi\,\gamma(\alpha, 1)} \frac{N_c}{N_L} N(\nu_0 t)^{-1+\alpha}, \tag{17}$$

where $\alpha = \beta_0 kT$, N is the total number of carriers, N_L is the number of localized states in the exponential band and $\gamma(\alpha, 1)$ is the incomplete gamma function. The numerical factor $\sin(\alpha\pi)/\alpha\pi\gamma(\alpha, 1)$ goes to zero as α for α approaching zero, and as $1-\alpha$ for $1-\alpha$ approaching zero, but is otherwise unexceptional.

The above argument is rigorous only for an exact exponential DOS and a power law which extends back to zero time. However, it can be seen that the integral which gives the total number of carriers is sharply peaked around $-E_d$ (with a width of the order of kT or β_0^{-1}), except when $\beta_0 kT$ is close to either one or zero. Thus a DOS which varies in a roughly exponential way with energy will still give rise to a slope which is given by $\alpha = \beta_0 kT$, with β_0 evaluated at $-kT \ln(\nu_0 t)$. A change in α will also change the numerical prefactor in eqn. (17), but this effect will generally be unimportant except for α near zero or one.

All the other transients we discussed may be treated within the trapping/release framework. For instance, in the example we have been discussing, as the number of deep trapping states decreases with time, the removal of carriers from transport states will eventually be dominated by some process other than trapping at $-E_d$. At that point, the decay will proceed much faster, and very soon the lagging part of the emission term will be negligible with respect to the uncovering term given by eqn. (9). Since the decay is faster than t^{-1}, as is shown below, the integral in eqn. (9) is sensibly constant once the decay is well under way, so the emission rate is just proportional to the DOS at $-E_d$ (the various contributions are again simply functions of νt) and to the release rate $1/t$ at $-E_d$. Therefore the current is given by

$$n(t) \propto \Gamma(\alpha+1)(\nu_0 t)^{-1-\alpha}. \tag{18}$$

It is worth noting that the argument leading up to eqn. (18) does not depend on $\beta_0 kT$ being less than one, and in fact that equation is still valid if $\beta_0 kT > 1$,

as long as emission is dominated by states at $-E_d$ and trapping is dominated by deep states (or recombination or transit across the sample). Thus, if emission is dominated by uncovered carriers, then the transient provides a spectroscopy of the DOS : the slope of the log–log plot is either $-(1-\beta_0 kT)$ or $-(1+\beta_0 kT)$, depending on whether trapping is at $-E_d$ or deeper. The first case corresponds to slopes shallower than -1, the second to steeper decays.

In contrast, if the DOS rises more rapidly at shallower energies, and trapping is not dominated by deep states, then the decay will be slow and the lagging term large, and the emission will come primarily from states which are shallower than $-E_d$. We now discuss that case. The emission from the shallow states results from the fact that their occupancy is lagging behind $n(t)$, and is therefore proportional to $-dn/dt$. The effect of this term is to slow the rate at which the thermalized shallow carriers are trapped, since they spend only a fraction of their time in the transport states. That fraction is given by $N_c/\tilde{N}_c$, where

$$\tilde{N}_c = \int_{-kT \ln \nu_0 t}^{\infty} g(E) \exp(-E/kT)\, dE \tag{19}$$

is the effective number of states at the band edge, including the shallow traps. If emission is truly dominated by the shallow states, then the lower limit of the integral is not critical and $\tilde{N}_c$ is not a function of time. (The integrand in eqn. (19) is proportional to the emission from lagging traps at energy E, so if shallow states dominate the emission they must also dominate the integral.) The time dependence is thus determined by the number of deep traps :

$$\frac{\tilde{N}_c}{N_c}\frac{dn}{dt} = -bN_d(t)n(t), \tag{20}$$

so that

$$n(t) = n(t_1) \exp\left[-\frac{N_c}{\tilde{N}_c}\int_{t_1}^{t} bN_d(t')\, dt'\right]. \tag{21}$$

