Thermally stimulated conductivity in disordered semiconductors at low temperatures

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Theoretical interpretation of the thermally stimulated conductivity (TSC) is suggested for the temperatures at which transport is via hopping of carriers through localized bandtail states. The description is not based on specific assumptions used in the most of the previous TSC theories, such as, e.g., neglect of the retrapping of mobile carriers, etc. Our approach is based on the general concept of the transport energy according to which the transport path of hopping electrons in the bandtail is temperature dependent. This theory allows for a natural extension to higher temperatures and accounts for all existing experimentally observed trends in the TSC including the puzzling so far pinning of the low-temperature maximum on the TSC curves at different initial temperatures. Experimental results for the low-temperature TSC are presented, which are consistent with the theoretical predictions. [S0163-1829(97)00224-5]

I. INTRODUCTION

Thermally stimulated conductivity (TSC) has been being measured since more than 50 years in various crystalline and amorphous semiconductors.[1–14] In these measurements a sample is cooled to a low temperature T_0, photoexcited for a time t_e, and after a delay period t_0, the sample is heated in darkness at a constant rate β while the thermostimulated current is measured. The TSC technique has attracted increasing attention over the last years due to the ease with which experiments can be performed and the hope to obtain with its help important information on the energy distribution of the density of states (DOS) in the gap. It is worth noting, however, that the information on the DOS extracted from the TSC measurements essentially depends on the interpretation of the TSC phenomenon.

Simmons, Taylor, and Tam[15] suggested a consistent theory of the TSC in a system with a continuous energy distribution of localized states below the band edges. In this theory only carriers in extended states above the mobility edges were considered as mobile and it was assumed that the carriers that are thermally emitted from the traps are swept out of the sample before they can recombine. Such a theory can be valid perhaps at high electric fields at which carriers are swept out very efficiently and also at high enough temperatures at which hopping via localized band-tail states does not contribute to the transport properties significantly.

Experiments with the TSC technique are usually carried out at low electric fields at which recombination processes cannot be neglected. A theory of the TSC taking recombination into account was suggested by Fritzsche and Ibaraki.[8] The authors assumed that after a long delay t_0 (about 1 h) the distribution of photoexcited carriers in the trapping states corresponds to the thermal equilibrium at temperature T_0. Only carriers in the extended states above the mobility edge were considered as contributing to the current. The TSC was assumed to arise from a balance between thermal emission and recombination. As the sample is heated in the darkness, the thermal emission occurs from progressively lower-lying trapping states, and the magnitude of the TSC $\sigma_{\rm TSC}$ is therefore expected to be proportional to the product of the density of states $g(\epsilon)$ of the traps and the occupation probability $f_0(\epsilon,T_0)$ at the end of the delay time[8]

$$\sigma_{\rm TSC}\propto e\mu_0\tau_0 g(E_m)f_0(E_m,T_0), \tag{1}$$

where e is the electronic charge, $\mu_0\tau_0$ is the free-electron mobility-lifetime product, $g(\epsilon)$ is the density of gap states, and E_m is the maximum—TSC—emission energy, which moves towards midgap with time and temperature.[10] The crucial assumptions of this approach are: (i) the complete neglecting of the retrapping processes and (ii) the treatment of the system as being in the ''steady state,'' i.e., the exact balance between thermal emission and recombination was assumed.[8,12]

In reality, the thermostimulated conductivity $\sigma_{\rm TSC}$ arises from the interplay between the thermal emission of electrons

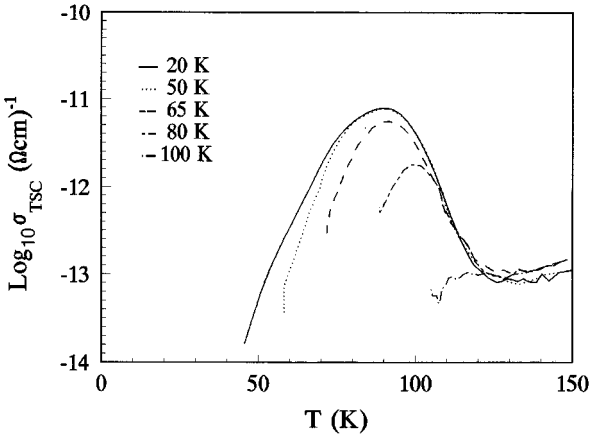

FIG. 1. The TSC curves for *a* Si:H with different starting temperatures T_0 in the range from 20 to 100 K.

