Simulation of hydrogenated amorphous silicon: temperature dependence of nonequilibrium distribution functions for trap states

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Abstract

Nonequilibrium distribution functions (NDFs) for trap states in the mobility gap under photoillumination and zero bias voltage are derived by a constructed self-consistent drift–diffusion simulator consisting of the Poisson equation and current continuity equations for hydrogenated amorphous silicon (a-Si:H). Regarding the temperature dependence of the NDF, we find that the values of the NDF decrease with increasing temperature (negative temperature dependence) in the energy region near the conduction band for $p$-type a-Si:H. This is the reverse of the temperature dependence of the equilibrium distribution functions (EDFs) for the trap states in the mobility gap. Furthermore, we show that this new physical characteristic can be applied in explaining the temperature characteristic of the photoconductivity caused by electron hopping in the conduction band tail for a-Si:H. The photoconductivity of a-Si:H decreases with increasing temperature, which is called thermal quenching (TQ). We show that the TQ observed at low temperatures of approximately 200 K for $p$-type a-Si:H can be explained by the electron hopping model, with the $p$-type NDF having a negative temperature dependence.

Keywords Temperature dependence · Nonequilibrium distribution function · Hopping · Amorphous silicon · Photoconductivity · Thermal quenching

1 Introduction

Many theoretical models for the capture and emission processes between trap states in the mobility gap and the bands [the valence band (VB) and the conduction band (CB)] have been proposed. Simmons and Taylor [1–4] proposed a simple model based on the Shockley–Read–Hall recombination model [5]. The key idea of the model is that the nonequilibrium steady-state condition is applied to each energy state in the mobility gap. The main advantage of this approach is that NDFs for the trap states in the mobility gap can be uniquely determined. The temperature dependence of the EDFs for the trap states in the mobility gap is well known, and it is the same as the Fermi–Dirac distribution function. However, the temperature dependence of NDFs has not been precisely argued in the past. The density of trap carriers in the mobility gap is derived by integrating the product of the NDF and the density of states (DOS) at each trap energy for the interval from the VB to the CB. Therefore, the temperature dependence of the trap carrier density in the mobility gap is determined by that of the NDF. This is extremely important for the argument of the temperature dependence of some physical phenomena related to the electron density in the conduction band tail for a-Si:H. We rigorously study the temperature dependence of the NDF under photoillumination and zero bias voltage and find a new characteristic. Furthermore, we aim to show that the new physical characteristic is applicable to the explanation of the temperature characteristic of the photoconductivity caused by electron hopping [6–9] in the conduction band tail of a-Si:H.

Figure 1 shows the typical measured photoconductivity of a-Si:H for $p$-type, $i$-type, and $n$-type samples as a function of temperature [10, 11]. In the area surrounded by the dashed line, the photoconductivity changes from increasing to decreasing with increasing temperature: the temperature coefficient of the photoconductivity changes from positive to negative. Subsequently, the photoconductivity changes from decreasing to increasing as the temperature increases further. This temperature characteristic of the photoconductivity is called thermal quenching (TQ). Physical explanations of TQ...
in a-Si:H have been reported in many studies [10–21]. Tran assumed that the recombination center changed from the VB tail to the dangling bond (DB) with increasing temperature and that the capture rate of the DB was larger than that of the VB tail. However, the quantitative fit of the temperature dependence of the photoconductivity with experimental data had to be explained by hopping processes [12]. Merazga et al. [13] followed the approach of Tran; they assumed that the capture rate of the DB was larger than that of the VB tail and included the process of electron hopping in the CB tail states. However, Merazga calculated the density of the hopping carriers in steady-state quasi-equilibrium despite the nonequilibrium condition under photoirradiation. Regarding this matter, we treat the nonequilibrium capture and emission process rigorously.

We study the degree of the effect of electron hopping on photoconductivity and find that TQ can be explained by electron hopping at low temperatures. That is, TQ at low temperatures can be explained by the temperature dependence of the NDF only.

As a supplemental explanation, the aim of this study is to study the temperature dependence of the NDF for p-type and n-type a-Si:H and to show that the new physical property can be applied to the explanation of TQ as being caused by electron hopping in the conduction band tail at low temperatures of approximately 200 K but not to accurately reproduce the data of Fig. 1. The dark conductivity is orders of magnitude smaller than the photoconductivity, so it can be neglected. This paper is organized as follows: Sect. 2 introduces the theoretical model and the numerical simulation method. In Sect. 3, we present the simulation results of the temperature dependence of the NDF, the TQ of the photoconductivity, and their physical interpretation. Finally, we describe the conclusions in Sect. 4.

