

## Determination of activation energies by using the widths of peaks of thermoluminescence and thermally stimulated depolarisation currents

C Christodoulides

Department of Physics, National Technical University, Polytechnioupolis Zografou, GR 157 73 Zografou, Athens, Greece

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**Abstract.** Expressions are presented for the determination of the activation energies,  $E$ , of first-order peaks of thermoluminescence or thermally stimulated depolarisation currents, using the widths or half-widths of the peaks. These widths correspond to temperatures at which the signal level is  $\frac{1}{4}$ ,  $\frac{1}{2}$  or  $\frac{3}{4}$  of the peak height, on either side of the peak temperature,  $T_M$ . Very exact expressions are derived, valid in the region of  $E/kT_M$  values between 10 and 100. Also given are expressions for the widths of the peaks when their energies and peak temperatures are known.

### 1. Introduction

Of the methods used in determining the thermal activation energy of a peak in thermoluminescence (TL) or thermally stimulated depolarisation currents (TSDC), by far the easiest to apply is the one based on the geometrical shape of the peak. By this we usually mean the width or half-width of the peak at a signal level equal to a fraction of the peak's maximum. The various formulae used assume that the kinetics involved in the process are known, and that the parameters in the expressions giving the activation energy depend on the order of kinetics. In this work we will be concerned with peaks obeying first-order kinetics only.

The various expressions suggested for use in determining the activation energy  $E$  were reviewed by Bräunlich (1968) and Chen (1969). In discussing these,  $T_M$  denotes the absolute temperature at which the peak maximum appears and  $T_1$  and  $T_2$  denote the temperatures at which the signal drops to half its maximum value on the low-temperature and high-temperature sides respectively. We will also make use of a result to be proved in § 2, namely that the value of the variable  $\varepsilon = E/kT$  for which the signal drops to a certain fraction  $\alpha$  of the maximum, depends only on  $\alpha$  and the value of  $\varepsilon$  at  $T_M$ , namely on  $\varepsilon_M = E/kT_M$  ( $k$  is Boltzmann's constant). The error in  $E$  as determined by a particular method based on the widths of the peak will therefore be a function of the parameter  $\varepsilon_M$  only. We will also state here that we will be mainly interested in the range of  $\varepsilon$  values between 10 and 100, which covers most, if not all, of the cases met in TL and TSDC.

Starting with the first of these expressions which was given by Urbach (1930), i.e.  $E = T_M/500$ , we may mention that it was meant as a very rough guide and as such it is of

limited accuracy. It is equivalent to assuming that  $\varepsilon_M = 23.2$  and gives energy values which may be wrong by up to a factor of two either way.

Lushchik (1955) gave the formula

$$E = \frac{kT_M^2}{T_2 - T_M}$$

which we find to be in error by 3.3% for  $\varepsilon_M = 10$ , reducing to 1.7% for  $\varepsilon_M = 100$ , in all cases giving a higher value of  $E$  than the actual one.

Halperin and Braner (1960) suggested

$$E = 1.72 \frac{kT_M^2}{T_M - T_1} \left( 1 - 3.16 \frac{kT_M}{E} \right).$$

By calculating  $T_1/T_M$  for a range of values between  $\varepsilon_M = 10$  and 100 in the manner to be described in § 2 (equation (7)), we found that this formula underestimates  $E$  by 4.2% for  $\varepsilon_M = 10$ , is exact for  $\varepsilon_M = 11$  approximately, over-estimates  $E$  by 12% for  $\varepsilon_M = 20$  and by 17% for  $\varepsilon_M = 100$ .

Grosswiener (1953) gave

$$E = 1.51 \frac{kT_M T_1}{T_M - T_1}$$

with a claimed accuracy of 5% for  $\varepsilon_M > 20$  and  $s/\beta > 10^7 \text{ K}^{-1}$ , where  $s$  is the frequency factor and  $\beta$  the heating rate. Dussel and Bube (1967) showed that the errors can be as high as 7%. We find that the second condition,  $s/\beta > 10^7 \text{ K}^{-1}$ , is not needed and that the formula overestimates  $E$  by 10.4% for  $\varepsilon_M = 10$ , by 7.1% for  $\varepsilon_M = 20$  and by 4.1% for  $\varepsilon_M = 100$ .