from the traps to the transport states and their retrapping and recombination. The concentration of the conducting electrons n obeys the equation

$$\frac{dn}{dt}=\dot{n}_+-\dot{n}_--\frac{n}{\tau_0}, \tag{2}$$

where $\dot{n}_+$ and $\dot{n}_-$ are the rates of the increase of n due to thermal emission and its decrease due to retrapping, respectively, and τ_0 is the lifetime of the conducting electrons, which depends on n, T and also on the whole concentration of trapped and free carriers in the system. In the approach, of Fritzsche and Ibaraki[8] term $\dot{n}_-$ was neglected and it was assumed that $dn/dt=0$, i.e., $n=\tau_0\dot{n}_+$, which automatically leads to Eq. (1).

Predictions of this approach were verified experimentally. Zhou and Elliott[16] found inconsistencies between the experimental data and the theoretical results at low temperatures. Analyzing the similarity between the temperature dependence of the TSC and that of the steady-state photoconductivity, Zhou and Elliott came to the conclusion that the TSC is probably controlled by recombination, rather than by thermal emission of trapped electrons. Under such circumstances Eq. (1) is not valid. Concerning this equation, it is also very difficult to justify the neglecting of the retrapping processes in the description of the TSC.[13] The relative efficiency of the retrapping of free electrons as compared to their recombination was recently evaluated from the experimental data on the photoconductivity decay after terminating the excitation.[17] It was found that even at room temperatures the recombination time for free carriers is larger by many orders of magnitude than the trapping time. At lower temperatures at which TSC is usually measured the relation must be even more drastic. Therefore the retrapping processes should be undoubtedly taken into account in the theoretical interpretation of the TSC.

A theory of the TSC taking into account all three important processes, i.e., thermal emission, retrapping, and recombination, has been suggested by Gu, Xu, and Dong.[18] This theory has not been put to extensive use perhaps due to its quantitative and not qualitative formulation. One should also note that Gu, Xu, and Dong[18] assumed that only free carriers, i.e., those in the extended states above mobility edges, can contribute to the TSC. This is correct at high enough temperatures. However, many interesting peculiarities in the temperature dependence of the TSC are usually observed at low temperatures, at which transport is via hopping of electrons between localized bandtail states. In Fig. I typical temperature dependences of the TSC are shown for different initial temperatures T_0 which were obtained at the heating rate $\beta=2$ K min^{-1} (see Ref. 19 for experimental details). For $T_0<65$ K a pronounced maximum at $T_m\approx 90$ K is observed, which is independent of the value of T_0. Similar curves were obtained by other authors,[16,9] though with different values of T_m also independent of T_0.

In the temperature range below ≈ 120 K the hopping of electrons via localized band-tail states will probably dominate the transport mechanism,[20] and the corresponding theory of the TSC, taking hopping transport into account. Below we present such a theory based on the picture of the temperature-dependent hopping in band tails suggested by Shklovskii *et al.*[20] At high enough T when the transport path of carriers emerges into the mobility edge, our description automatically converges with that of Gu, Xu, and Dong.[18]

The paper is arranged as follows. In Sec. II we present a new qualitative interpretation of the low-temperature TSC. New experimental results on the temperature dependence of the σ_{TSC} at different heating rates and for annealed and degradated samples are also present, which agree well with the suggested qualitative picture. In Sec. III a complete set of rate equations is presented that allows one to describe the TSC at low temperatures at which hopping is the dominant transport mechanism. This approach is based on the concept of the ''transport energy'' for hopping of electrons in the band tails. Quantitative numerical solution of these equations gives results in excellent agreement with the observed trends of the low-temperature TSC. Concluding remarks are gathered in Sec. IV.

II. QUALITATIVE PICTURE OF THE LOW-TEMPERATURE TSC

At low temperatures the hopping of electrons via localized band-tail states determines various transport phenomena in disordered semiconductors, in particular, in amorphous materials. It was shown to be the case for the equilibrium dark conductivity,[21,22] for nonequilibrium relaxation of excess electrons[23] and for the steady-state photoconductivity.[20] It is reasonable therefore to assume that in the TSC experiments at low temperatures, hopping of carriers through localized band-tail states also plays a dominant role. The main feature of this hopping is as follows:[20–24] At very low temperatures the transport path of electrons lies deep in the band tail and the hopping mobility of carriers is low due to the large distances between the localized states involved in the hopping processes. When raising temperature progressively, more shallow states are used by electrons in their hopping and the carrier mobility increases drastically because localized states involved become closer in space and the tunneling between them becomes exponentially easier. At some particular temperature T_{crit} the transport path emerges into the mobility edge and the mobility achieves its value for free carriers μ_0. At $T>T_{\mathrm{crit}}$ movement of electrons in extended states above the mobility edge determines the transport prop-