2 Numerical method

2.1 Capture and emission processes

Regarding the capture and emission processes, we follow the approaches taken by Hack et al. [22–25], Fantoni et al. [26, 27] and Walker et al. [28], which consider the Simmons and Taylor model [1–4]. For the Shockley–Read–Hall model, two capture and two emission processes are considered for each trap state, which are shown in Fig. 2. The transition $\alpha^A$ is an electron capture process from the CB via the acceptor-like trap states located at energy $E$, and $b^A$ is an electron emission process from that state to the CB. The transition $c^A$ is a hole capture process from the VB via the acceptor-like trap states located at energy $E$, and $d^A$ is a hole emission process from that state to the CB. The solid arrows and dashed arrows indicate the transition directions of the electrons and holes, respectively, in Fig. 2. Similarly, four capture and emission processes of electrons and holes via the donor-like trap states located at energy $E$ are shown in Fig. 2: $a^D$, $b^D$, $c^D$, and $d^D$. We assume that the capture and emission processes at the different energy levels $E$ in the mobility gap do not have a relationship to each other. Then, by employing the Shockley–Read–Hall model, the electron capture and electron emission rates per unit volume for the acceptor-like trap states are expressed as follows:

$$r_{\alpha^A} = \nu_{th} \sigma_n^A n N_i^A (1 - f^A(E)),$$

where $\nu_{th}$ is the thermal velocity, $\sigma_n^A$ is the capture cross-section for acceptor-like traps, $n$ is the carrier density, $N_i^A$ is the density of states per unit volume for acceptor-like traps, and $f^A(E)$ is the Fermi–Dirac distribution function.

Fig. 2 Two capture and two emission processes of electrons and holes via the acceptor-like trap states located at energy $E$ ($\alpha^A$, $b^A$, $c^A$, and $d^A$) and via the donor-like trap states located at energy $E$ ($a^D$, $b^D$, $c^D$, and $d^D$) under photoillumination. The solid arrows and the dashed arrows indicate the transition directions of electrons and holes, respectively. The electron photogeneration process $G$ is also shown.

Fig. 1 Typical measured photoconductivity in a-Si:H for $p$-type, $i$-type and $n$-type samples as a function of temperature [10, 11]. In the area surrounded by the dashed line, the photoconductivity changes from increasing to decreasing with increasing temperature. Subsequently, the photoconductivity changes from decreasing to increasing as the temperature increases further. This temperature characteristic is called thermal quenching (TQ).
\[ r_{\rho A} = v_{\text{th}} \sigma_n^A N_A \exp \left( \frac{E - E_C}{k_B T} \right) N_A^{-1} f^A(E), \]

where \( n \) is the density of electrons in the CB, \( N_A \) is the density of the acceptor-like trap, \( E_C \) is the energy of the CB edge, \( k_B \) is the Boltzmann constant, and \( T \) is the system temperature. \( v_{\text{th}}, \sigma_n^A, \) and \( N_A \) are described in Table 1. \( f^A(E) \) is the NDF for the acceptor-like trap states, which is different from the Fermi–Dirac distribution function under photoillumination in general. Likewise, the capture and emission rates per unit volume for holes are expressed as follows:

\[ r_{cA} = v_{\text{th}} \sigma_p^A p N_V f^A(E), \]

\[ r_{dA} = v_{\text{th}} \sigma_p^A p N_V \exp \left( \frac{E_V - E}{k_B T} \right) N_V^{-1} (1 - f^A(E)), \]

where \( p \) is the density of holes in the VB and \( E_V \) is the energy of the VB edge. \( \sigma_p^A \) and \( N_V \) are described in Table 1.

The capture and emission rates per unit volume of electrons and holes via the donor-like trap states are expressed by changing the suffix “A” to “D”; \( r_{\rho D}, r_{D_D}, r_{\rho D}, \) and \( r_{D_D} \) correspond to the capture and emission processes \( d^D, b^D, c^D, \) and \( d^D \), respectively.

Under the nonequilibrium steady-state condition at each trap state, the formulas for the acceptor-like trap states and the donor-like trap states are as follows:

\[ r_{\rho A} - r_{\rho D} = r_{cA} - r_{D_D}, \]

\[ r_{\rho D} - r_{\rho D} = r_{cD} - r_{D_D}. \]

The formula of the NDF for the acceptor-like trap states is derived from Eq. (5) and is expressed as follows:

\[ f^A(E) = \frac{n + c^A N_V \exp \left( \frac{E-E_C}{k_B T} \right)}{n + c^A + p + N_V \exp \left( \frac{E-E_C}{k_B T} \right)} : C^A = \frac{\sigma_p^A}{\sigma_n^A}. \]

