

# A New Model of Multiphonon Excitation Trap-Assisted Band-to-Band Tunneling

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**Abstract.** *The paper describes a new approach to calculating the currents in a pn-diode based on the extension of the Shockley-Read-Hall recombination-generation model. The presented theory is an alternative to Schenk's model of trap-assisted tunneling. The new approach takes into account generation and recombination as well as tunneling processes in pn-junctions. Using this model, the real "soft" I-V curve usually observed in the case of switching diodes and transistors was modeled as a result of the high concentration of traps that assist in the process of tunneling.*

## Keywords

Shockley-Read-Hall model, Schenk model, trap assisted tunneling, pn-junction, I-V curve.

## 1. Introduction

Electrical characteristics of gate dielectric stacks strongly affect the reliability and non-volatility of memory devices. Leakage currents in these stacks are adversely influenced by defects present in the dielectrics that act as deep energy levels and bring about indirect, trap-assisted tunneling (TAT) of charge carriers. Under certain densities and distributions of the traps in the dielectrics, the TAT leakage current may assume dominant magnitudes.

In the last decade a number of models of TAT have been proposed [1 - 5]. In common, they allow to retrieve the energy levels and the densities of trapping centers by fitting the parameters of the models to experimentally obtained data. More recently, also a simple graphical method was developed for extraction of TAT parameters in thin n-Si/SiO<sub>2</sub> structures [6].

Attempts have been made to formulate compact unified models of TAT [7 - 9], nevertheless, some questions remain still open and new approaches to the issue can be expected.

Trap-assisted tunneling results in a reduction of the Shockley-Read-Hall (SRH) recombination lifetimes in the regions of strong electric fields [10, 11]. I-V characteristics

of a reverse biased pn-junction are extremely sensitive to defect-assisted tunneling. The classical SRH model assumes that intermediate trap centers with concentration  $N_t$  lie on a discrete energy level  $E_t$ . In our model we assume that the discrete energy level  $E_t$  is broadened due to interactions of intermediate trap centers with multiphonon lattice vibrations, which gives rise to a band of multiphonon excitation traps.

## 2. Theory

In our model, the distribution function  $D_t^i$  of the density of traps (index  $i$  denotes a particular donor or acceptor band of traps) in the band gap satisfies the normalizing condition

$$N_t^i = \int_{E_V(x)}^{E_C(x)} D_t^i(x, \varepsilon) d\varepsilon \quad (1)$$

where  $N_t^i$  are donor or acceptor trap concentrations, and

$$D_t^i(x, \varepsilon) = \frac{N_t^i M^i(\varepsilon)}{\int_{E_V}^{E_C} M^i(\varepsilon) d\varepsilon} \quad (2)$$

Here,  $M(\varepsilon)$  is the multiphonon non-radiative transition probability for electron and hole capture [10]

$$M^i(\varepsilon, x) = \frac{1}{\sqrt{2\pi\varepsilon_r}} \frac{(\theta \mp S)^2}{(\theta^2 + z^2)^{\frac{1}{4}}} \times \exp\left(\sqrt{z^2 + \theta^2} - \theta \ln\left(\frac{\theta}{z} + \sqrt{1 + \left(\frac{\theta}{z}\right)^2}\right) - S(2f_B + 1) - \frac{\varepsilon_t^i}{2kT}\right) \quad (3)$$

where  $S$  is the Huang-Rhys factor representing the electron-phonon coupling,  $\hbar\omega_0$  is the effective phonon energy,  $\varepsilon_r = S \hbar\omega_0$  is the lattice relaxation energy,  $\theta = \varepsilon_t^i / (\hbar\omega_0)$ ,  $\varepsilon_t^i = |\varepsilon - E_C(x) + E_t^i|$ ,  $f_B$  is the Bose distribution function  $f_B = \left(\exp\left(\frac{\hbar\omega_0}{kT}\right) - 1\right)^{-1}$  and  $z = 2S\sqrt{f_B(1+f_B)}$ . The sign inside

the bracket in the nominator is negative for  $\varepsilon > E_C(x) - E_t$  and positive for  $\varepsilon < E_C(x) - E_t$ .