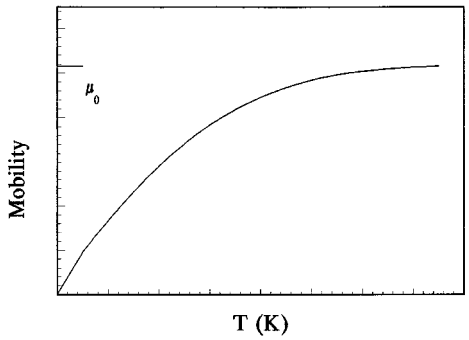

FIG. 2. Schematic temperature dependence of the hopping mobility.

erties. Schematic temperature dependence of the electron mobility $\mu(T)$ is shown in Fig. 2. In order to calculate the dependence $\mu(T)$ and the value of $T_{\rm crit}$ quantitatively, it is necessary to possess particular information on the density of states in the tail $g(\epsilon)$ and also the dependence of the localization length $\alpha(\epsilon)$ of carriers in the localized tail states on the localization energy ϵ in the vicinity of the mobility edge, as well as the magnitude of the microscopic mobility μ_0 of free electrons. As long as these parameters cannot be calculated from the first principles, we do not want to speculate on the value of $T_{\rm crit}$.

Thermally stimulated conductivity $\sigma_{\rm TSC}(T)$ is determined by the equation

$$\sigma_{\rm TSC}=e\mu(T)n(T), \tag{3}$$

where $n(T)$ is the concentration of mobile electrons. The term ''mobile electrons'' should be specified more clearly, of course. We clarify this in the next section and here we assume that $n(T)$ is the concentration of carriers possessing the mobility $\mu(T)$, which contribute mostly to the transport phenomena at temperature T.

The main feature of our model of the low-temperature TSC is that it is determined by the interplay between the hopping mobility $\mu(T)$ increasing with T and the concentration of carriers in the system, decreasing in the course of time due to recombination. We do not assume that the concentration of mobile carriers $n(T)$ obeys the steady-state condition $dn/dt=0$ as has been done in the most of the previous theoretical descriptions of the TSC.

Let us compare the values of $\sigma_{\rm TSC}$ at $T\approx 55$ K in Fig. 1 for $T_0=20$ K and $T_0=50$ K. We see that at $T_0=50$ K the value of $\sigma_{\rm TSC}$ (55 K) is much lower than that at $T_0=20$ K. The mobility $\mu(T)$ determined just by the actual temperature ($T=55$ K) is the same for these two cases. Therefore, in accordance with Eq. (3), the only reason for the difference in the values of $\sigma_{\rm TSC}$ (55 K) can be the difference in the values of n in these two cases. As long as the light intensity F and the excitation duration t_e were the same in these two cases,[19] the total amount of generated carriers was also the same. Hence the only reason why there are more carriers at $T=55$ K in the case of $T_0=20$ K than in the case of $T_0=50$ K is that the recombination process at $T_0=50$ K is more efficient than at $T_0=20$ K. Therefore, after the delay period $t_0=30$ min, which was the same in both cases,[19] there were much more electrons at the start of the heating at $T_0=20$ K than at $T_0=50$ K. During the slow heating process the carriers continue to recombine and the number of carriers that disappear from the system per second per cm^3 is higher for higher total amount of carriers in the system, i.e., recombination at $T\approx 55$ K is more intensive in the case of $T_0=20$ K than in the case of $T_0=50$ K. The shape of $\sigma_{\rm TSC}(T)$ at low T is determined by the interplay between the increase of $\mu(T)$ due to the movement of the transport path towards more shallow tail states and the decrease of $n(T)$ due to the successive recombination. Therefore initial increase of $\sigma_{\rm TSC}$ (T) is steeper for $T_0=50$ K than for $T_0=20$ K, because $\mu(T)$ for these two cases is the same and the recombination is less pronounced for $T_0=50$ K due to the lower total amount of carriers in the system. After the curve of $\sigma_{\rm TSC}$ (T) for $T_0=50$ K emerges into that for $T_0=20$ K there is no difference between these two cases anymore. Curves for larger values of T_0 emerge into the curve for $T_0=20$ K at higher temperatures, respectively.