### Table 1 Parameter list for the present simulations

| Parameter | Character (unit) | Value |
|-----------|-----------------|-------|
| Length of the device | \( L \) (nm) | 150 |
| Mobility gap | \( E_g \) (eV) | 1.72 |
| Electron mobility | \( \mu_n \) (cm\(^2\)V\(^{-1}\)s\(^{-1}\)) | 10.0 |
| Hole mobility | \( \mu_p \) (cm\(^2\)V\(^{-1}\)s\(^{-1}\)) | 1.0 |
| Electron–hole pair generation rate per unit volume at the center of the device | \( G \) (cm\(^{-3}\)s\(^{-1}\)) | 1.74 \times 10^{12} |
| Effective density of states of the CB | \( N_C \) (cm\(^{-3}\)) | 1 \times 10^{19} |
| Effective density of states of the VB | \( N_V \) (cm\(^{-3}\)) | 1 \times 10^{19} |
| Ionized donor density | \( N_D^+ \) (cm\(^{-3}\)) | 1 \times 10^{19} |
| Ionized acceptor density | \( N_A^- \) (cm\(^{-3}\)) | 1 \times 10^{19} |
| Thermal velocity | \( v_{\text{th}} \) (cm\(\cdot\)s\(^{-1}\)) | 1 \times 10^{7} |
| DOS of the tail states at \( E = E_m \) | \( g_0 \) (cm\(^{-3}\) eV\(^{-1}\)) | 5.0 \times 10^{16} |
| Characteristic energies for acceptor-like tail states | \( E_s \) (eV) | 0.053 |
| Characteristic energies for donor-like tail states | \( E_{sl} \) (eV) | 0.088 |
| Energy at which both tail states coincide with the value of \( g_0 \) | \( E_m \) (eV) | 1.07 |
| Effective number density of states associated with acceptor-like deep states | \( N_A^\text{th} \) (cm\(^{-3}\)) | 1 \times 10^{18} |
| Effective number density of states associated with donor-like deep states | \( N_D^\text{th} \) (cm\(^{-3}\)) | 1 \times 10^{18} |
| Peak positions of acceptor-like deep states | \( E_A^\text{th} \) (eV) | 1.0 |
| Peak positions of donor-like deep states | \( E_D^\text{th} \) (eV) | 0.70 |
| Standard deviation in energy space of acceptor-like deep states | \( \sigma_n^A \) (eV) | 0.10 |
| Standard deviation in energy space of donor-like deep states | \( \sigma_p^A \) (eV) | 0.10 |
| Electron capture cross section of acceptor-like states | \( \sigma_n^A \) (cm\(^2\)) | 1 \times 10^{-16} |
| Hole capture cross section of acceptor-like states | \( \sigma_p^A \) (cm\(^2\)) | 1 \times 10^{-14} |
| Electron capture cross section of donor-like states | \( \sigma_n^D \) (cm\(^2\)) | 1 \times 10^{-14} |
| Hole capture cross section of donor-like states | \( \sigma_p^D \) (cm\(^2\)) | 1 \times 10^{-16} |
| Escape attempt frequency | \( v_{\text{at}} \) (s\(^{-1}\)) | 7 \times 10^{12} |
| Localization radius of the trap state | \( a \) (cm) | 5.12 \times 10^{-8} |
| Energy mesh interval in the mobility gap | \( d\text{EG} \) (meV) | 10 |
The formula of the NDF for the donor-like trap states is derived from Eq. (6) and is expressed as follows:

\[
f^D(E) = \frac{C^D n + N_D \exp \left( \frac{E - E_m}{k_B T} \right)}{C^D (n + N_D \exp \left( \frac{E - E_m}{k_B T} \right)) + p + N_C \exp \left( \frac{E - E_m}{k_B T} \right)} = \frac{C^D}{C^D + C^p}.
\]

When trap states exist successively in the mobility gap, the total capture and emission rates per unit volume are calculated by integrating the capture and emission rates per unit volume at each energy level for the interval from the VB to the CB, as was proposed by Simmons and Taylor [1–4]. This is expressed at each energy level for the interval from the VB to the CB, as total capture and emission rates per unit volume are calculated as given below for the acceptor-like states;

\[
R_{\alpha^A} = \int_{E_v}^{E_c} \nu_{\alpha^A} g^A_T(E) \left( 1 - f^A(E) \right) dE,
\]

\[
R_{\alpha^D} = \int_{E_v}^{E_c} \nu_{\alpha^D} g^D_T(E) \left( 1 - f^D(E) \right) dE,
\]

\[
R_{\beta^A} = \int_{E_v}^{E_c} \nu_{\beta^A} g^A_D(E) dE,
\]

\[
R_{\beta^D} = \int_{E_v}^{E_c} \nu_{\beta^D} g^D_D(E) dE.
\]

Regarding the donor-like states, the total capture and emission rates per unit volume are expressed by changing the suffix “A” to “D”; \( R_{\alpha^A}, R_{\beta^A}, R_{\beta^D}, \) and \( R_{\beta^D} \) correspond to the capture and emission processes \( a^A, b^A, c^A, \) and \( d^A, \) respectively, \( g^A_T(E) \) and \( g^D_T(E) \) are the DOSs of a-Si:H in the mobility gap, which are shown in the next section.

2.2 Density of states of a-Si:H

For the DOSs in the mobility gap for a-Si:H, we employ tail states and deep states [24, 26, 29–32]. The tail states caused by material disorder are modeled with an exponential tail from the CB edge or the VB edge. In the present study, the tail state DOSs are modeled as given below for acceptor-like states \( g^A_T(E) \) and donor-like states \( g^D_T(E) \).

\[
g^A_T(E) = g_0 \exp \left( \frac{E - E_m}{E_A} \right),
\]

\[
g^D_T(E) = g_0 \exp \left( \frac{E_m - E}{E_D} \right),
\]

where \( E_m, g_0, E_A, \) and \( E_D \) are described in Table 1. On the other hand, the deep states associated with the DB of a-Si:H are modeled by a Gaussian distribution with respect to energy. The DOS of the acceptor-like deep states \( g^A_D(E) \) and that of the donor-like deep states \( g^D_D(E) \) are expressed as follows:

\[
g^A_D(E) = \frac{N^A}{\sigma_A} \exp \left( - \frac{(E - E^A_g)^2}{2\sigma_A^2} \right),
\]

\[
g^D_D(E) = \frac{N^D}{\sigma_D} \exp \left( - \frac{(E - E^D_g)^2}{2\sigma_D^2} \right),
\]

where \( E^A_g, E^D_g, \sigma_A, \sigma_D, N^A, \) and \( N^D \) are as described in Table 1.