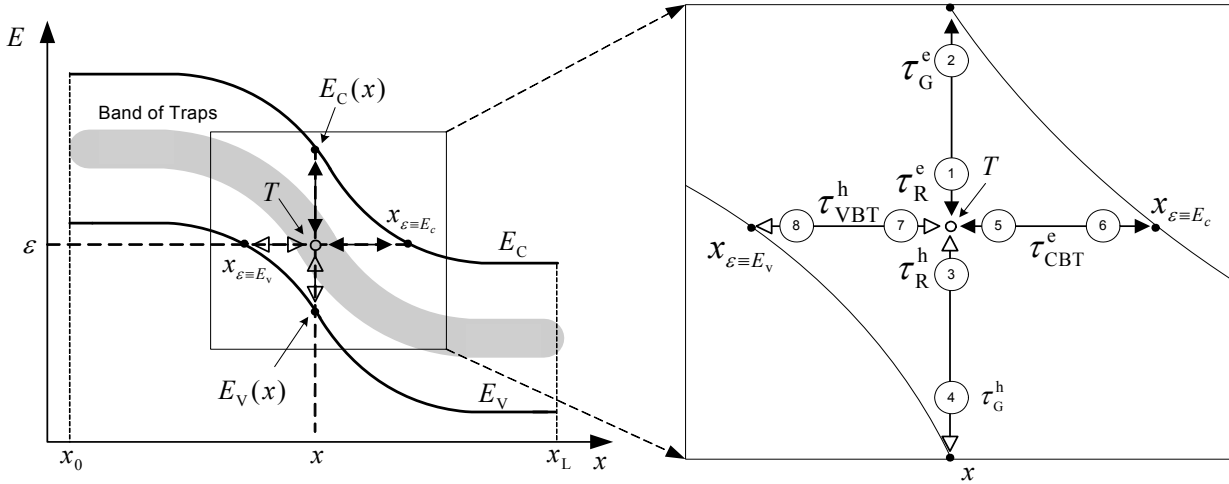


Fig. 1. Eight exchange processes considered in the new model of trap-assisted band-to-band tunnelling.

The current densities in the considered structures are calculated by solving the basic semiconductor laws, – the Poisson equation and continuity equation.

The continuity equations for electrons and holes can be written as

$$\frac{dJ_D^e(x)}{dx} = q \left( U_{SRH}(x) + U_{TAT}^{e(THER)}(x) + U_{TAT}^{e(TUN)}(x) \right), \quad (4)$$

$$\frac{dJ_D^h(x)}{dx} = -q \left( U_{SRH}(x) + U_{TAT}^{h(THER)}(x) + U_{TAT}^{h(TUN)}(x) \right) \quad (5)$$

where  $J_D^e$ ,  $J_D^h$  are the drift-diffusion electron/hole current densities.

In our model of recombination we do not work with recombination lifetimes. Instead of them we introduce a set of the so-called escape times characterizing the exchange of electrons between the trap and the conduction or valence band. The physical model of the generation-recombination terms  $U_{SRH}$ ,  $U_{TAT}^{e(THER)}$ ,  $U_{TAT}^{e(TUN)}$ ,  $U_{TAT}^{h(THER)}$  and  $U_{TAT}^{h(TUN)}$  taking into account the effect of trap-assisted tunneling is based on exchange processes of free charge carriers between the trap and the conduction or valence band (see Fig. 1). Four processes of electron and hole generation and recombination described by the classical SRH model are completed by four electron and hole capture and release processes of tunneling to and from the traps, giving together 8 exchange processes characterized by 6 escape times  $\tau_R^e$ ,  $\tau_G^e$ ,  $\tau_R^h$ ,  $\tau_G^h$ ,  $\tau_{CBT}^e$  and  $\tau_{VBT}^h$  [12 - 14]. From these 6 escape times one can derive the generation-recombination rates present in the continuity equations for electrons and holes.

## 2.1 Thermal Escape Times

1) Escape time  $\tau_{R,i}^e$  describes the transition of the electron from position  $x$  in the CB (conduction band edge) to a trap lying at position  $x$  with a loss of electron energy (phonon transition)

$$\tau_{R,i}^e(x) = \frac{1}{v_{th}^e \sigma^i n(x)} \quad \text{where} \quad v_{th}^e = \sqrt{3kT/m_e^*} \quad (6, 7)$$

and  $\sigma^i$  is the trapping cross-section.

2) Escape time  $\tau_{G,i}^e$  describes the transition of the electron from the trap lying at position  $x$  to CB at position  $x$  with an increase of electron energy (phonon transition)

$$\frac{1}{\tau_{G,i}^e(x, \varepsilon)} = \left( v_{th}^e \sigma^i N_C \exp\left(-\frac{E_C(x) - \varepsilon}{kT}\right) \right). \quad (8)$$

3) Escape time  $\tau_{R,i}^h$  describes the transition of the hole from position  $x$  in the VB (valence band edge) to a trap lying at position  $x$ , with an increase of hole energy (phonon transition)

$$\tau_{R,i}^h(x) = \frac{1}{v_{th}^h \sigma^i p(x)} \quad \text{where} \quad v_{th}^h = \sqrt{3kT/m_h^*}. \quad (9)$$

4) Escape time  $\tau_{G,i}^h$  describes the transition of the hole from the trap lying at position  $x$  to VB at position  $x$  with a loss of hole energy (phonon transition)

$$\frac{1}{\tau_{G,i}^h(x, \varepsilon)} = \left( v_{th}^h \sigma^i N_V \exp\left(-\frac{\varepsilon - E_V(x)}{kT}\right) \right). \quad (10)$$