In previous studies of the TSC, particular attention has been given to the dependence of $\sigma_{\rm TSC}(T)$ on the value of the starting temperature T_0. Concerning this dependence, it is well seen in Fig. 1 that there is some universal curve (for given values of F, t_e, and t_0) obtained at $T_0=20$ K and all curves for $T_0>20$ K just emerge into it at some higher temperatures. This behavior is absolutely natural. The higher is T_0 the lower is the starting concentration of carriers in the system, because more of them recombine during the delay period t_0 at higher T_0. Recombination is less efficient for lower concentration of carriers and, hence, for higher T_0. Carrier mobility depending just on T does not depend on the starting temperature T_0. Therefore, the increase of $\sigma_{\rm TSC}$ with T is always steeper for higher T_0 in good agreement with the experimental data in Fig. 1. In the ''steady-state'' description provided by Eq. (1) the tendency should be just opposite:[19] the initial rise of $\sigma_{\rm TSC}$ with T should be steeper for lower T_0 being determined by the function f_0 at $T=T_0$. The pinning of the position T_m of the low-temperature TSC maximum for low T_0 is also inherent in the suggested picture. All $\sigma_{\rm TSC}(T)$ curves at different T_0 that emerge into the universal TSC curve (that at very low $T_0\approx 20$ K) at temperatures smaller than T_m have the same maximum position T_m because they just do not differ from each other after they converge. If the measurements of the TSC start at some T_0 which is higher than T_m corresponding to lower values of T_0, the maximum in the suggested picture has to shift toward higher temperatures, if it appears at all.

Up to now we discussed qualitatively the behavior of $\sigma_{\rm TSC}(T)$ at low temperatures. The main idea was that the TSC at low T is provided by hopping of electrons via localized band-tail states and that the concentration of the carriers is controlled by their recombination. When the temperature is increased in the heating process, the transport path of carriers in the tail moves toward more shallow states and at some $T_{\rm crit}$ emerges into the mobility edge. At $T>T_{\rm crit}$ the mobile carriers are those in the extended states which have almost temperature-independent mobility μ_0. The temperature dependence of the TSC at $T>T_{\rm crit}$ is therefore completely controlled by the recombination as was already suggested by Zhou and Elliott[16] and by Gu, Xu, and Dong.[18]

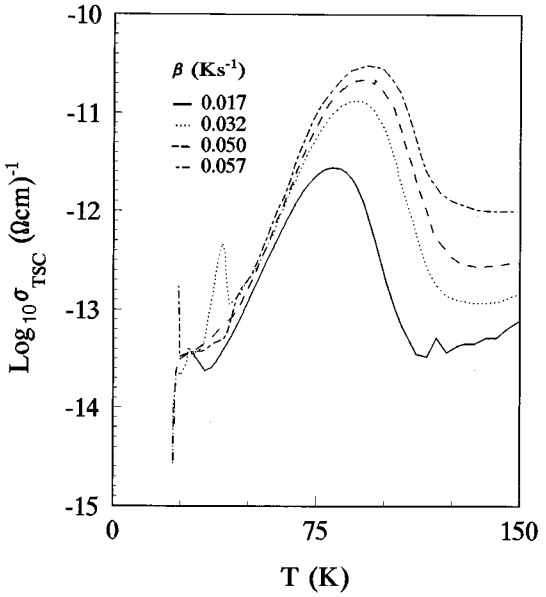

FIG. 3. The TSC spectra in *a* Si:H for different heating rates β.

In order to check whether it is indeed the interplay between the progressive recombination of mobile carriers and the increase of their mobility with T which determines the behavior of the TSC at low temperatures, we have carried out measurements of the TSC at different heating rates β. If our picture is correct, one would expect that at higher β the low-temperature maximum in the TSC shifts to higher values of T_m and also increases in the amplitude, because the higher is β, the less pronounced is the effect of recombination at a particular temperature due to the shorter time at which the temperature was achieved. Experimental data obtained are presented in Fig. 3. They clearly confirm the expected trend. Results similar to those in Fig. 1 were obtained by Zhou and Elliott[16] and by Misra, Kumar, and Agarwal,[9] though with the low-temperature maximum at $T_m \approx 110$ K, i.e., shifted to higher T as compared to the data in Fig. 1. It is now easy to understand this shift. Zhou and Elliott and Misra, Kumar, and Agarwal used considerably higher heating rates and hence the effect of recombination at each particular temperature was not as strong as it was for the results in Fig. 1.

