Experimental Evidence for the Applicability of an Effective Temperature Concept in *a*-Si:H

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We have tested the validity of the effective temperature approach in amorphous semiconductors by performing high electric field (10^4-10^5 V/cm) photoconductivity measurements in intrinsic hydrogenated amorphous silicon (*a*-Si:H) films at low temperatures. Our results on thermal quenching in *a*-Si:H conclusively show that there is an equivalence between electric field and temperature as required by the effective temperature approach for electrons. We find a different functional dependence of the electron effective temperature on the actual temperature and field from the one previously proposed. We propose that a similar effective temperature can be formulated for holes.

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The deepest valence band-tail states in *a*-Si:H have the lowest capture-rate coefficient for electrons to trapped holes ($\sim 10^{-13}$ cm^3 s^{-1}) [1,2]. The holes trapped in these states reside there for long times, safe from recombination, as a result of which these states have been named as "safe hole traps" (SHT) [1]. The energy location of SHTs within the band gap of *a*-Si:H has been determined to be about 0.4 eV above the valence band edge from dual-beam photoconductivity [3] and photoinduced absorption [4]. From the secondary photocurrent spectroscopy [2], it has been suggested that on increasing the temperature the holes trapped in SHTs are excited to shallower, more dense, less localized states located ~0.15 eV above the valence band edge where they tunnel to dangling bonds and complete the recombination process. This results in the commonly observed low-temperature peak in the photoconductivity (σ_p) versus temperature plot in low defect density *a*-Si:H films [5]. Depending on the sample properties, the thermal quenching peak occurs in the temperature range between 130 and 200 K.

In this temperature range the transport in *a*-Si:H is believed to take place by the hopping of carriers through localized tail states including thermal activation from deeper states to shallower ones. The concept of the so-called transport energy has been shown to allow for a lucid interpretation of transport phenomena [6,7] in this regime. Shklovskii *et al.* [6] have proposed that the transport at a finite temperature is equivalent to the transport at $T = 0$ in the presence of a strong electric field F with the equivalence defined by an effective temperature given by

$$T_{\text{eff}} = eFa/2, \tag{1}$$

where a is the localization length, e is the electronic charge, and k is the Boltzmann constant. From actual numerical calculations, Marianer and Shklovskii [8] found that the effective temperature is close to $0.67eFa/k$ for high electric fields. On the basis of their numerical results, they have further suggested a formula

$$T_{\text{eff}}^2 = T^2 + (0.67eFa/k)^2 \tag{2}$$

for the case of finite temperature and electric field. It has also been proposed that the photoconductivity in this temperature region can also be described by such an effective temperature approach [6]. The phenomenon of thermal quenching offers a unique opportunity to monitor electron and hole populations in *a*-Si:H which is not available in any other temperature range. In this Letter we report the effect of high electric fields up to 10^5 V/cm on the thermal quenching in *a*-Si:H and suggest an explanation based on the effective temperature concept.

The steady-state photoconductivity as a function of temperature was measured on a number of films prepared using glow discharge technique at University of Kaiserslautern. The defect densities of the films were measured to be in the range of $(2-6) \times 10^{16}$/cm^3 by photothermal deflection spectroscopy (PDS). The films were deposited on roughened Corning 7059 glass substrates with a coplanar geometry of chromium electrodes separated by 0.5 mm for concurrent measurements of photoluminescence and photoconductivity. The photoconductivity as a function of temperature was recorded from 50 to 200 K with the samples kept in a closed cycle refrigeration system. The samples were illuminated with the 632.5 nm line from the He-Ne laser using the appropriate line filter. The photon flux was varied using different neutral density filters ($10^{14}-10^{16}$/cm^2 s). The electric field was varied from 2×10^3 to 10^5 V/cm at each temperature. The photocurrents were recorded using a Keithley model 485 picoammeter and averaged using a personal computer. The results from only the sample with a defect density of 3.1×10^{16}/cm^3 are reported here for consistency as the results on other samples are similar. At higher generation rates ($\sim 10^{16}$/cm^2 s), we have verified that there is no degradation of the sample by monitoring the photocurrent

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and photoluminescence of the sample over various time intervals.