## 2.2 Tunneling Escape Times

5) Escape time  $\tau_{CBT,i}^e$  describes the transition of the electron from the cross-section  $x_{\varepsilon=E_C}$  lying in CB to the trap  $T$  lying at position  $x$  and in the opposite direction without any change in electron energy (tunnel transition)

$$\begin{aligned} \frac{1}{\tau_{CBT,i}^e(x, \varepsilon)} &= \\ &= \frac{m_R^e \sigma^i}{2\pi^2 \hbar^3} \int_{E_C(x_L)}^{\varepsilon} |\varepsilon - \varepsilon'| \Gamma_{TAT}^e(\varepsilon', x_{\varepsilon=E_C} - x) d\varepsilon' \quad (11) \end{aligned}$$

where  $m_R^e$  is the effective mass for calculating the electron Richardson constant in the semiconductor and  $\Gamma_{TAT}^e$  is the

probability of electron tunneling. In WKB approximation it is expressed as

$$\Gamma_{\text{TAT}}^e(\varepsilon, x_{\varepsilon=E_C} - x) = \exp\left(-\frac{2}{\hbar} \int_{x_{\varepsilon=E_C}}^x \sqrt{2m_T^e |E_C(x) - \varepsilon|} dx\right). \quad (12)$$

Here,  $m_T^e$  is the electron effective tunneling mass.

6) Escape time  $\tau_{\text{VBT},i}^h$  describes the transition of the hole from the cross-section  $x_{\varepsilon=E_V}$  lying in VB to trap T at position  $x$  and in the opposite direction without any change in hole energy (tunnel transition)

$$\frac{1}{\tau_{\text{VBT},i}^h(x, \varepsilon)} = \frac{m_R^h \sigma^i E_V(x_L)}{2\pi^2 \hbar^3} \int_{\varepsilon}^{\varepsilon'} |\varepsilon - \varepsilon'| \Gamma_{\text{TAT}}^h(\varepsilon', x - x_{\varepsilon=E_V}) d\varepsilon' \quad (13)$$

where  $m_R^h$  is the effective mass for calculating the hole Richardson constant in the semiconductor and  $\Gamma_{\text{TAT}}^h$  is the probability of hole tunneling. In WKB approximation it is expressed as

$$\Gamma_{\text{TAT}}^h(\varepsilon, x - x_{\varepsilon=E_V}) = \exp\left(-\frac{2}{\hbar} \int_{x_{\varepsilon=E_V}}^x \sqrt{2m_T^h |E_V(x) - \varepsilon|} dx\right), \quad (14)$$

where  $m_T^h$  is the hole effective tunneling mass.

### 2.3 Generation-Recombination Terms

After computing the density of traps  $D_t^i(x, \varepsilon)$  and single escape times we can evaluate the generation-recombination terms occurring in (4) and (5). The generation-recombination terms are expressed in (17) to (21), where  $f_{F_n}$  and  $f_{F_p}$  are the Fermi-Dirac distribution function for electrons and holes defined as

$$f_{F_n}(x_{\varepsilon=E_C}) = 1 / \left(1 + \exp\left(-\frac{\varepsilon - E_{F_n}(x_{\varepsilon=E_C})}{kT}\right)\right). \quad (15)$$

and 
$$f_{F_p}(x_{\varepsilon=E_V}) = 1 / \left(1 + \exp\left(-\frac{E_{F_p}(x_{\varepsilon=E_V}) - \varepsilon}{kT}\right)\right). \quad (16)$$

Parameter  $E_{F_n}(x_{\varepsilon=E_C})$  in (15) denotes the Fermi quasi-level for electrons at cross-section  $x_{\varepsilon=E_C}$  and  $E_{F_p}(x_{\varepsilon=E_V})$  in (16) denotes the Fermi quasi-level for holes at cross-section  $x_{\varepsilon=E_V}$ , see Fig. 1. In (20) and (21),

$$F_C = \frac{dE_C(x_{\varepsilon=E_C})}{dx} \quad \text{and} \quad F_V = \frac{dE_V(x_{\varepsilon=E_V})}{dx}$$

are the electron and hole driving forces, respectively.