Another interesting feature of the TSC curves is the dependence of the maximum position T_m on the state of a sample. We have carried out experiments with the heating rate $\beta = 2\ \mathrm{K\ min^{-1}}$ with samples in the annealed state (A) and the degradated state (B). In Fig. 4 the values of T_m are shown for states A and B along with the corresponding results obtained by Misra, Kumar, and Agarwal[9] and Zhou and Elliott[16] at higher heating rates β. Compared to samples in the state A, all low-temperature maximum positions of the TSC in the state B are shifted to lower values of T_m at the same initial temperature T_0. In the suggested picture of the TSC the maximum at T_m results from the interplay between increasing with T-hopping mobility of the carriers and their decreasing concentration due to recombination. It is well known that the recombination in the state B is more effective than in the state A and therefore the maximum of the TSC appears at lower temperatures for the degradated samples in good agreement with our model.

We see that all trends observed so far, including the dependences of the TSC on the initial temperature T_0, on the heating rate β and even on the state of a sample are inherent properties of our qualitative model of the TSC, according to which it is the interplay between the carrier mobility increasing with temperature and the decreasing concentration of carriers in the course of time, which determines the temperature dependence of the TSC.

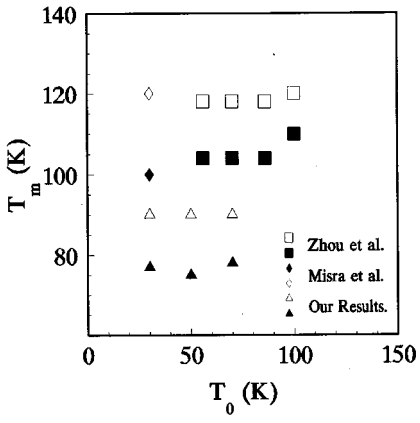

FIG. 4. The low-temperature maximum position of the TSC in *a* Si:H as a function of T_0. Open symbols correspond to the state *A* and closed symbols-to the state B.

In the next section we present a set of rate equations that allow one to describe the TSC at low temperatures quantitatively. This quantitative part is based on the theory of hopping conductivity via the band-tail states developed by Shklovskii *et al.*[20] At $T \approx T_{\mathrm{crit}}$ our equations converge with those of Gu, Xu, and Dong[18] suggested previously under the assumption that only carriers in the extended states are mobile.

III. MODEL AND RATE EQUATIONS FOR THE LOW-TEMPERATURE TSC

The quantitative theory of the low-temperature TSC, which we present below, is essentially based on the concept of the transport energy. It is known that a particular energy level ϵ_t in the band tail called the transport energy plays a crucial role in hopping transport of carriers via localized band-tail states in both equilibrium and nonequilibrium conditions and for both steady-state and transient phenomena.[20–23] Recently it was shown[24] why this energy level is so universal that hopping of electrons in its vicinity dominates various transport phenomena. It is the transport energy, which maximizes the hopping rate as a final electron energy in the hopping transition between two localized states, independently of the initial energy.[24]

Most theories of the transport phenomena determined by hopping of electrons via localized band-tail states have been developed so far for the exponential DOS in the band tail,

$$g(\epsilon) = \frac{N_0}{\epsilon_0} \exp\left(\frac{\epsilon}{\epsilon_0}\right), \tag{4}$$

where the localization energy ϵ is measured negatively from the mobility edge ($\epsilon = 0$) towards the gap center; N_0 is the total concentration of localized tail states, and ϵ_0 is the tail-

ing parameter. For the exponential tail a narrow-energy band of the width $W=(6\epsilon_0 kT)^{1/2}$ centered at the transport energy

$$\epsilon_t \approx -3\epsilon_0 \ln \frac{3\epsilon_0 N_0^{1/3}\alpha}{2kT}, \tag{5}$$

plays the decisive role in the hopping transport.[20] Here α is the localization length in the tail states. It is worth noting, however, that the mathematical expressions for ϵ_t and W depend on the DOS. Recently it was shown[25] that such transport energy exists not only for the exponential DOS, but for any DOS function, which rapidly decreases into the mobility gap. As long as we do not want to specify a particular shape of the DOS in the discussion below, we will assume that the quantities ϵ_t and W exist in the system under consideration, having in mind that they have to be calculated for each particular shape of the DOS separately.