Figures 1(a), 1(b), and 1(c) show the variation of steady-state photoconductivity as a function of temperature with different applied electric fields at three photon flux values. Since we are primarily interested in investigating the effect of high electric fields on the thermal quenching, only the relevant range of temperatures is shown in these figures. From these curves, it can be clearly seen that at a constant photon flux, the temperature (T_m) at which the photoconductivity shows a maximum (σ_m) decreases with an increase in the electric field. This shift in T_m becomes more apparent on increasing the incident photon flux from $10^{14}/\text{cm}^2\,\text{s}$ to $10^{16}/\text{cm}^2\,\text{s}$. At the lowest field ($2 \times 10^3$ V/cm), the temperature T_m moves toward higher values on increasing the photon flux in agreement with the previous results [9]. The change from high to low photoconductivity in the temperature dependence occurs when with rising temperature the hole demarcation level moves from below to above the trapping level. The temperature T_m where the demarcation level crosses the trapping level E_t can be determined by setting the capture rate of an electron equal to the rate of thermal emission of a hole to less localized states near the valence band edge located at E_{tnl} [2,9]. So

$$nC_tN_t = \nu_0 N_t \exp[-(E_t - E_{tnl})/kT_m], \qquad (3)$$

where N_t denotes the concentration of safe hole traps at E_t, C_t is the capture coefficient for electron capture, n is the free electron concentration which is proportional to σ_{ph}, and ν_0 is the attempt to escape frequency. With an increase in the generation rate, the free electron concentration and, hence, the photoconductivity increases, and the temperature T_m has to increase to satisfy the equality in Eq. (3). In other words, as the generation rate increases the demarcation level moves toward the valence band edge and more thermal energy is required to move the demarcation level to the trap level. From this dependence of T_m on the generation rate at the lowest field, we get an average activation energy ($E_t - E_{tnl}$) of ~0.23 eV comparable to 0.25 eV proposed by McMahon and Crandall [2].

According to the effective temperature approach, an electron can increase its energy relative to the mobility edge by hopping over some distance against the electric field in a process similar to thermal activation. McMahon and Crandall [2] have reported that the photoconductivity in a-Si:H shows an activated behavior with an activation energy in the range of 0.04–0.05 eV in the temperature region before thermal quenching sets in. We also find such an activated behavior with similar activation energy. The activation energy in this case refers to the energy separation between the quasi Fermi level for electrons and the conduction band edge. Since this activation energy does not change with the applied electric field, the photoconductivity still follows an activated behavior with