Keating (1961) gave an expression which may be written as

$$\frac{1}{\varepsilon_M} = \frac{T_2 - T_1}{T_M} \left( 1.2 \frac{T_2 - T_M}{T_M - T_1} - 0.54 \right) + 0.0055 - \frac{1}{4} \left( \frac{T_2 - T_M}{T_M - T_1} - 0.75 \right)^2$$

with the restrictions that  $0.75 \leq (T_2 - T_M)/(T_M - T_1) \leq 0.9$  and  $10 \leq \varepsilon_M \leq 35$ . As we prove in § 2,  $T_1/T_M$  and  $T_2/T_M$  are functions of  $\varepsilon_M$  only, so that the first restriction is found to be equivalent to  $6 \leq \varepsilon_M \leq 18$  which combined with the second restriction implies that Keating's formula is valid for  $10 \leq \varepsilon_M \leq 18$ . At any rate, we find that this expression overestimates  $E$  by 3% at  $\varepsilon_M = 10$ , by a maximum 10% at  $\varepsilon_M = 20$ , is exact at  $\varepsilon_M = 60$  and underestimates  $E$  by 12.5% for  $\varepsilon_M = 100$ .

Chen (1969), after critically reviewing all the above equations, calculates  $T_1$ ,  $T_M$  and  $T_2$  for a range of  $E$  between 0.1 and 2 eV and values of  $s/\beta$  between  $2 \times 10^5$  and  $2 \times 10^{13} \text{ K}^{-1}$ . These values correspond to  $\varepsilon_M$  between 14 and 42. He thus derived the equation

$$E = 2kT_M \left( 1.26 \frac{T_M}{T_2 - T_1} - 1 \right)$$

giving quite accurate results for  $E$ . In particular, we find that the equation underestimates  $E$  by 4% at  $\varepsilon_M = 10$ , by 1.6% at  $\varepsilon_M = 14$ , is exact at  $\varepsilon_M = 22$  and overestimates  $E$  by 1.6% at  $\varepsilon_M = 40$  and 2.4% at  $\varepsilon_M = 100$ . Chen also derived a less accurate version of the above equation,

$$E = 2.29 \frac{kT_M^2}{T_2 - T_1}$$

which however is wrong by up to 3% for  $\varepsilon_M$  between 14 and 40, and by 5% for  $\varepsilon_M$  down to 10 or up to 100.

Chen (1969) also corrected the coefficient in Lushchik's equation, which now becomes

$$E = 0.976 \frac{kT_M^2}{T_2 - T_M}.$$

This is quite accurate, the errors being less than 0.5% for  $\varepsilon_M$  between 14 and 40 and less than 0.8% when  $\varepsilon_M$  is as low as 10 or as high as 100.

Finally, Chen (1969) gives the equation

$$E = 1.52 \frac{kT_M^2}{T_M - T_1} - 3.16kT_M$$

which expresses  $E$  in terms of  $T_M$  and the low-temperature half-width of the peak,  $T_M - T_1$ . We find that this expression underestimates  $E$  by 5.3% at  $\varepsilon_M = 10$ , by 2.5% at  $\varepsilon_M = 14$ , is exact at  $\varepsilon_M = 22$  and overestimates  $E$  by 2% at  $\varepsilon_M = 43$  and by 3.2% at  $\varepsilon_M = 100$ .

