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On the Computation of the Integral Appearing in Glow Curve Theory*

Dealing with the theories of thermoluminescence (TL) [1] and thermally stimulated currents (TSC) [2] one always has in the expression giving the intensity of the phenomenon the integral $\int_{T_0}^{T} \exp(-E/kT')\,dT'$, where E is the activation energy (ev), k—the Boltzmann constant (ev/°K), T_0 is the temperature (°K) at which the crystal is excited before being heated, and T the variable temperature (°K). A method which is usually simpler and more accurate than numerical integration for evaluating the value of the integral is found by integration in parts [3, 4] of the same integral when the lower limit of integration is 0 instead of T_0:

$$F(T, E) = \int_0^T \exp(-E/kT')\,dT' = T\exp(-E/kT) \sum_{n=1} (kT/E)^n (-1)^{n-1}\, n! \quad (1)$$

Thus the value of the needed integral is [5]

$$\int_{T_0}^{T} \exp(-E/kT')\,dT' = F(T, E) - F(T_0, E). \quad (2)$$

Since $F(T, E)$ is a very strongly increasing function of T, it is conventional to neglect $F(T_0, E)$ in comparison to $F(T, E)$, so that the right hand side of Eq. (1) is considered to represent the value of the integral (from T_0) very well. The series on the right hand side of Eq. (1) is divergent but may give a good approximation for the value of the integral as follows. If one takes N terms of this asymptotic series

$$S_N = \sum_{n=1}^{N} (kT/E)^n (-1)^{n-1}\, n! \quad (3)$$

the absolute value of the maximal possible error, $|R_N|$ would not exceed the absolute value of the $(N+1)$th term, a_{N+1}. Thus,

$$|R_N| = |a_{N+1}| = (kT/E)^{N+1} (N+1)!. \quad (4)$$

The series in Eqs. (1) and (3) is very closely related to the Euler series [6].

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In previous treatment of Eq. (1) usually only the first term [3, 7] or first two terms [8] were taken as an approximation for the value of the integral. The former approach includes an error of 10–20%. The latter one is reasonably good for the usual cases where E/kT is about 20 (error of about 1.5%), but becomes worse for extreme cases of $E/kT \approx 10$ appearing in certain cases, when the error can be of 6% or more. This is specially undesirable when first order glow curves are investigated since in this case the expression for the glow intensity includes the above mentioned integral appearing in the exponent:

$$I(T) = sn_0 \exp(-E/kT) \exp\left[-(s/\beta) \int_{T_0}^{T} \exp(-E/kT')\, dT'\right] \tag{5}$$

where s is the frequency factor ($\sec^{-1}$), n_0 the initial concentration of electrons (cm^{-3}) and β the heating rate (°K/sec). In these cases it is desirable to take more terms in the series. This does not pose a serious problem when the glow curve is evaluated by the use of a computer [9, 10]. It is, however, of primary importance to decide the number of terms to be taken for optimal results and to evaluate the possible error for each case.

The simple procedure for having the optimal value of the integral is taking the terms in the series down to the smallest one (or the preceding one), when the possible error would be about the same as this last term. Thus it is worthwhile taking N to be the highest number for which $|a_N/a_{N-1}| \leqslant 1$. This can be written as

$$(kT/E)N \leqslant 1. \tag{6}$$

Thus the number of terms, N, to be taken is the largest integer smaller than E/kT. The absolute value of the last term taken is $(kT/E)^N N!$ and the possible error is given again by Eq. (4) for the N fixed by Eq. (6). Since E/kT (and thus N too) is about 10 or more for all physically interesting cases, a_N and a_{N+1} differ only slightly from one another, but have opposite signs. One can take, therefore, $\frac{1}{2}a_N$ instead of a_N as the last term in the series and by this reduce the maximal possible error to

$$|R_N| \approx |\tfrac{1}{2}a_{N+1}| = \tfrac{1}{2}(kT/E)^{N+1}(N+1)! \approx \tfrac{1}{2}(kT/E)^N N! \tag{7}$$

Let us define $0 \leqslant \alpha < 1$ such that

$$E/kT = N + \alpha \tag{8}$$

and thus have

$$1/|R_N| \approx 2(N+\alpha)^N/N! = 2N^N(1+\alpha/N)^N/N! \tag{9}$$

Since we are dealing with $N \approx 10$ or more, we can use the Stirling formula $N! \approx \sqrt{2\pi}\, N^{N+1/2}e^{-N}$ and write $(1+\alpha/N)^N \approx e^{\alpha}$. The possible error in the former would not exceed 1% and in the latter, about 5%.

Thus we have now

$$1/|R_N| \approx (2/\sqrt{2\pi N})\, e^N e^\alpha \tag{10}$$

or

$$|R_N| \approx \tfrac{1}{2}\sqrt{2\pi N}\, e^{-(N+\alpha)}. \tag{11}$$

$N + \alpha$ is E/kT by Eq. (8). By inserting E/kT instead of N in the square root. we may add an error of up to about 5 %, therefore

$$|R_N| \approx \sqrt{\tfrac{1}{2}\pi E/kT}\, \exp(-E/kT). \tag{12}$$

Thus we have: an effective method to decide the number of terms to be taken in the series, an improvement by taking half of the last term thereby reducing the possible error to a half, and an effective method for estimating the error. In order to find the relative error we have to divide the term in Eq. (12) by the sum of the series, which can, for this purpose, be approximated by the first term kT/E,

$$|R_N/a_1| \approx \sqrt{\tfrac{1}{2}\pi(E/kT)^3}\, \exp(-E/kT). \tag{13}$$

For the case of interest, $E/kT \approx 10$, one has to take about 10 terms in the series and the possible relative error would be about 2×10^{-3}, which would give very reasonable results for the calculated glow intensities. For $E/kT \approx 20$ one may take 20 terms in the series, thus having a possible relative error of about 10^{-7}. This accuracy is not necessary in most cases and less terms can be taken when N is much larger than 10.

As for the possible error generated by neglecting $F(T_0, E)$, it would be sufficient to compare the first terms in $F(T, E)$ and $F(T_0, E)$. One has

$$F(T_0, E)/F(T, E) \approx (kT_0^2/E)\exp(-E/kT_0)/[(kT^2/E)\exp(-E/kT)] \tag{14}$$

which can be written

$$F(T_0, E)/F(T, E) \approx (T_0/T)^2 \exp[(E/kT)(1 - T/T_0)]. \tag{15}$$

Since $T > T_0$, this ratio will be smaller for larger values of E/kT. For the extreme cases of $E/kT \approx 10$ one has to have $T/T_0 \approx 1.55$ in order to get an error which would not exceed 2×10^{-3} which was the possible error in evaluating $F(T, E)$ Thus the value of T_0 should be as low as possible when $E/kT \approx 10$ in order to have small errors while neglecting $F(T_0, E)$. In cases where the expression in (15) is quite high, one should calculate separately the value of $F(T_0, E)$ by Eq. (1) and subtract it from $F(T, E)$. This would not cause any substantial difficulty as long as the calculations are carried out by the computer.

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