There is a consent among all researchers studying the TSC theoretically that at the start of the heating, thermal equilibrium corresponding to the initial temperature T_0 is established in the system due to the long delay t_0. Since the heating rate is slow compared to the trapping, recombination and thermal emission rates, it is reasonable to assume that the thermal equilibrium is valid at all temperatures during the heating process, i.e., that electrons can equilibrate to a new T and their energy distribution can be described by the function

$$f(\epsilon)=\frac{1}{1+\exp[(\epsilon-\epsilon_q(T))/kT]}, \tag{6}$$

with an appropriate value of the effective Fermi level $\epsilon_q(T)$.
Then we can express the concentration of mobile carriers as

$$n(\epsilon_t)=W\, g(\epsilon_t)\exp\left(\frac{\epsilon_t-\epsilon_q}{kT}\right). \tag{7}$$

The effective Fermi level ϵ_q at low temperatures is determined by the total concentration N_t of electrons introduced by the excitation[20]

$$N_t=\int_{-\infty}^{\epsilon_q} g(\epsilon)\,d\epsilon. \tag{8}$$

The rate equations governing $n(\epsilon_t)$ and the occupation function of trap states $f(\epsilon)$ are

$$\frac{dn}{dt}=-\frac{n}{\tau(T)}+\int_{\epsilon_q}^{\epsilon_t} d\epsilon\, g(\epsilon)[\nu(\epsilon,\epsilon_t)f(\epsilon)-b_t n(1-f(\epsilon))], \tag{9}$$

$$\frac{df(\epsilon)}{dt}=b_t n[1-f(\epsilon)]-\nu(\epsilon,\epsilon_t)f(\epsilon), \tag{10}$$

where $\nu(\epsilon,\epsilon_t)$ is the hopping activation rate from a deep state at energy ϵ to the transport energy ϵ_t and b_t is the trapping coefficient of electrons at the transport energy into deeper tail states. $\tau(T)$ is the lifetime of the carriers at ϵ_t with respect to recombination. The value of the effective Fermi level is equal to

$$\epsilon_q(T)=\epsilon_t-kT\,\ln\frac{Wg(\epsilon_t)}{n}. \tag{11}$$

Using Eqs. (9) and (10) and the relation $T=T_0+\beta t$, one easily obtains

$$\beta\frac{dn}{dT}=-\frac{n}{\tau(T)}-\beta\int_{\epsilon_q}^{\epsilon_t}\frac{df(\epsilon)}{dT}\,g(\epsilon)\,d\epsilon. \tag{12}$$

Using Eqs. (6) and (11) one obtains

$$\frac{df}{dT}=\frac{df}{d\epsilon}\,kT\left[-\frac{\epsilon-\epsilon_q}{kT^2}-\frac{1}{kT}\frac{d\epsilon_t}{dT}-\frac{1}{T}\ln\frac{n}{Wg(\epsilon_t)}-\frac{1}{n}\frac{dn}{dT}+\frac{1}{W}\frac{dW}{dT}+\frac{1}{g(\epsilon_t)}\frac{dg(\epsilon_t)}{dT}\right]. \tag{13}$$

Substituting Eq. (13) into Eq. (12) and replacing $df/d\epsilon$ by $-\delta(\epsilon-\epsilon_q)$ we obtain

$$\frac{dn}{dT}=\frac{nkTg(\epsilon_q)\left[\frac{1}{T}\ln\frac{Wg(\epsilon_t)}{n}-\frac{1}{kT}\frac{d\epsilon_t}{dT}+\frac{1}{W}\frac{dW}{dT}+\frac{1}{g(\epsilon_t)}\frac{dg(\epsilon_t)}{dT}\right]-\frac{n^2}{\beta\tau(T)}}{n+kTg(\epsilon_q)}. \tag{14}$$

Thermally stimulated conductivity in the hopping regime is

$$\sigma_{\mathrm{TSC}}=\frac{e^2}{kT}\,n(\epsilon_t)D(\epsilon_t), \tag{15}$$

where the diffusion coefficient of electrons at the transport energy is[20]

$$D=\frac{1}{3}\,r^2(\epsilon_t)\nu_0\,\exp\left\{-\frac{2r(\epsilon_t)}{\alpha}\right\}, \tag{16}$$