We will show below that expressions for  $E$  can be found, which have accuracies of better than 0.1% as compared to the exact Randall–Wilkins equation, and involve  $T_M$ ,  $T_1$  and  $T_2$ , or the temperatures  $S_1$  and  $S_2$  at which the signal is  $\frac{1}{4}$  of the peak's maximum, and  $U_1$  and  $U_2$  at which the signal is  $\frac{3}{4}$  of the maximum. Of course the experimental uncertainties in determining these temperatures lead to errors in  $E$  which are larger than 0.1%. In this respect, it is felt that using the pairs  $(S_1, U_1)$ ,  $(U_2, S_2)$  or  $(S_1, S_2)$ , which can be determined more accurately, will reduce the errors in the final results.

## 2. Theory

We will initially use the terminology of thermoluminescence. The final results however are presented in such a form as to be applicable to peaks of thermally stimulated depolarisation currents as well.

### 2.1. The equation of the peak

For peaks obeying first-order kinetics, the variation of light intensity with temperature is described, apart from a constant of proportionality, by the Randall–Wilkins equation:

$$I = n_0 s \exp \left\{ -\frac{E}{kT} - \int_0^T \frac{s}{\beta} \exp \left( -\frac{E}{kT} \right) dT \right\} \quad (1)$$

where  $E$  is the trap depth,  $s$  is the frequency factor,  $k$  is Boltzmann's constant,  $n_0$  the initial number of trapped charge carriers the liberation of which causes the peak to appear,  $\beta$  is the heating rate and  $T$  the absolute temperature.

For constant heating rate, the peak has a maximum at temperature  $T_M$ , which satisfies the equation

$$\frac{\beta E}{kT_M^2} = s \exp \left( -\frac{E}{kT_M} \right). \quad (2)$$

In terms of the variable  $\varepsilon = E/kT$  and its value at peak maximum,  $\varepsilon_M = E/kT_M$ , equations (1) and (2) give

$$I = n_0 s \exp \left\{ -\varepsilon - \varepsilon_M^2 \exp(\varepsilon_M) \int_{\varepsilon}^{\infty} \frac{e^{-z}}{z^2} dz \right\}. \quad (3)$$

The integral can be expressed in terms of the second exponential integral

$$E_2(\varepsilon) = \int_1^{\infty} \frac{e^{-\varepsilon t}}{t^2} dt = \varepsilon \int_{\varepsilon}^{\infty} \frac{e^{-z}}{z^2} dz$$

so that equation (3) becomes

$$I = n_0 s \exp \left\{ -\varepsilon - \varepsilon_M^2 \exp(\varepsilon_M) \frac{E_2(\varepsilon)}{\varepsilon} \right\} \quad (4)$$

which has a maximum value, for  $\varepsilon = \varepsilon_M$ , equal to

$$I_M = n_0 s \exp \{ -\varepsilon_M - \varepsilon_M \exp(\varepsilon_M) E_2(\varepsilon_M) \}$$

so that finally

$$I = I_M \exp \left\{ -(\varepsilon - \varepsilon_M) - \varepsilon_M^2 \exp(\varepsilon_M) \left[ \frac{E_2(\varepsilon)}{\varepsilon} - \frac{E_2(\varepsilon_M)}{\varepsilon_M} \right] \right\}. \quad (5)$$

This expression gives the signal output  $I$  as a function of  $\varepsilon$  for a TL or TSDC peak of given  $I_M$  and  $\varepsilon_M$ . It should be noted that given a value of  $\varepsilon_M$ , the ratio  $I/I_M$  depends only on  $\varepsilon$ .

## 2.2. The values of $\varepsilon$ for a given ratio $I/I_M$

To solve equation (5) for  $\varepsilon$ , given a ratio  $I/I_M$ , we must use an iteration procedure. We must ensure that this procedure converges.

Equation (5) may be written as

$$(\varepsilon - \varepsilon_M) + \left( \frac{\varepsilon_M}{\varepsilon} \right)^2 \exp(\varepsilon_M - \varepsilon) [\varepsilon e^{\varepsilon} E_2(\varepsilon)] = [\varepsilon_M \exp(\varepsilon_M) E_2(\varepsilon_M)] + \ln \left( \frac{I_M}{I} \right). \quad (6)$$

From tables of the exponential integrals such as those of Abramowitz and Stegun (1965), we find that for  $5 \leq \varepsilon \leq \infty$  we have  $0.7 \leq \varepsilon e^{\varepsilon} E_2(\varepsilon) \leq 1$  and therefore the terms in square brackets in equation (6) are of order unity.