2.3 Drift–diffusion simulation model

Under the drift–diffusion simulation method, we solve the Poisson equation and the current continuity equations for the electrons and holes self-consistently. All quantities are evaluated at the center of the device length. The Poisson equation is expressed as follows:

\[
\frac{d^2 \varphi}{dx^2} = -\frac{q}{\epsilon} \left( p - n + p_h - n_h + p_i - n_i + N_D^+ - N_A^- \right),
\]

where \( x \) is the distance from the top of the device, \( \varphi \) is the electrostatic potential, \( \epsilon \) is the dielectric constant of a-Si, \( q \) is the elementary charge, and \( N_D^+ \) and \( N_A^- \) are the densities of the ionized donor and acceptor, respectively. The densities of trapped electrons and holes in the tail states are denoted by \( n_h \) and \( p_h \), respectively. The densities of trapped electrons and holes in the DB are denoted by \( n \) and \( p_i \), respectively. \( n_h, p_h, n_i, \) and \( p_i \) are calculated as follows:

\[
n_h = \int_{E_v}^{E_c} g^A_T(E) f^A(E) dE,
\]

\[
p_h = \int_{E_v}^{E_c} g^D_T(E) (1 - f^D(E)) dE,
\]

\[
n_i = \int_{E_v}^{E_c} g^D_D(E) dE,
\]

\[
p_i = \int_{E_v}^{E_c} g^A_D(E) dE.
\]
\[ n_i = \int_{E_v}^{E_c} g^A_D(E)f^A(E)\text{d}E, \tag{20} \]
\[ p_i = \int_{E_v}^{E_c} g^B_D(E)(1-f^B(E))\text{d}E. \tag{21} \]

Under a steady state, the current continuity equations for the electrons and the holes are expressed as follows:

\[ -\frac{1}{q} \frac{\text{d}J_n}{\text{d}x} = G - R_{c\varepsilon} + R_{d\varepsilon} - R_{\varepsilon d} + R_{\varepsilon p}, \tag{22} \]
\[ \frac{1}{q} \frac{\text{d}J_p}{\text{d}x} = G - R_{c\varepsilon} + R_{d\varepsilon} - R_{\varepsilon d} + R_{\varepsilon p}. \tag{23} \]

where \( J_n \) is the electron current density and \( J_p \) is the hole current density. Electron–hole pairs are generated under photoillumination; \( G \) is the electron–hole pair generation rate per unit volume. \( G \) is expressed as the product of the absorption coefficient, the incident photon flux, and the attenuation of photons inside the device. The value of \( G \) at the center of the device length is shown in Table 1. The current density consists of drift and diffusion current densities; \( J_n \) and \( J_p \) are expressed as follows, with the electron (hole) mobility \( \mu_n(\mu_p) \) and the electron (hole) diffusion coefficient \( D_n(D_p) \) in the CB (VB):

\[ J_n = -q\mu_n\frac{\text{d}\phi}{\text{d}x} + qD_n\frac{\text{d}n}{\text{d}x}, \tag{24} \]
\[ J_p = -q\mu_p\frac{\text{d}\phi}{\text{d}x} - qD_p\frac{\text{d}p}{\text{d}x}. \tag{25} \]

2.4 Hopping model

According to Mott’s hopping model, trap state electron hopping occurs from the initial state at energy level \( E_i \) to the destination state at energy level \( E_j \) [6–9, 13]. The single hopping rate \( \Gamma_{ij} \) (s\(^{-1}\)) is calculated under the condition of the energy level \( E_i \) and \( E_j \) as follows:

\[ \Gamma_{ij} = v_0 \left( \frac{g^A_i(E_i)dEG}{GT_i} \right) \exp \left( -\frac{2R_{ij}}{a} \right), \tag{26} \]
\[ GT_i = \int_{E_v}^{E_i} g^A_i(E)\text{d}E. \tag{27} \]

\[ R_{ij} = \left( \frac{4\pi}{3} GT_i \right)^{-1/3}, \tag{28} \]
\[ \text{if } E_i < E_j \Gamma_{ij} = v_0 \left( \frac{g^A_i(E_i)dEG}{GT_i} \right) \exp \left( -\frac{2R_{ij}}{a} \right) \exp \left( -\frac{E_j - E_i}{k_BT} \right), \tag{29} \]
\[ GT_j = \int_{E_v}^{E_j} g^A_j(E)\text{d}E, \tag{30} \]
\[ R_{ij} = \left( \frac{4\pi}{3} GT_j \right)^{-1/3}. \tag{31} \]

where \( v_0, a \) and \( dEG \) are as described in Table 1. \( g^A_i(E) \) is given in Eq. (13). \( \frac{g^A_i(E)dEG}{GT_i} \) from Eq. (26) and \( \frac{g^A_j(E)dEG}{GT_j} \) from Eq. (29) are the weight coefficients of the hopping probability for \( E_i \geq E_j \) and \( E_i < E_j \), respectively. \( GT_i \) and \( GT_j \) are the total DOSs of the tail states under energy levels \( E_i \) and \( E_j \), respectively. \( R_{ij} \) is the hopping length from the initial state at energy level \( E_i \) to the destination state at energy level \( E_j \). The summation of the hopping rates per unit volume for the trapped electrons in the acceptor-like band tail (\( R_{hop}^a \)), which is a hop from the initial states at energy level \( E_i \) to many destination states at energy level \( E_j \), is calculated from the single hopping rate \( \Gamma_{ij} \) as follows:

\[ R_{hop}^a = n_h \sum_i \Gamma_{ij}, \tag{32} \]
\[ n_h = g^A_i(E)\int f^A(E_i)dEG, \tag{33} \]

where \( n_h \) is the trapped electron density in the acceptor-like tail states and \( f^A(E_i) \) is the NDF for the acceptor-like trap states at energy level \( E_i \). The temperature dependence of \( f^A(E_i) \) is especially important for studying TQ. The trap state electron hopping photoconductivity at energy level \( E_i \) (\( \sigma_{hop}(E_i) \)) is shown as follows, as given in Mott [6]:

\[ \sigma_{hop}(E_i) = \frac{q^2}{6k_BT}R_{ij}^2R_{hop}^a, \tag{34} \]

The total trap state electron hopping photoconductivity (\( \sigma_{hop} \)) is the summation of all the acceptor-like band tail energy levels in Eq. (34):

\[ \sigma_{hop} = \frac{q^2}{6k_BT} \sum_i \left( R_{ij}^2R_{hop}^a \right). \tag{35} \]

The band carrier photoconductivity (\( \sigma_{ext} \)) is calculated as follows with the electron density (\( n \)) in the CB and the hole density (\( p \)) in the VB:
\[ \sigma_{\text{ext}} = q(\mu_n n + \mu_p p), \]  

where \( \mu_n \) and \( \mu_p \) are the mobility of the electrons in the CB and that of the holes in the VB, respectively. Trap state hopping and band conduction occur simultaneously. Therefore, the total photoconductivity \( \sigma_{\text{ph}} \) is the sum of the trap state electron hopping photoconductivity and the band carrier photoconductivity as follows:

\[ \sigma_{\text{ph}} = \sigma_{\text{hop}} + \sigma_{\text{ext}}. \]

### 2.5 Simulation parameters

The parameter list for the present simulations is shown in Table 1 [13, 24, 26]. The device consists of p-type and n-type a-Si:H. The length of the device is set to be sufficient to examine the temperature dependence of the NDF; the longer the device size is, the worse the convergence of the simulations at low temperatures.

The temperature of this simulation is in the range of 150–400 K. It has been shown in previous studies that some of the parameters have temperature dependence and energy dependence. However, we assume some of the parameters to be as described below, and we determine the parameter values.

- The mobility of the electrons in the CB and that of the holes in the VB are constant values at 300 K, without temperature dependence. It has been shown that the mobility of band carriers decreases with decreasing temperature [33, 34], which has advantages in explaining the cause of TQ.
- The conventional simulation method used in this study does not allow the simulation to converge under extremely small mobility conditions at low temperatures, as shown in Ref. [33, 34]. From the above, to enable simulations at low temperatures and to clarify the effect of the temperature dependence of the NDF on the cause of TQ, we deal with the mobility of band carriers as the constant values shown in Table 1 without temperature dependence. That is, based on the assumption that the mobilities are large enough to be simulated at low temperatures and the ratio of the temperature dependence of the mobilities is kept the same as in Ref. [33, 34], it is confirmed that the temperature dependence of the NDF without the temperature dependence of mobility shows the same tendency as that with the temperature dependence of mobility, but there are slight shifts in the NDF values on the CB side.
- The values of \( N_C \) and \( N_V \) are set to be smaller than those of the tail states at the band edges. The reasons for this are as follows: The measured photoconductivities in Fig. 1 have a positive temperature dependence on the mobility of the band carriers [33, 34]. However, the simulations employ mobilities without temperature dependence, as described above. This results in the large simulation value of \( \sigma_{\text{ext}} \) at low temperatures and the large deviation from the measured value in Fig. 1. To discuss the TQ observed at approximately 200 K for p-type samples, the values of \( \sigma_{\text{ext}} \) are shifted to lower values by setting the values of \( N_C \) and \( N_V \) to smaller values.
- The capture cross sections of the carriers are constant values at 300 K (Table 1) without energy dependence, without temperature dependence, and without a difference between the tail states and the DB.
- It is assumed that 80% of the donor and acceptor atoms are ionized at 150 K and 90% of the donor and acceptor atoms are ionized at 200 K [35].

### 2.6 Simulation method

The simulation scheme of the present study is the conventional drift–diffusion method; the numerical method is Scharfetter and Gummel’s scheme with the iterative technique [36–40]. The device is divided into meshes of 10 nm for calculating points. Imposing the nonequilibrium steady-state condition on each trap state, the NDF (the occupation probability of carriers for the trap states in the mobility gap) is calculated self-consistently during the simulations, which treat the capture and emission processes rigorously. Figure 3 shows the flowchart of the drift–diffusion simulation in the present study [41]. The Poisson equation derives the electrostatic potential \( \varphi \). The current continuity equation for the electrons derives the electron density \( n \) and that for the holes derives the hole density \( p \). The simulation derives \( \varphi, n, p, n_h, p_h, n_t, \) and \( p_t \) self-consistently under the control of the distribution functions derived by employing the principle of the nonequilibrium steady-state condition, which assumes that the capture and emission processes at the different energy levels \( E \) in the mobility gap do not have a relationship with each other. Furthermore, employing Mott’s hopping models, \( \sigma_{\text{hop}}, \sigma_{\text{ext}}, \) and \( \sigma_{\text{ph}} \) are derived with the results of the self-consistent drift–diffusion simulation.