ν_0 being the attempt-to-escape frequency for hopping between localized states ($\nu_0\approx 10^{13}\ \mathrm{s}^{-1}$) and $r(\epsilon_t)$ is the typical hopping distance for electrons at ϵ_t

$$r(\epsilon_t)=\left\{(4\pi/3)\int_{-\infty}^{\epsilon_t} g(\epsilon)\,d\epsilon\right\}^{-1/3}. \tag{17}$$

The temperature derivative of σ_{TSC} is

$$\frac{d\sigma_{\mathrm{TSC}}}{dT}=\frac{e^2}{kT}\left\{D(\epsilon_t)\,\frac{dn(\epsilon_t)}{dT}+n(\epsilon_t)\,\frac{dD(\epsilon_t)}{dT}-\frac{n(\epsilon_t)D(\epsilon_t)}{T}\right\}. \tag{18}$$

The quantity $\epsilon_t(T)$ can be calculated for a given energy dependence of the DOS as described in Refs. 24, 25. Possessing the DOS and the function $\epsilon_t(T)$, one can easily calculate $D(\epsilon_t)$ and dD/dT using Eqs. (16) and (17). In order to find $d\sigma_{\mathrm{TSC}}/dT$ via Eq. (18), it is, however, necessary to calculate $n(\epsilon_t)$ and dn/dT determined by Eqs. (7) and (14) respectively. This calculation can be carried out, provided the temperature dependence of the recombination time $\tau(T)$ is known. According to Eq. (14), this function plays a crucial role in the calculation of dn/dT and hence that of $n(\epsilon_t)$. Therefore, a theoretical treatment of the TSC depends on the chosen recombination mechanism.

The recombination problem for electrons, which move by hopping via localized band-tail states has been solved by Shklovskii *et al.*[20] in their treatment of the low-temperature steady-state photoconductivity. Shklovskii *et al.* considered the system of electrons in the localized states to be in the thermal equilibrium and therefore one can use their recombination picture for the description of the TSC. At low temperatures, recombination is limited by the diffusion of carriers through the states in the vicinity of ϵ_t and the recombination flux is[20]

$$Q=4\pi R_{\mathrm{rec}}D(\epsilon_t)n(\epsilon_t)N_D, \tag{19}$$

where it is assumed, as usual, that recombination occurs via recombination centers[26] as, e.g., dangling bonds with concentration N_D; R_{rec} is the distance at which an electron is captured by the recombination center with a probability near unity. This distance was shown to be[20,27]

$$R_{\mathrm{rec}}=\frac{r^2(\epsilon_t)}{3\alpha}, \tag{20}$$

where the right-hand side is the correlation length of the infinite cluster of localized sites of the percolation problem that determines the conductivity at the transport energy.
Recombination flux Q determines the number of electrons recombining in the system per cm^3 per second. The recombination time $\tau(T)$ of the mobile electrons at the transport energy in Eqs. (9), (12), and (14) is determined as $\tau(T)=n(\epsilon_t)/Q$, and according to Eqs. (19) and (20), equals to

$$\tau(T)=\left\{\frac{4\pi}{3}\,\frac{r^2(\epsilon_t)}{\alpha}\,D(\epsilon_t)N_D\right\}^{-1}. \tag{21}$$

The recombination picture described above is based on the assumption that recombination is limited by diffusion.[20] This assumption is valid for low temperatures at which the transport energy is situated deep in the tail, so that hopping is slow due to the low concentration of localized states available, and the diffusion is slower than a recombination event, limiting therefore the whole recombination process.[20] With rising temperature the transport energy moves towards the mobility edge. Hence a higher number of localized states become available for hopping of electrons and the diffusion coefficient determined by Eq. (16) increases exponentially

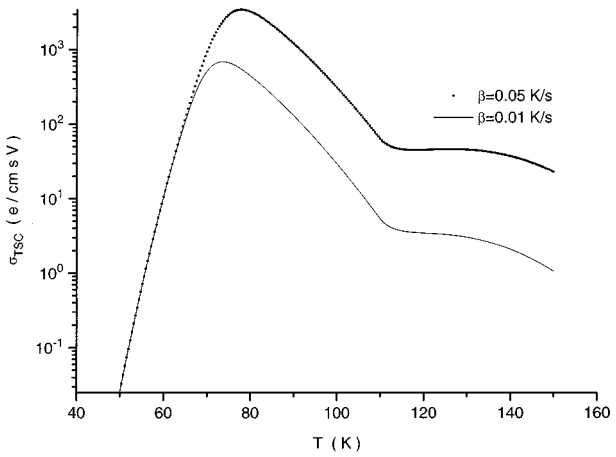

FIG. 5. Calculated functions $\sigma_{\mathrm{TSC}}(T)$ at two different heating rates β. Values of material parameters are specified in the text.