For temperatures  $T < T_M$ , i.e.  $\varepsilon > \varepsilon_M$ , we have  $\exp(\varepsilon_M - \varepsilon) < 1$  and the term  $(\varepsilon - \varepsilon_M)$  dominates in equation (6), so we can solve for  $\varepsilon$  as

$$\varepsilon = \ln \left( \frac{I_M}{I} \right) + \varepsilon_M [1 + \exp(\varepsilon_M) E_2(\varepsilon_M)] - \varepsilon_M^2 \exp(\varepsilon_M) \frac{E_2(\varepsilon)}{\varepsilon}. \quad (7)$$

For  $T > T_M$ , i.e.  $\varepsilon < \varepsilon_M$ ,  $\exp(\varepsilon_M - \varepsilon)$  is greater than and dominates over  $(\varepsilon - \varepsilon_M)$  in equation (6) so that

$$\varepsilon = \varepsilon_M - \ln \left\{ \frac{\ln(I_M/I) + \varepsilon_M [1 + \exp(\varepsilon_M) E_2(\varepsilon_M)] - \varepsilon}{\varepsilon_M^2 e^{\varepsilon} E_2(\varepsilon)/\varepsilon} \right\}. \quad (8)$$

Given a value of  $I/I_M$ , the corresponding value of  $\varepsilon$  on the low-temperature side of the peak can be found by using equation (7), while that at the high-temperature side of the peak is given by equation (8). Both iteration procedures converge if  $\varepsilon_M$  is used on

the right-hand side of the equations as starting values for  $\epsilon$ . Each time, a better estimate for  $\epsilon$  is found, which is then fed into the right-hand side of the equation. This iteration procedure is continued until the required accuracy in  $\epsilon$  is achieved.

In numerical work, a rational approximation may be used for the transcendental function  $E_2(\epsilon)$ . Such expressions were given by Hastings (1955) and are also quoted by Abramowitz and Stegun (1965). One such expression is

$$e^\epsilon E_2(\epsilon) = \frac{0.99997\epsilon + 3.03962}{\epsilon^2 + 5.03637\epsilon + 4.19160} + \Delta(\epsilon) \tag{9}$$

where  $|\Delta(\epsilon)| < 10^{-7}$  for  $10 \leq \epsilon$ .

### 3. Results

#### 3.1. Expressions for the energy

We were interested in finding the values of  $\epsilon$  for which  $I/I_M = \frac{1}{4}, \frac{1}{2}$  and  $\frac{3}{4}$ . These are denoted by  $\delta_1, \epsilon_1$  and  $\zeta_1$  respectively for the low-temperature side of the peak, and by  $\delta_2, \epsilon_2$  and  $\zeta_2$  for the high-temperature side (see figure 1). The temperatures corresponding to  $\delta_1, \epsilon_1, \zeta_1, \epsilon_M, \zeta_2, \epsilon_2$  and  $\delta_2$  are  $S_1, T_1, U_1, T_M, U_2, T_2$  and  $S_2$  respectively, in increasing order. These values of  $\epsilon$  were found for a range of  $\epsilon_M$  values between 10 and 100, using equations (7) and (8) with the approximation for  $E_2(\epsilon)$  given by equation (9).