### 3 Results and discussion

#### 3.1 Temperature dependence of the distribution functions

##### 3.1.1 p-type

Figure 4 shows the NDF for the acceptor-like trap states at the center of the device length for p-type samples under photoillumination and zero bias voltage at temperatures.
Fig. 3 Flowchart of the present drift–diffusion simulator. All calculations are carried out in terms of the distribution functions derived by employing the principle of the nonequilibrium steady-state condition for the acceptor-like and donor-like states self-consistently. \( V_{\text{app}} \) (the bias voltage) is 0 V in this study. Furthermore, employing Mott’s hopping models, the photoconductivity is derived with the results of the self-consistent drift–diffusion simulation.

Fig. 4 The NDFs for the acceptor-like trap states for \( p \)-type samples at temperatures of 150 K, 200 K, 250 K, 300 K, and 400 K. These functions have stair-shaped structures; these are the energy regions that keep the values of the NDF constant ([Region1]). In terms of the temperature dependence of these functions, the values of the functions decrease with increasing temperature (negative temperature dependence) in [Region1], [Region2], and [Region3].

Fig. 5 The EDFs for the acceptor-like trap states for \( p \)-type samples at temperatures of 150 K, 200 K, 250 K, 300 K, and 400 K. Additionally, Fig. 5 shows the EDF for the acceptor-like trap states at the center of the device length for \( p \)-type samples at the same temperatures. Both figures are shown on a semilogarithmic scale graph, with the abscissa denoting energy (eV) and the ordinate denoting the electron occupation probability (logarithmic scale). The slopes (gradient of the occupation probability to energy) of the NDF become gentler with increasing temperature, as shown in the area surrounded by dashed lines in Fig. 4; this is caused by the carriers’ thermal excitation to the band. The same tendency for the slopes of the EDF is shown in Fig. 5.

Fig. 6 Schematics of the capture and emission processes via the acceptor-like states located at energy \( E \). a The energy level \( E \) is far from the conduction band and the valence band, and the capture process of the electrons and that of the holes \((a^A \text{ and } c^A)\) are dominant. b The energy level \( E \) approaches the edge of the conduction band, and the electron emission process \( b^A \) comes into play. c The energy level \( E \) is remarkably close to the edge of the conduction band, the electron capture and emission processes \((a^A \text{ and } b^A)\) become dominant, and the small difference between \( a^A \) and \( b^A \) balances with the hole capture process \( c^A \). (a–c) Correspond to the energy levels [Region1], [Region2] and [Region3] in Fig. 4, respectively.
capture process of the electrons and that of the holes ($a^h$ and $c^h$). Therefore, the transition rate of the electron capture process $a^h$ is mostly the same as that of the hole capture process $c^h$ ($r_{a^h} = r_{c^h}$); the electrons combine with the holes rapidly in the trap states. Under this condition, $f^A(E)$ has constant values that decrease with increasing temperature, as shown in Fig. 4 [Region1]; this is negative temperature dependence. The width of [Region1] becomes narrower with increasing temperature because the transition rate of the hole emission process $d^h$ and that of the electron emission process $b^h$ become larger with increasing temperature. The constant values agree with the calculation value $n/(n + C^4 p)$. This is the value derived from Eq. (7). When the trap energy level $E$ is far from $E_V$ and $E_C$ ($E_V \ll E \ll E_C$), the electron and hole emission rates become exceedingly small; \(\exp\left(\frac{E-V}{kT}\right) \approx 0\) and \(\exp\left(\frac{E-E_C}{kT}\right) \approx 0\) are satisfied. This means that the distribution functions are calculated exactly during the simulations by employing the nonequilibrium steady-state condition for each trap state.

When the energy level $E$ approaches the edge of the CB, the electron emission process $b^h$ comes into play, as shown in Fig. 6b. This makes the values of the NDF small (Fig. 4 [Region2]). Focusing on the temperature dependence of the NDF at each energy level, the function values decrease with increasing temperature; this is negative temperature dependence. This occurs because with increasing temperature, the constant values of the NDF with respect to energy decrease (Fig. 4 [Region1]), and the energy levels at which the NDF changes from constant to decreasing become lower; the width of [Region1] becomes narrower.

Furthermore, the energy level $E$ approaches the edge of the CB (Fig. 4 [Region3]), and the electron capture and emission processes ($a^h$ and $b^h$) become dominant. In [Region3], according to the imposed nonequilibrium steady-state condition, the small difference between $d^h$ and $b^h$ balances with the hole capture process $c^h$, as shown in Fig. 6c. These capture and emission processes are rather similar to the equilibrium condition. However, the condition of Fig. 6c is definitely not the equilibrium condition.

On the other hand, under the equilibrium condition, the values of the EDF near the CB for $p$-type samples become larger with increasing temperature, as shown in Fig. 5; this is positive temperature dependence. That is, the temperature dependence of the distribution functions for the trap states near the CB for $p$-type samples under nonequilibrium circumstances is the reverse of that under equilibrium circumstances. This causes the difference in the temperature dependence of the trap state carriers’ density and that of the hopping photoconductivity between these two circumstances.