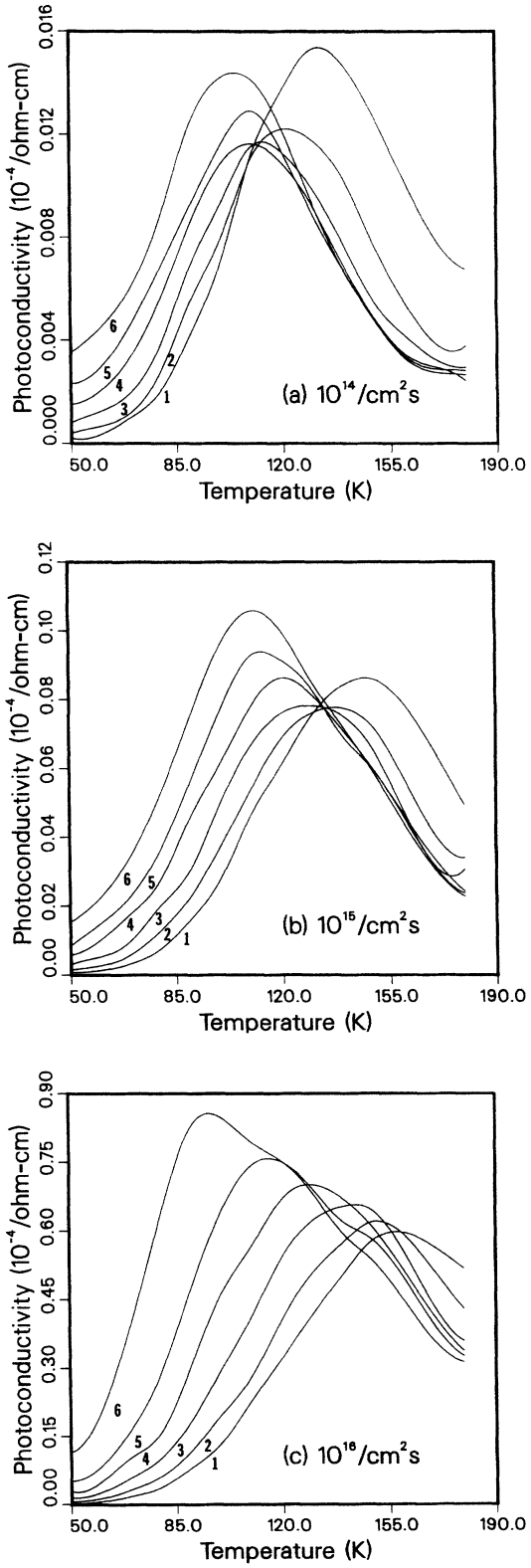

FIG. 1. Photoconductivity versus temperature at (1) 2×10^3 V/cm, (2) 2×10^4 V/cm, (3) 4×10^4 V/cm, (4) 6×10^4 V/cm, (5) 8×10^4 V/cm, and (6) 1×10^5 V/cm for a photon flux of (a) $10^{14}/\text{cm}^2\,\text{s}$, (b) $10^{15}/\text{cm}^2\,\text{s}$, and (c) $10^{16}/\text{cm}^2\,\text{s}$.

the temperature replaced by the effective temperature and can be expressed as

$$\sigma = \sigma_0 \exp(-E_a/kT_{\text{eff}}), \tag{4}$$

where E_a is the activation energy of photoconductivity and T_{eff} is the effective temperature, which is a function of the actual temperature and the applied electric field. At the lowest field the effect of field is negligible, so the peak temperature (T_m) is the same as the effective temperature allowing us to find σ_0 in Eq. (4). For all the other fields, from the measured peak conductivity and σ_0, the effective temperature can be extracted accurately. We picked the peak temperature (T_m) as the representative temperature for performing the calculations, but the results are valid at all temperatures in this range. Figure 2 shows the variation of $\frac{T_{\text{eff}}}{T} - 1$ with $\frac{F}{T}$ for electrons at $T = T_m$ at the three generation rates. The dotted line in the figure shows the calculated T_{eff} values according to Eq. (2) for $a = 1$ nm. Since the $\frac{F}{T}$ values for the three generation rates are similar, the three curves corresponding to Eq. (2) almost overlap each other. Hence, for clarity of presentation only the plot for the lowest generation rate is shown. From the comparison of this plot with our extracted effective temperature values, it is quite obvious that the relation in Eq. (2) is not suitable for our data and some other functional form needs to be used. From the experiments conducted at high fields [10,11] it has been found that the change in photoconductivity at high fields in coplanar geometry a-Si:H samples follows

$$\frac{\sigma(F,T) - \sigma(0,T)}{\sigma(0,T)} = A(T)F^{\gamma}, \tag{5}$$

where $\sigma(F,T)$ is the photoconductivity at field F, $\sigma(0,T)$ is the photoconductivity at zero field, $A(T)$ decreases with an increase in temperature, and the value of γ is between 1 and 2. In this temperature range, the term $A(T)F^{\gamma}$ is less than 1, and the photoconductivity shows activated behavior. Thus, to a first order approximation the previous