Some simple relation was searched for, connecting the quantities in each of the following pairs:  $(\epsilon_1, \epsilon_M), (\epsilon_2, \epsilon_M), (\epsilon_1, \epsilon_2), (\delta_1, \epsilon_M), (\delta_2, \epsilon_M), (\delta_1, \delta_2), (\delta_1, \zeta_1)$  and  $(\delta_2, \zeta_2)$ . We illustrate this procedure by using the results for the pair  $(\epsilon_1, \epsilon_M)$ . A plot of  $\epsilon_M$  as a function of  $\epsilon_M/(\epsilon_1 - \epsilon_M)$  was found to be very linear (see figure 2(b)), so that we can assume that

$$\epsilon_M = c_1 \left( \frac{\epsilon_M}{\epsilon_1 - \epsilon_M} \right) + c_2. \tag{10}$$

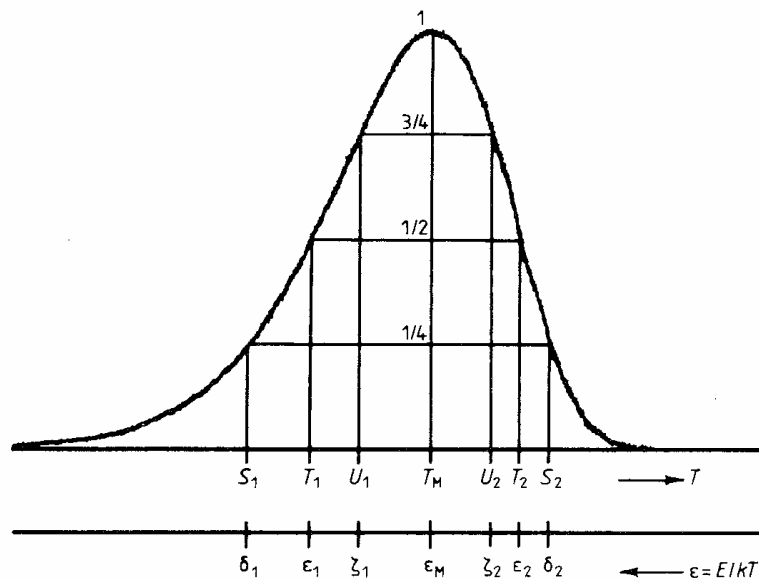
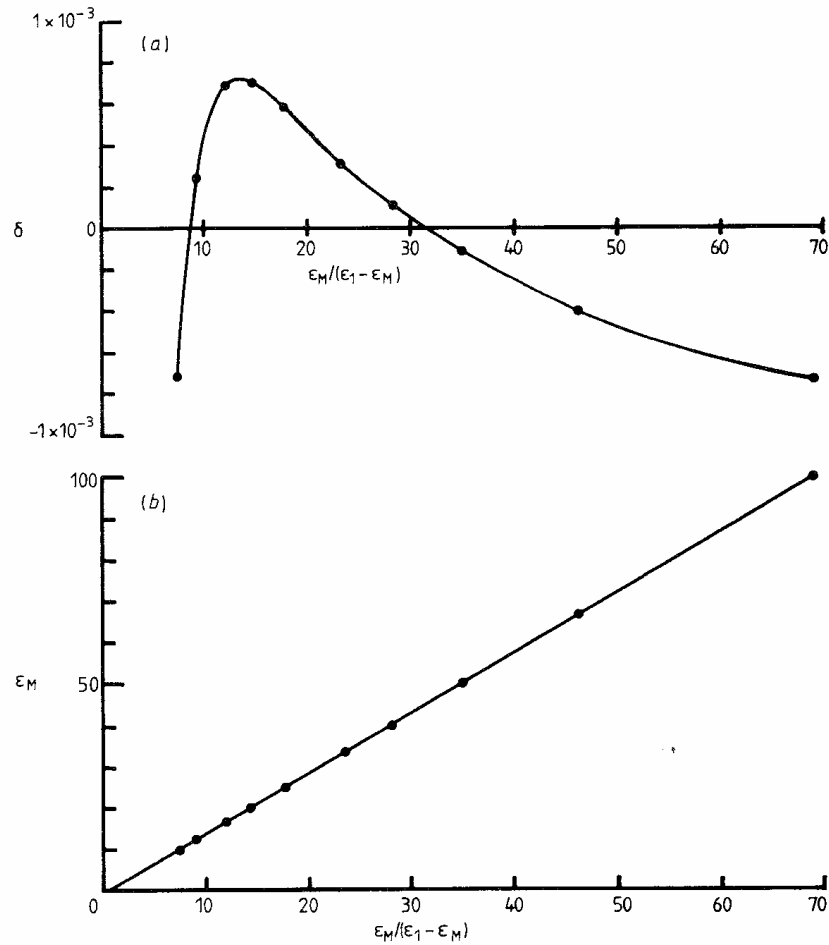