Now, we discuss the reason for the negative temperature dependence of the NDF near the CB for $p$-type samples. Employing the Shockley–Read–Hall recombination model for each energy level, the NDF values are determined by the density of the electrons in the CB and that of the holes in the VB. Therefore, we discuss the temperature dependence of the density of the electrons in the CB and that of the holes in the VB below. Considering the material temperature dependence, the carriers’ generation rate per unit volume of photoillumination is constant without temperature dependence. Figure 7a, b shows the density of the electrons in the CB and that of the holes in the VB as a function of temperature for $p$-type and $n$-type samples, respectively. For $p$-type samples, the density of the majority carrier holes produced by photogeneration and the thermal excitation in the VB increases exponentially with increasing temperature. On the other hand, the density of the minority carrier electrons in the CB is constant without temperature dependence because the density of the photogenerated electrons without temperature dependence is much larger than that of the thermal excitation electrons. In the Shockley–Read–Hall recombination model, the abovementioned temperature dependence of the band carrier density makes the capture rate of holes for the trap states become larger with increasing temperature; in other words, the electron occupation probability for the trap states.

![Fig 7](image-url)
states decreases with increasing temperature. This explains why the NDF values decrease with increasing temperature in the energy region near the CB for $p$-type samples.

### 3.1.2 n-type

Figure 8a, b shows the same NDF for the acceptor-like trap states at the center of the device length for $n$-type samples at temperatures of 150 K, 200 K, 250 K, 300 K, and 400 K. Figure 8a is shown on a linear scale graph; the inset is the enlarged figure in the area surrounded by the dashed line. On the other hand, Fig. 8b is shown on a semilogarithmic scale graph.

The common characteristics between the NDF for $n$-type samples and that for $p$-type samples (Fig. 4) are as follows:

- Both NDFs have stair-shaped structures: these are energy regions that keep the values of the NDF constant.
- The widths of the energy regions that keep the values of the NDF constant become narrower with increasing temperature because the transition rate of the hole emission process $d^h$ and that of the electron emission process $b^A$ become larger with increasing temperature.
- The slopes (gradients of occupation probability with respect to energy) of the NDF become gentler with increasing temperature, which is caused by the carriers’ thermal excitation to the band.

On the other hand, the characteristics that are different between the NDF for $n$-type samples and that for $p$-type samples are as follows:

- The constant values of the NDF against the energy for $n$-type samples become larger with increasing temperature (positive temperature dependence), as shown in the vicinity of the energy area surrounded by the dashed line in Fig. 8a, which is the reverse of the temperature characteristic for $p$-type samples.
- In the vicinity of the CB, the values of the NDF at each respective energy level become larger with increasing temperature, similar to the EDF (positive temperature dependence), as shown in the area surrounded by the dashed line in Fig. 8b. Therefore, the temperature dependence of the NDF near the CB for $n$-type samples is the reverse of that for $p$-type samples.

We show the difference of the temperature characteristic between the NDF for $n$-type samples and that for $p$-type samples by using the explanatory figures (Fig. 9a for $n$-type samples and Fig. 9b for $p$-type samples). The solid lines show the NDF for the lower temperature, and the dashed lines show the NDF for the higher temperature. The NDFs are calculated exactly during the simulations by employing the nonequilibrium steady-state condition for each trap state. As mentioned earlier, when the energy level $E$ is far from the CB and the VB, the transition rate of the electron capture process $c^A$ is largely the same as that of the hole capture process $c^A$ ($r_{c^A} = r_{c^A}$), and the NDF has constant values against energy. Regarding the temperature dependence of the constant values of the NDF against energy, the values become larger for $n$-type samples, and they decrease for $p$-type samples with increasing temperature because of the temperature dependence of the densities of the band carriers (Fig. 7a, b).

Concerning the values of the NDF near the CB, the values are affected by the constant values of the NDF against the energy, the energy levels at which the NDF changes from constant to decreasing, and the slope of the NDF. For $n$-type samples, the constant values of the NDF at higher temperatures are larger than those at lower temperatures, and the slopes of the NDF at higher temperatures are gentler.

![Fig. 8](image_url) The nonequilibrium distribution functions for the acceptor-like trap states for $n$-type samples at temperatures of 150 K, 200 K, 250 K, 300 K, and 400 K. a This is shown on a linear scale graph; the inset is the enlarged figure in the area surrounded by the dashed line. These functions have stair-shaped structures: these are the energy regions that keep the values of the NDF constant. The constant values become larger with increasing temperature (positive temperature dependence). b This is shown on a semilogarithmic scale graph. In the vicinity of the CB, the values of the NDF at the respective energy levels become larger with increasing temperature, similar to the EDF (positive temperature dependence), as shown in the area surrounded by the dashed line.
than those at lower temperatures. This makes the values of the NDF at the respective energy levels become larger with increasing temperature near the CB for \( n \)-type samples.

The doping densities and light intensity influence the temperature characteristics of the NDF. In this study, the densities of ionized donors and acceptors have typical values, and the photon flux is approximately AM1.5, as shown in Table 1.

The differences between both types of NDFs, as shown in Fig. 9, are the cause of the TQ that is observed for \( p \)-type samples but not observed for \( n \)-type samples at low temperatures of approximately 200 K. This is explained in detail in the next section.

