# On the relation between thermally stimulated conductivity and thermoluminescence maxima

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The temperatures of thermoluminescence (TL) peaks and their corresponding thermally stimulated conductivity (TSC) counterparts are investigated for the case of temperature-dependent recombination probabilities and mobilities. The conditions under which the TL peaks will occur at higher temperatures than the TSC peaks, i.e., the normal order is inverted, are derived.

The relation between corresponding thermally stimulated conductivity (TSC) and thermoluminescence (TL) peaks has previously[1] been theoretically investigated under the assumption that the recombination probability of free carriers with recombination centers is temperature independent. It was shown that, under this assumption, a TL peak appears at a lower temperature than the associated maximum in the concentration of free carriers; the TSC peak will coincide with the carrier concentration peak provided that the mobility is temperature independent. In most simultaneous TL–TSC measurements discussed in the literature, the TL peaks occur at lower temperatures than the TSC peaks (see Refs. 2–9 in Ref. 1). However, exceptions in which the TL peaks occur at higher temperatures have also been observed.[2,3]

We discuss now the possibility of inversion of TL and TSC peak temperatures when temperature dependence of the recombination probability and the carrier mobility is taken into account.

One of the basic equations[4] governing the TL phenomenon is

$$I(t) = -\frac{dm}{dt} = Amn_c, \qquad (1)$$

where $I$ is the TL intensity, $t$ is the time (sec), $m$ is the concentration of empty recombination centers ($cm^{-3}$), $n_c$ is the concentration of free charge carriers, and $A$ is the recombination probability ($cm^3\,sec^{-1}$). $A$ is known to be the product of the cross section for recombination and the thermal velocity of free carriers.[4] According to Keating,[5] Bemski,[6] and Lax,[7] the cross section for recombination varies with temperature as $T^{\alpha}$, where $-4 \leq \alpha \leq 0$. Since the thermal velocity depends on $T^{1/2}$, we have

$$A = A'T^{a}, \quad -\tfrac{7}{2} \leq a \leq \tfrac{1}{2}. \qquad (2)$$

The solution of Eq. (1) for a temperature-dependent recombination probability will be considered now. Assuming any heating function $T = T(t)$, we have $A = A(t)$, and the solution of Eq. (1) is

$$I(t) = m_0 A(t) n_c(t) \exp[-\textstyle\int_0^t A(t')n_c(t')\,dt'], \qquad (3)$$

where $m = m_0$ at $t = 0$. Differentiating with respect to time,

$$\frac{dI}{dt} = m_0 \exp[-\textstyle\int_0^t A(t')n_c(t')\,dt']\left[n_c\left(\frac{dA}{dt}\right) + A\left(\frac{dn_c}{dt}\right) - A^2 n_c^2\right]. \qquad (4)$$

The condition for the maximum of the TL curve is thus

$$\left(\frac{dn_c}{dt}\right)_m = A_m n_{c_m}^2 - n_{c_m}\left(\frac{d\ln A}{dt}\right)_m, \qquad (5)$$

where the subscript $m$ designates values corresponding to the TL maximum. Equation (5) certainly reduces to $(dn_c/dt)_m = An_{c_m}^2$ for a temperature-independent $A$, as shown previously.[1] For any monotonically increasing heating function $T = T(t)$, Eq. (5) can be written as

$$\left(\frac{dn_c}{dt}\right)_m = A_m n_{c_m}^2 - \beta_m n_{c_m}\left(\frac{d\ln A}{dT}\right)_m, \qquad (6)$$

where $\beta_m = (dT/dt)_m$ is the heating rate at the TL maximum point. In order to determine whether the TL peak precedes the peak of $n_c(T)$ or not, it is necessary to examine the right-hand side of Eq. (6). If this expression is negative, then $(dn_c/dt)_m$ is negative when the TL reaches its maximum value, and therefore the $n_c$ peak must have occurred at a lower temperature than the TL peak. Writing $A = A'T^a$, the right-hand side of Eq. (6) will be negative if

$$A_m T_m n_{c_m} < a\beta_m. \qquad (7)$$

This inequality will be true under certain circumstances, provided that $a > 0$.

If the recombination cross section is temperature independent, we have $a = \frac{1}{2}$. Taking a reasonable value of cross section for recombination $S = 10^{-18}$ cm$^2$, a TL peak at $T_m = 300$ K and a heating rate at the peak $\beta_m = 0.5$ K/sec, any $n_{c_m} < 7\times10^7$ cm$^{-3}$ would yield $(dn_c/dt)_m < 0$, implying an inversion of the TL and $n_c$ peak temperatures.

If one now wishes to compare peak temperatures of TL and TSC, as distinct from TL and carrier concentration, the possible temperature dependence of the carrier mobility must be taken into account.

According to Lax,[7] the mobility $\mu$ of free carriers is given by

$$\mu = \mu' T^{b}, \qquad (8)$$

where $b$ assumes usually a value of $-\frac{3}{2}$, or sometimes $-2.3$. The conductivity $\sigma$ is given by

$$\sigma = e\mu n_c, \qquad (9)$$

where $e$ is the charge of an electron. Since $\mu$ decreases with increasing temperature, $\sigma(T)$ may assume its maximum value at a lower temperature than the $n_c(T)$ function. Combining Eqs. (9) and (1) one obtains, at the TL peak temperature,

$$I(t)=-\frac{dm}{dt}=\left(\frac{A}{\mu e}\right)\sigma m=\bar{A}\sigma m\,, \tag{10}$$

where $\bar{A}=A/\mu e$. Combining Eqs. (2) and (8) we obtain

$$\bar{A}=A/\mu e=(A'/\mu' e)T^c, \tag{11}$$

where $c=a-b$, and $A'$ and $\mu'$ are constants. One has $-2\leqslant c\leqslant 2$ for the previously described temperature dependence of the recombination probability, assuming that $b$ takes on its usual value of $-\frac{3}{2}$.

Because of the resemblance between Eqs. (1) and (10), the conclusions drawn from the former can be used for the latter. Thus the equivalent of Eq. (6) is

$$\left(\frac{d\sigma}{dt}\right)_m=\bar{A}_m\sigma_m^2-\beta_m\sigma_m\left(\frac{d\ln\bar{A}}{dT}\right)_m. \tag{12}$$

Any inversion of corresponding TL and TSC peak temperatures is governed by the sign of the right-hand side of Eq. (12). If that expression is negative, and assuming $\bar{A}$ given by Eq. (11), the condition for the appearance of a TL peak at a higher temperature than the corresponding TSC peak is then similar to condition (7),

$$\bar{A}_m T_m\sigma_m<c\beta_m. \tag{13}$$

This is a less stringent condition (in terms of $n_{c_m}$) than Eq. (7), since the range of possible positive $c$ values (of necessity $c\geqslant 0$) is broader.

Thus, writing $c=2$, as compared to $a=\frac{1}{2}$ earlier, $n_{c_m}<2.8\times10^8$ cm$^{-3}$ gives peak inversion. In cases where $c$ is negative or zero, or even if it is positive but the right-hand side of Eq. (13) is smaller than the left-hand side, the "usual" order of appearance of TL and TSC peaks prevails. The two terms in Eq. (13) can, under very specific conditions, be equal, in which case the TL and TSC peak temperatures will coincide.


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