Figure 1. A TL or TSDC peak showing the various temperatures defined in the text. Also shown are the corresponding  $\epsilon$  values.



**Figure 2.** (a) The fractional error in  $E$ , defined as  $\delta = (E/E_{\text{corr}}) - 1$  where  $E$  is the value of energy found by using the expression  $E = T_1 T_M / 7954 (T_M - T_1) - T_M / 17158$  derived from the linear relationship in (b), and  $E_{\text{corr}}$  is the correct value of the energy. (b) A plot of  $\epsilon_M$  as a function of  $\epsilon_M / (\epsilon_1 - \epsilon_M)$  illustrating their linear relationship for  $\epsilon_M$  between 10 and 100.

If we choose  $c_1$  and  $c_2$  such as to minimise the maximum of the absolute value of the fractional error in  $\epsilon_M$  as given by equation (10), in the range of  $\epsilon_M$  values between 10 and 100, we find:

$$c_1 = 1.45899 \quad c_2 = -0.67635.$$

For these values of  $c_1$  and  $c_2$  the fractional error in  $\epsilon_M$  as given by equation (10) is less than 0.07% for  $\epsilon_M$  between 10 and 100 (see figure 2(a)).

Equation (10) can be expressed in terms of temperatures as

$$E = \frac{T_1 T_M}{7954(T_M - T_1)} - \frac{T_M}{17158}$$

in eV when  $T$  is in K.

In fact this equation was not chosen to be presented in the final results. Considering instead  $\epsilon_1$  as a function of  $\epsilon_M / (\epsilon_1 - \epsilon_M)$ , a similar relation was found which is accurate to within 0.015%, so the latter was finally chosen (equation (11) below).

This procedure was followed for each of the pairs listed above, each time finding two linear relationships connecting the pair of variables and choosing the more accurate one. The results were surprisingly accurate, with fractional errors in  $E$  of no more than 0.1% and in some cases as low as 0.005%.

The results, giving the value of  $E$  in eV in terms of the various temperatures, are presented below. We also define the fractional error in  $E$  as  $\delta = E/E_{\text{corr}} - 1$  where  $E$  is the value of energy as found by the use of the formula and  $E_{\text{corr}}$  is the correct value. Given next to each expression for  $E$  and in parentheses, is the value of  $100|\delta|_{\text{max}}$ , i.e. the maximum absolute value of the percentage error in  $E$  as given by the expression. The expressions for  $E$  are:

$$E = \frac{T_1 T_M}{7940(T_M - T_1)} - \frac{T_1}{14866} \quad (\pm 0.015\%) \quad (11)$$

$$E = \frac{T_2 T_M}{11780(T_2 - T_M)} - \frac{T_M}{10010} \quad (\pm 0.005\%) \quad (12)$$

$$E = \frac{T_1 T_2}{4738(T_2 - T_1)} - \frac{T_1}{11616} \quad (\pm 0.06\%) \quad (13)$$

$$E = \frac{S_1 T_M}{5077(T_M - S_1)} - \frac{S_1}{16813} \quad (\pm 0.04\%) \quad (14)$$

$$E = \frac{S_2 T_M}{8881(S_2 - T_M)} - \frac{T_M}{9439} \quad (\pm 0.015\%) \quad (15)$$

$$E = \frac{S_1 S_2}{3225(S_2 - S_1)} - \frac{S_1}{11797} \quad (\pm 0.10\%) \quad (16)$$

$$E = \frac{S_1 U_1}{8192(U_1 - S_1)} - \frac{S_1}{22121} \quad (\pm 0.008\%) \quad (17)$$

$$E = \frac{S_2 U_2}{18351(S_2 - U_2)} - \frac{U_2}{9018} \quad (\pm 0.03\%) \quad (18)$$