For reference, regarding the hole distribution functions, the values of the nonequilibrium hole distribution functions for the donor-like trap states in the mobility gap \((1 - f_D(E))\) decrease with increasing temperature (negative temperature dependence) in the energy region near the VB for \( n \)-type samples.

### 3.2 Temperature dependence of photoconductivity

We consider that electron hopping occurs between two energy levels in conduction band tail states. Figure 10a shows the summations of the hopping rates per unit volume \( R_{\text{ho}}^n \) (Eq. 32) for the trapped electrons in the acceptor-like band tail for \( p \)-type samples as a function of the initial energy level \( E_i \) at temperatures of 150 K, 200 K, 250 K, 300 K, and 400 K. a This is shown in the overall energy level of the mobility gap. It is found that \( R_{\text{ho}}^n \) is dominant near the conduction band. b This is shown in the vicinity of the conduction band; regarding the temperature dependence of \( R_{\text{ho}}^n \), the values of \( R_{\text{ho}}^n \) decrease with increasing temperature (negative temperature dependence).
250 K, 300 K, and 400 K. Figure 11b is the enlargement of Fig. 11a near the CB. It is also found that $R_{n}^{e}$ changes exponentially with respect to the initial energy level $E_i$, and $R_{n}^{e}$ is dominant near the conduction band. Regarding the temperature dependence of $R_{n}^{e}$, the values of $R_{n}^{e}$ become larger with increasing temperature (positive temperature dependence). The temperature dependence of $R_{n}^{e}$ for n-type samples is the reverse of that for p-type samples.

Figure 12a shows the electron hopping photoconductivity $\sigma_{\text{hop}}$ calculated from Eq. (35) as a function of temperature for p-type and n-type samples. The photoconductivity is normalized by the illumination intensity. a The electron hopping photoconductivity $\sigma_{\text{hop}}$ is calculated from Eq. (35). b The band carriers’ photoconductivity $\sigma_{\text{ext}}$, which consists of the photoconductivity of the electrons in the conduction band and that of the holes in the valence band, is calculated from Eq. (36). c The total photoconductivity $\sigma_{\text{ph}}$, which is the sum of $\sigma_{\text{hop}}$ and $\sigma_{\text{ext}}$, is calculated from Eq. (37). Thermal quenching is shown at low temperatures of approximately 200 K for p-type samples.
a positive temperature dependence, at less than 200 K. At 200 K or more, the band carrier photoconductivity is greater than the electron hopping photoconductivity. For these reasons, the total photoconductivity $\sigma_{\text{ph}}$ changes from decreasing to increasing with increasing temperature at approximately 200 K. According to these results, the TQ is explained by the negative temperature dependence of the NDF near the CB for $p$-type samples. For $n$-type samples, $\sigma_{\text{ph}}$ increases monotonicly, and the minimum value of $\sigma_{\text{ph}}$ is not shown in Fig. 12c because the NDF for $n$-type samples does not have a negative temperature dependence but a positive temperature dependence.

It is considered that the TQ observed around a temperature of 350 K for $n$-type samples in Fig. 1 is explained not by the hopping model with a positive temperature dependence for the NDF but by Tran’s assumption described in the introduction.

### 4 Conclusions

The NDFs for the trap states in the mobility gap under photoluminescence and zero bias voltage are derived by the constructed self-consistent drift–diffusion simulator consisting of the Poisson equation and current continuity equations for a-Si:H. Regarding the temperature dependence of the NDF for $p$-type samples, we find that the values of the NDF decrease with increasing temperature (negative temperature dependence) in the energy region near the CB, which is the reverse of the temperature dependence of the EDFs for the trap states in the mobility gap, as shown for the first time. Regarding $n$-type samples, the values of the NDF increase with increasing temperature (positive temperature dependence) in the energy region near the CB, which is the same as for the EDF. The temperature dependence of the NDF is caused by that of the densities of the carriers produced by the photogeneration and thermal excitation in the bands and the balance between the capture and emission rates of the majority carriers and the minority carriers in the bands.

Furthermore, we show that this new physical characteristic can be applied in the explanation of the temperature characteristic of the photoconductivity caused by electron hopping in the conduction band tail for a-Si:H. Employing Mott’s hopping models, the electron hopping photoconductivity is derived from the summation of the hopping rates for all hopping paths, which is related to the product of the DOS of the trap states in the mobility gap and the NDF. The DOS of the tail states near the CB is large, which makes the hopping rates near the CB dominant. Regarding the temperature dependence of the NDF near the CB for $p$-type samples, the values of the NDF decrease with increasing temperature (negative temperature dependence). These factors make the electron hopping photoconductivity decrease with increasing temperature for $p$-type samples. At temperatures lower than 200 K, the electron hopping photoconductivity, with a negative temperature dependence, is larger than the band carrier photoconductivity, with a positive temperature dependence. At 200 K or more, the band carriers’ photoconductivity exceeds the electron hopping photoconductivity. Therefore, the temperature dependence of the total photoconductivity, which is the sum of the electron hopping photoconductivity and the band carrier photoconductivity, changes from decreasing to increasing with increasing temperature at approximately 200 K.

Thus, we show for the first time that the TQ observed at low temperatures of approximately 200 K for $p$-type a-Si:H can be explained by an electron hopping model with a $p$-type NDF that has a negative temperature dependence.

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