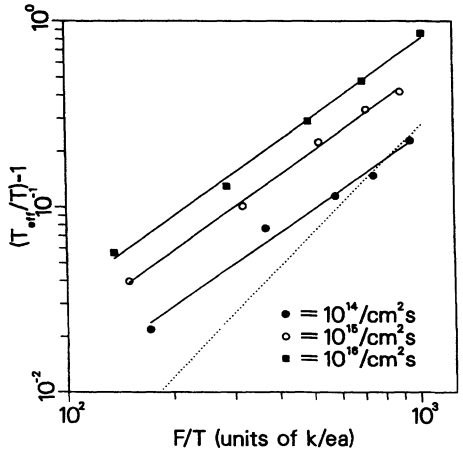

FIG. 2. $\frac{T_{\text{eff}}}{T} - 1$ vs $\frac{F}{T}$ for electrons with $T = T_m$ for the three generation rates in Fig. 1. The dotted line shows the calculated T_{eff} values according to Eq. (2) in the text for $a = 1$ nm.

equation can be rewritten as

$$\sigma_0 e^{-\frac{E_a}{kT_{\text{eff}}}} = \sigma_0 e^{-\frac{E_a}{kT}} [e^{A(T)F^{\gamma}}]. \tag{6}$$

By comparing the exponents and using the fact that $E_a \sim 0.04$–0.05 eV and $kT \sim 0.01$–0.015 eV, the equation can be simplified as

$$T_{\text{eff}} = T + kT^2 A(T) F^{\gamma}/E_a. \tag{7}$$

The exact functional temperature dependence of $A(T)$ is not known, but its value decreases with an increase in temperature. Hence, it will tend to complement the temperature dependence of T^2. So we decided to use the functional form

$$T_{\text{eff}} = T + CT^{\gamma_1} F^{\gamma_2}, \tag{8}$$

where C is a constant that can be expressed in terms of localization length, electronic charge, and Boltzmann constant by comparing with Shklovskii's relation [Eq. (1)]. From the least squares fits using Eq. (8) we found the best fits for $\gamma_1 = -\frac{1}{3}$ and $\gamma_2 = \frac{4}{3}$ leading to

$$\frac{T_{\text{eff}}}{T} = 1 + \left(\frac{eFa(E)/2k}{T}\right)^{4/3}, \tag{9}$$

where F is the applied electric field, $a(E)$ is the localization length, e is the electronic charge, and k is the Boltzmann factor. From the best fits we obtain $a(E) = 0.58$, 1.04, and 1.44 nm for 10^{14}, 10^{15}, and 10^{16}/cm^2 s, respectively. The localization length depends on the depth from the band edge as [6]

$$a(E) = a_0 (E_{0c}/E)^{\frac{1}{2}}, \tag{10}$$

where $a_0 = N^{-1/3} = 3$ nm, N is the total density of conduction band-tail states in a-Si:H, and E_{0c} is the inverse slope of the conduction band tail. So an increasing localization length implies decreasing localization of the electrons, which is consistent with the fact that with an increase in the generation rate, the quasi Fermi level moves toward the band edges, i.e., toward less localized states.

The functional form of effective temperature [Eq. (9)] is different from the one proposed by Marianer and Shklovskii [8]. It is important to note that Marianer and Shklovskii [8] have not provided any justification for the exact form of Eq. (2) and their calculations are directly applicable to dark conductivity. Our relation is based on the actual photoconductivity measurements in coplanar geometry samples as opposed to numerical simulations of dark conductivity in their case. In addition, since there is a possibility that at high electric fields the space charge effects might cause systematic differences in conductivity between coplanar and sandwich geometry intrinsic samples, the physical consequences of the departure from Eq. (2) are difficult to interpret from our experiment alone.