### 3.2. Peak widths

It is sometimes of interest to know the widths of a peak whose  $E$  and  $T_M$  are known. Relations between these widths and  $\varepsilon_M$  and  $T_M$  were obtained using the procedure illustrated below for the case of  $T_M - T_1$ . It is assumed that

$$\frac{\varepsilon_1}{\varepsilon_1 - \varepsilon_M} = \frac{\varepsilon_M + B}{A} \quad (19)$$

where  $A$  and  $B$  are constants to be determined. The plot of  $\varepsilon_1/(\varepsilon_1 - \varepsilon_M)$  as a function of  $\varepsilon_M$  is a straight line to a very high accuracy.  $A$  and  $B$  were determined, such as to minimise the maximum of the absolute value of the fractional error in  $\varepsilon_1/(\varepsilon_1 - \varepsilon_M)$ , for  $\varepsilon_M$  between 10 and 100. Having determined  $A$  and  $B$  we can then rewrite equation (19) as

$$\frac{1}{\varepsilon_M} - \frac{1}{\varepsilon_1} = \frac{A}{\varepsilon_M(\varepsilon_M + B)}$$

and finally

$$T_M - T_1 = \frac{AT_M}{\varepsilon_M + B} \quad (20)$$

Such expressions for the widths and half-widths of a peak were obtained as described above. By comparison with the exact values given by equations (7) and (8), we also determined in each case the maximum value of the magnitude of the fractional error in the region  $10 \leq \varepsilon_M \leq 100$ . These are given in parentheses next to each expression listed below.

$$T_M - T_1 = \frac{1.4591}{\varepsilon_M + 2.137} T_M \quad (\pm 0.07\%) \quad (21)$$

$$T_2 - T_M = \frac{0.98516}{\varepsilon_M + 0.174} T_M \quad (\pm 0.004\%) \quad (22)$$

$$T_2 - T_1 = \frac{2.4404}{\varepsilon_M + 1.252} T_M \quad (\pm 0.11\%) \quad (23)$$

$$T_M - S_1 = \frac{2.2810}{\varepsilon_M + 2.837} T_M \quad (\pm 0.07\%) \quad (24)$$

$$S_2 - T_M = \frac{1.3067}{\varepsilon_M - 0.077} T_M \quad (\pm 0.014\%) \quad (25)$$

$$S_2 - S_1 = \frac{3.5759}{\varepsilon_M + 1.577} T_M \quad (\pm 0.20\%) \quad (26)$$

It should be mentioned finally that the frequency factor  $s$  can be found from equation (2) by using the values of  $\varepsilon_M$  determined by equations (11) to (18).

#### 4. Discussion

The theory presented is based on the Randall–Wilkins equation for peaks obeying first-order kinetics. Based on this assumption, expressions were derived for the energy of the peak in terms of various temperatures at which the signal is a certain fraction of the maximum. It was demonstrated that the values of  $\varepsilon_1$ ,  $\varepsilon_2$ ,  $\delta_1$ ,  $\delta_2$ ,  $\zeta_1$ ,  $\zeta_2$  depend only on the  $\varepsilon_M$  value of the peak. The inverse problem was also studied, of determining the peak's widths, given its  $\varepsilon_M$  and  $T_M$ . In all situations, relations between these quantities were found which were remarkably linear, resulting in very exact expressions for both the energy and the widths of the peak. It should be stressed that this accuracy refers to the range of  $\varepsilon_M$  values between 10 and 100 which covers most of the experimentally possible situations. The expressions may however be used for values outside this region, but with an increase of the uncertainties in the results.