Here t_1 is the time at which emission begins to be dominated by shallow states. We give a specific example of this behaviour below, but some comments on the general case are in order here. Equations (20) and (21) represent a process in which the rate of decay decreases with time (proportional to $N_d(t)$). However, the requirement that the emission be dominated by lagging, shallow states and the trapping by states near $-E_d$ also places restrictions on the decrease in the decay rate. Specifically, the rate of decay must decrease at least as fast as $1/t$ (since the DOS must decrease faster than the Boltzmann factor increases, for deeper energies). What this restriction on the decay rate means is that the decay, plotted on a log–log plot, must have positive curvature as long as the system is in this regime.

This situation will continue until either (1) the trapping becomes dominated by deep traps, or (2) emission from $-E_d$ or deeper begins to dominate emission. If (1) occurs, and shallow states still dominate the emission, then from eqn. (21) we see that the decay is a simple exponential. It should be noted that the shallow carriers increase the lifetime by a simple (time-independent) factor $(\tilde{N}_c/N_c)$. In contrast, if (2) occurs the current will

change smoothly to the appropriate limit : either the power law-like behaviour of eqn. (17) (for emission from $-E_d$) or a constant (for emission from deeper levels, which is described next).

The third case to consider is when deep states dominate the emission. For this to occur, the DOS must rise very rapidly at deeper energies (faster than a Boltzmann factor). The capture must therefore also be dominated by deep states. The current in this trivial case is simply a constant until $-E_d$ reaches the states dominating the emission, at which time the states being uncovered can finally deplete themselves down to an occupation in equilibrium with the shallow states. The various possible types of decay we have discussed are summarized in the table.

Possible decay types.

Dominant emission	Dominant trapping	
	Near $-E_d$	Deep
Shallow (lagging)	$n(t)=n(t_1)\times\exp\left[\frac{bN_c}{\tilde{N}_c}\int_{t_1}^{t}N_d(t')\,dt'\right]$	$n(t)=n(t_1)\times\exp\left(\frac{-N_dN_c}{\tilde{N}_c}bt\right)$
Near $-E_d$ (uncovering)	$n(t)\propto t^{-1+\beta_0kT}$, $0<\beta_0kT<1$	$n(t)\propto t^{-1-\beta_0kT}$, $\beta_0kT>-1$
Deep	Not possible	$n(t)$ constant

§ 6. Examples

To give the reader a better feeling for the relationship between the various types of decay, we examine a particular DOS in detail. We look at the decay for an exactly exponential DOS with $\beta_0kT>1$. (The case $0<\beta_0kT<1$ has been adequately described by Tiedje and Rose (1981) and Orenstein and Kastner (1981 a, b).) Specifically, we assume that

$$g(E)=N_L/kT_0\exp(E/kT_0),\quad T>T_0. \tag{22}$$

When the decay begins, there may be transient associated with time initial condition of the carrier distribution. For t greater than a few ν_0^{-1}, however, a condition such as that depicted in fig. 1 will arise. Since the DOS falls away from $E=0$ more rapidly than the Boltzmann factor, the emission will be dominated by lagging, shallow states. By inserting eqn. (22) into eqns. (14), (19) and (21), we obtain

$$\left.\begin{aligned} n(t)&=N\frac{N_c}{\tilde{N}_c}\exp\left[\frac{N_L}{\tilde{N}_c}\frac{\alpha\Gamma(\alpha)}{\alpha-1}(\nu_0t)^{-(\alpha-1)}\right],\\ \ln[n(t)]&=\ln\left(\frac{N_c}{\tilde{N}_c}N\right)+\frac{N_L}{\tilde{N}_c}\frac{\alpha\Gamma(\alpha)}{\alpha-1}\exp[-(\alpha-1)\ln(\nu_0t)].\end{aligned}\right\} \tag{23}$$