The peak photoconductivities for the curves with the same excitation intensity but different electric fields are different, suggesting that the number of holes needed for thermal quenching of the photoconductivity through

recombination has to change accordingly. The holes trapped in SHTs can gain energy by moving in the direction of the field at a certain temperature. Since the activation energy for the release of holes from SHTs [$E_t - E_{tnl}$ from Eq. (3)] is not affected by the electric field, the effective temperature for holes can be extracted in the same way as electrons using the proper activation energy. The variation of $\frac{T_{\rm eff}}{T} - 1$ as a function of $\frac{F}{T}$ for holes at $T = T_m$ is shown in Fig. 3. We find that the hole effective temperature follows

$$\frac{T_{\rm eff}}{T} = 1 + \left(\frac{eFa(E)/2k}{T}\right)^{\gamma}, \qquad (11)$$

where $\gamma = \frac{2}{3}, 1, \frac{4}{3}$ with $a(E) = 0.2, 0.65$, and 1.19 nm for 10^{14}, 10^{15}, and $10^{16}/\mathrm{cm}^2\,\mathrm{s}$, respectively. So the variation of the hole effective temperature with actual temperature and field is identical in functional form to the electron effective temperature at the highest generation rate, but at other generation rates the dependence is different. This suggests that for holes trapped in deeper SHTs the effect of field is very small due to a significantly reduced density of states, larger separation between states, and a smaller localization length. At higher generation rates, the shallower SHTs get filled, where the density of states is larger, separation between the states is smaller, and the localization length is larger. Hence, at higher generation rates the field effect is similar to those of electrons which are generally in less localized states as compared to holes due to the asymmetry in the density of states.

Physically the effective temperature concept represents the fact that in high electric fields electrons and holes in the band-tail states of a-Si:H can redistribute themselves by moving in the appropriate direction. So the shift of the peak temperature T_m toward lower temperatures can also be interpreted as a shift of the effective trap energy E_t toward lower energies due to a redistribution of the trapped holes in SHTs in the presence of high electric fields. Thus, the occupation of holes in deeper SHTs in which the hole residence times are longer is either inhibited or significantly reduced in the presence of high electric fields. The indirect evidence for this may be that in these experiments we do not see light degradation of the samples at higher generation rates. This is important because it has been reported [5] that exposure to a photon flux of $7 \times 10^{15}/\mathrm{cm}^2\,\mathrm{s}$ at 163 K causes degradation of a-Si:H samples resulting in a reduction in photoconductivity. The conversion of these deep SHTs into dangling bonds has been proposed as a mechanism for such light degradation of a-Si:H samples [5]. Since the high electric fields prevent the occupation of these deep SHTs by holes, the probability of the conversion of a SHT into a dangling bond is greatly reduced. The effect of high electric fields on light degradation needs to be studied in more detail to provide more support to this suggestion.

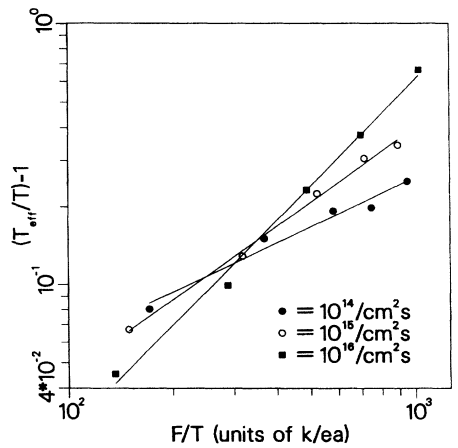

FIG. 3. $\frac{T_{\rm eff}}{T} - 1$ vs $\frac{F}{T}$ for holes with $T = T_m$ for the three generation rates in Fig. 1.

In conclusion, we have provided experimental evidence for the validity of effective temperature approach in a-Si:H. In these experiments, we find that with an increase in the electric field, the temperature T_m at which the thermal quenching sets in decreases and the corresponding peak photoconductivity changes. In the effective temperature approach, every temperature and field combination corresponds to an effective temperature, and the photoconductivity has an activated dependence on the effective temperature. The localization lengths of the states in which the electrons and the holes reside determine the average hopping distance against the field, and, hence, the energy gained by the carrier and its effective temperature. With an increase in the generation rate, the states in which the carriers reside become less localized and the effective temperature is higher. At higher generation rates, the effective temperatures of electrons and holes show identical functional dependence on the actual temperature and field.

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