Apart from widening the range of  $\varepsilon_M$  values for which the expressions apply, and substantially improving the accuracy of the results as compared to existing formulae, expressions were also derived which are based on the temperatures at which the height is  $\frac{1}{4}$  or  $\frac{3}{4}$  of the peak height. These may be used even when only one side of the peak is available, undisturbed by other peaks. The main advantage of these expressions, however, is that they depend on temperatures which are measured at points where the



slope of the curve is high, leading to higher accuracy in their values. This is of great value since all expressions for  $E$  depend on the difference of two similar temperatures (in the denominators of equations (11) to (18)) and this has the effect of producing large fractional errors in  $E$  from small uncertainties in the temperatures.

It should be emphasised that the percent errors given for the expressions presented in this work refer to the degree of agreement between the approximate expressions for the energy and peak widths and the exact predictions of the Randall–Wilkins equation.

Serious limitations may exist in some cases in the applicability of the theory described. As the theory is based on the first-order equation for the peak, the results do not apply to peaks not obeying first order kinetics. As this is not known *a priori*, the method can be used as a means of obtaining a first estimate of the energy of the peak which may then be used in a curve-fitting procedure to verify the order of kinetics involved.

In polymers and many crystalline systems, peaks are due not to a single energy value but to a distribution of energy values. The method presented does not give any meaningful results in these cases. However, there exist experimental techniques such as that of thermal sampling in which, by means of both selective polarisation and subsequent peak cleaning by thermal treatment, relaxation mechanisms produced by a narrow range of energy values may be isolated. These then result in a peak of shape very similar to that of a single first-order process and the theory presented may be applied to determine the mean energy of the relaxations isolated.

The theoretical errors in the expressions presented in this work are much smaller than those resulting from the experimental difficulties in measuring the temperatures. It is in this respect that the use of the temperatures at  $\frac{1}{4}$  and  $\frac{3}{4}$  of peak height may be an advantage. Whenever possible, more than one expression should be used in determining  $E$ , so as to improve the accuracy of the final result, but also to check whether the kinetics of the peak is in fact of first order and as a means of detecting possible interference from other unresolved peaks, depending on whether consistent results are obtained using the different expressions.

## 5. Conclusions

Expressions were derived which give the energy of a first-order peak in terms of its widths or half-widths at various signal levels, these being fractions equal to  $\frac{1}{4}$ ,  $\frac{1}{2}$  and  $\frac{3}{4}$  of the maximum. The accuracy of these is better than 0.1% in the region of  $\epsilon_M$  values between 10 and 100. This is both an improvement in accuracy and in the range of applicability of the expressions as compared to previously available ones. In addition, the use of the expressions making use of the temperatures at which the signal is  $\frac{1}{4}$  or  $\frac{3}{4}$  of the maximum should improve the accuracy of the results as it reduces the errors in the measurement of the temperatures used. It has also been shown that  $\epsilon_M$  is the correct parameter to be used in determining the accuracy and range of applicability of the various expressions for the energy.

## References

- Abramowitz M and Stegun I A (eds) 1965 *Handbook of Mathematical Functions* (New York: Dover) ch 5  
Bräunlich P 1968 *Thermoluminescence of Geological Materials* ed. D J McDougall (London, New York: Academic) pp 61–88  
Chen R 1969 *J. Appl. Phys.* **40** 570–85

- Dussel G A and Bube R H 1967 *Phys. Rev.* **155** 746  
Grosswiener L I 1953 *J. Appl. Phys.* **24** 1306  
Halperin A and Braner A A 1960 *Phys. Rev.* **117** 408–15  
Hastings C Jr 1955 *Approximations for Digital Computers* (Princeton: University Press)  
Jenkins T R 1978 *J. Computat. Phys.* **29** 302–5  
Keating P N 1961 *Proc. Phys. Soc.* **78** 1408  
Lushchik C B 1955 *Dokl. Akad. Nauk. SSSR* **101** 641  
Urbach F 1930 *Weiner Ber. Ila* **139** 363