This expression describes an exponential on a log–log plot, decaying to a value $N_c/\tilde{N}_c$ times the total number of injected carriers, if there is sufficient time to reach this level. The time required for $n(t)$ to become greater than its final value by only a factor of e is

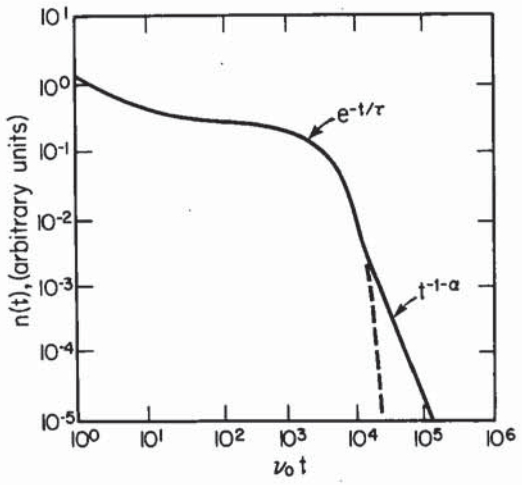
$$t_e = \nu_0^{-1}\left[\frac{N_L}{\tilde{N}_c}\frac{\alpha\Gamma(\alpha)}{\alpha-1}\right]^{1/(\alpha-1)}. \tag{24}$$

This time is very short (of the order of ν_0^{-1}) unless T is very close to T_0, at which temperature the remainder of this transient becomes infinite. The transient of eqn. (23) is very similar to those observed by Silver, Cohen and Adler (1981) in numerical simulations of MT.

The constant current, if it is reached, will continue as long as trapping is dominated by states near the mobility edge. At some time, however, some other mechanism will become dominant in removing carriers from transport states ; for example, recombination or transient across the sample. At this point the decay will become simply exponential (on a linear plot!) so the current will rapidly decrease.

With the rapid decay of the current, the emission due to lagging will become less and less important, while the emission due to uncovering of deep states will become more important (see the discussion of eqn. (9)). Shortly after the exponential decay begins, therefore, the lagging emission will cease being the dominant emission, and emission from uncovered carriers near $-E_d$ will dominate. We will then observe the power-law decay (steeper than t^{-2}!) of eqn. (18). The entire decay is illustrated in fig. 2.

Fig. 2



The form of the current transient for an exponential DOS, $N_L/kT_0 \exp(E/kT_0)$, with $T > T_0$. Three features are evident ; (1) A concave upward trace, which is exponential on this log–log plot, for short times, which becomes constant as the carriers achieve a steady-state distribution. (2) A truly exponential decay as thermalized carriers are trapped into a deep state. (3) A steep power-law decay for which the trapping rate is limited by the emission rate from states at the demarcation energy.

Finally, we note that this paper provides a basis for evaluating the proposal that there is an exponential DOS in several amorphous semiconductors (Tiedje, Cebulka, Morel and Abeles 1981, Orenstein and Kastner 1981 a). In previous discussions the possible effect of a barrier to trapping was not explored rigorously. In this paper, however, we have shown that a reduction in b by a factor has two effects : the time at which the states are observed is increased, and the effective DOS is decreased, both by the same factor. If one takes an activated form for the coefficients $b(E)$ it is possible to examine this possibility in detail.

Within the activated barrier approximation, the apparent DOS is approximately the true DOS $g(E)$ times a Boltzmann factor $\exp(-E_b/kT)$, evaluated where the release energy $E+E_b$ is equal to $kT\ln(\nu_0 t)$. In order to compare the currents corresponding to the same release energy (and therefore the same states), we therefore require a knowledge of ν_0. For power-law transients, however, the current looks the same on all observed time-scales, so no precise value for ν_0 is required (although it can be inferred from experiment ; see Orenstein and Kastner (1982).