with rising temperature. At some particular temperature T_r the diffusion becomes so fast that it no longer limits the recombination process. At $T>T_r$ recombination of electrons is limited by a recombination event and not by their diffusion.[20] The detailed theory of the transition from the diffusion-limited recombination to the recombination limited by a recombination event is described in Ref. 20, where it is shown that at $T>T_r$ the recombination flux is

$$Q=\frac{\alpha^3}{\tau_0}\,n(\epsilon_r)N_D, \tag{22}$$

where ϵ_r is the value of the transport energy at $T=T_r$, and τ_0 is the preexponential factor in the recombination rate of electrons $\tau(R)=\tau_0\exp(2R/\alpha)$ via recombination centers, R being the distance to the recombination center.[20]

In order to check the set of Eqs. (6)–(18), we carry out below a numerical calculation of the TSC. Our aim is not to fit the experimental data, but to check whether this set of equations can describe the $\sigma_{\mathrm{TSC}}(T)$ dependence of observed shape with a reasonable choice of material parameters. In particular, it is of high interest whether the low-temperature maximum at T_m arises due to the interplay between the increasing with T hopping mobility $\mu(T)$ and the decreasing with T (in the course of time t) total concentration of carriers, as we suggest in the qualitative discussion in Sec. II, or some peculiarities in the DOS are necessary to get such a maximum. If the latter alternative is the case, the TSC method would be a tool to determine such peculiarities of the DOS. If the former alternative is the case, as we expect in the qualitative consideration of Sec. II, the position and the height of the maximum is determined just by the experimental conditions, e.g., by the heating rate β.

For this test we choose the simplest exponential shape of the DOS function of Eq. (4) without any peculiarities. The parameters of the DOS are $\epsilon_0=0.025$ eV and $N_0=5\times10^{19}\ \mathrm{cm}^{-3}$. The transport energy in this case is determined[20–25] by Eq. (5). The concentration of recombination centers is chosen[26] equal to $N_D=10^{17}\ \mathrm{cm}^{-3}$. The localization length is assumed to be energy independent and equal to[26] $\alpha=10$ Å. The concentration of photoexcited carriers after the delay time t_0 i.e., at the start of the heating is taken as

$N_t = 10^{15}$ cm^{-3}. The temperature T_r at which recombination Eq. (19) should be replaced by Eq. (22), is assumed to be 110 K and the factor τ_0 is chosen equal to 10^{-7} s just to make the $\sigma_{\rm TSC}$ (T) curve continuous at $T = T_r$. Such a choice of τ_0 would be reasonable for both radiative recombination and nonradiative process with simultaneous emission of many phonons in a recombination event. The results for the dependence $\sigma_{\rm TSC}$ (T) are shown in Fig. 5 for two values of the heating rate β: 0.01 K/s and 0.05 K/s. It is clear that all experimental trends are present in Fig. 5, in particular, the position of the low-temperature maximum T_m and its height depend on the heating rate. At the higher heating rate β the maximum shifts to the higher value of T_m and also increases in its amplitude because the effect of recombination is less pronounced at higher β for each particular temperature due to the shorter time at which the temperature is achieved. Figure 5 obtained for the DOS of Eq. (4) clearly shows that no peculiarities of the DOS function are necessary for the existence of the low-temperature maximum on the $\sigma_{\rm TSC}(T)$ curve.

IV. CONCLUSIONS

A physical picture is suggested to interpret the TSC in disordered semiconductors at low temperatures at which transport is via hopping of carriers through the localized band-tail states. The picture provides reasonable understanding of all experimentally observed trends in the TSC including the puzzling so far pinning of the low-temperature maximum of the TSC at different initial temperatures. According to this picture, the low-temperature TSC is determined by the interplay between the hopping mobility $\mu(T)$ increasing with T and the decreasing concentration of carriers in the course of time due to their recombination.

A complete set of rate equations is derived for a quantitative description of the low-temperature TSC. Our equations converge at high temperatures with those of Gu, Xu, and Dong[18] derived under the assumption that transport is via extended states above the mobility edges.

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