In order to compare transients at different temperatures, one can simply plot the current at a given time and temperature versus $kT\ln(\nu_0 t)$. If the barrier to trapping E_b is the same for all states, then the curves for different temperatures should be parallel. This condition is in fact satisfied for power laws which have a slope of $-(1-T/T_0)$ at temperature T. This temperature dependence of the slope has been observed in time-of-flight measurements on a-Si : H (Tiedje *et al.* 1981) and transient photocurrent in a-As_2Se_3 (Orenstein and Kastner 1981 a). Recently Khan, Kastner and Adler (1983) have observed this temperature dependence in time-of-flight measurements on a-As_2Se_3, in contrast to previous work (Pfister and Scher 1978).

If the barrier E_b were different for different release energies, then the plot of current versus $kT\ln(\nu_0 t)$ would not give the same shape at different temperatures. A plot of the relative current at a given release energy versus $1/T$ will then determine the barrier to trapping, and the extrapolation of the curves to infinite temperature will give the true DOS $g(E)$, where E is determined from the release energy $kT\ln(\nu_0 t)$ and the barrier E_b at that release energy. For the photocurrent and time-of-flight data just mentioned, however, there is no reason to carry out this procedure, since the data require an exponential DOS with a constant barrier to trapping. Furthermore, the magnitude of the parameter ν_0 (related to b_0 by eqn. (12)), at around $10^{12}\,s^{-1}$, is as large as is physically reasonable, implying that there is no significant barrier to trapping into band tails in these amorphous semiconductors.

§ 7. Conclusions

In this paper we have focused on the trapping into and release from localized states, rather than their occupation as had been done previously. As a result we have been able to clarify the physical processes involved in multiple trapping (MT), and to facilitate the generalization of the model to a wider variety of situations. We have shown that the effect of a barrier to trapping on MT is simply to give an effective DOS, which is approximately the true DOS multiplied by the actual trapping coefficient. We have also extended the formalism to deal with transients at all temperatures, including

$\beta_0 kT > 1$, and we have demonstrated that these high-temperature transients will still reflect the DOS if the removal of carriers from mobile states is independent of time. We have also clarified the physical nature of the non-power-law transients observed at short times at all temperatures. In summary, our new outlook on the MT process, while remaining physical and relatively simple, enables the MT model to be extended to a variety of physical situations.

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References

Göbel, E. O., and Graudzus, W., 1982, *Phys. Rev. Lett.*, **48**, 1277.
Henry, C. H., and Lang, D. V., 1977, *Phys. Rev.* B, **15**, 989.
Khan, B. A., Kastner, M. A., and Adler, D., 1983, *Solid St. Commun.*, **45**, 187.
Mott, N. F., 1938, *Proc. R. Soc.* A, **167**, 384.
Noolandi, J., 1977, *Phys. Rev.* B, **16**, 4466.
Orenstein, J., and Kastner, M. A., 1981 a, *Phys. Rev. Lett.*, **46**, 1421 ; 1981 b, *Solid St. Commun.*, **40**, 85.
Orenstein, J., Kastner, M. A., and Vaninov, V., 1982, *Phil. Mag.* B, **46**, 23.
Pfister, G., and Scher, H., 1978, *Adv. Phys.*, **27**, 747, and references therein.
Schmidlin, F. W., 1977, *Phys. Rev.* B, **16**, 2362.
Silver, M., Cohen, L., and Adler, D., 1980, *Solid St. Commun.*, **40**, 535.
Stoneham, A. M., 1981, *Rep. Prog. Phys.*, **44**, 1251.
Struck, C. W., and Fonger, W. H., 1975, *J. Luminesc.*, **10**, 1.
Tiedje, T., and Rose, A., 1981, *Solid St. Commun.*, **37**, 49.
Tiedje, T., Cebulka, J. M., Morel, D. L., and Abeles, B., 1981, *Phys. Rev. Lett.*, **43**, 161.
Vardeny, Z., Strait, J., Pfost, D., Tauc, J., and Abeles, B., 1982, *Phys. Rev. Lett.*, **48**, 1132.