### 3. Results of Simulation

The new TAT model was employed in simulations of a pn-diode with a linear concentration profile (Fig. 2)

prepared on a phosphorous doped silicon substrate ( $N_D = 2.5 \times 10^{18} \text{ cm}^{-3}$ ) with orientation  $\langle 111 \rangle$  by boron diffusion from an infinite source with surface concentration  $N_A = 10^{19} \text{ cm}^{-3}$  at a temperature of  $1020^\circ\text{C}$  for 30 minutes. The structure was contaminated by gold, which forms one acceptor band of traps ( $i=A$ ) at a distance of  $E_t^A = 0.54 \text{ eV}$  from the conduction band edge. The concentration of the atoms of gold was assumed to be  $N_t^A = 10^{14} \text{ cm}^{-3}$ . The effective cross section was set for electrons and holes constant  $\sigma^A = 10^{-15} \text{ cm}^2$ . For evaluating the tunneling escape times  $\tau_{\text{CBT}}^e$ , effective masses  $m_R^e = 2.19 m_0$  and for  $\tau_{\text{VBT}}^h$ ,  $m_R^h = 0.66 m_0$  were used [15]. The tunneling probability was calculated using the WKB approximation and the effective masses were set as  $m_T^e = 0.26 m_0$  and  $m_T^h = 0.37 m_0$ .

Fig. 3 shows the simulated reverse  $I$ - $V$  curve. For comparing the influence of TAT mechanisms the  $I$ - $V$  curve calculated only with the SRH model is depicted as well. Trap-assisted-tunneling results in an increase of the current in the middle voltage region, resulting to a ‘‘soft’’ shape of the  $I$ - $V$  curve. At higher voltages, however, the influence of TAT mechanisms becomes negligible in comparison with band-to-band processes.

Fig. 4 displays  $I$ - $V$  characteristics with a constant Huang-Rhys factor  $S=4$ , for different effective energies  $\hbar\omega_0 = 12, 24, 36, 48$  and  $60 \text{ meV}$ . The change of  $\hbar\omega_0$  affects both the normalized distribution function  $D^A(\hbar\omega_0)$  and the

normalizing integral  $\int_{E_V}^{E_C} M^A(\varepsilon) d\varepsilon$ , thus the denominator

in (2), see Figs. 5 and 6. This eventually affects the multiphonon broadening of the deep trap level. A decrease in the multiphonon effective energy has a dramatic impact upon the growth of the current density even if the density of traps  $N_t$  in the band remains unchanged.

Fig. 7 shows the reverse  $I$ - $V$  curves with a constant multiphonon effective energy  $\hbar\omega_0 = 24 \text{ meV}$  for different values of the Huang-Rhys factor,  $S=2, 4, 6, 8$  and  $10$ . Similarly like the effective energy  $\hbar\omega_0$ , the Huang-Rhys factor has an influence on the broadening of the band of traps. In Figs. 8 and 9 one can see how the Huang-Rhys factor affects the distribution function  $D^A(S)$  and the normalization integral.

### 4. Conclusion

It is obvious that multiphonon broadening of the band of traps and trap-assisted tunneling markedly affect the reverse currents in heavily doped pn-junctions. Our simulations reveal that the effective energy  $\hbar\omega_0$  has a slightly stronger effect on the current than the Huang-Rhys factor. The new TAT model has the ability to describe the generation and recombination as well as the tunneling processes in pn-junctions. Using this model, the real ‘‘soft’’  $I$ - $V$  curve usually observed in the case of switching diodes and transistors was modeled as a result of the high concentration of traps that assist in the process of tunneling.

$$U_{\text{SRH}}(x) = \sum_{i=D,A} \int_{E_V(x)}^{E_C(x)} \frac{\left( \frac{1}{\tau_{R,i}^e(x)} \frac{1}{\tau_{R,i}^h(x)} - \frac{1}{\tau_{G,i}^e(x,\varepsilon)} \frac{1}{\tau_{G,i}^h(x,\varepsilon)} \right) D_t^i(x,\varepsilon) d\varepsilon}{\frac{1}{\tau_{R,i}^e(x)} + \frac{1}{\tau_{G,i}^e(x,\varepsilon)} + \frac{1}{\tau_{R,i}^h(x)} + \frac{1}{\tau_{G,i}^h(x,\varepsilon)} + \frac{1}{\tau_{\text{CBT},i}^e(x,\varepsilon)} + \frac{1}{\tau_{\text{VBT},i}^h(x,\varepsilon)}} \quad (17)$$

$$U_{\text{TAT}}^{e(\text{THER})}(x) = \sum_{i=D,A} \int_{E_V(x)}^{E_C(x)} \frac{\frac{1}{\tau_{R,i}^e} \left( \frac{1-f_{F_n}(x_{\varepsilon=E_C})}{\tau_{\text{CBT},i}^e} + \frac{f_{F_p}(x_{\varepsilon=E_V})}{\tau_{\text{VBT},i}^h} \right) - \frac{1}{\tau_{G,i}^e} \left( \frac{f_{F_n}(x_{\varepsilon=E_C})}{\tau_{\text{CBT},i}^e} + \frac{1-f_{F_p}(x_{\varepsilon=E_V})}{\tau_{\text{VBT},i}^h} \right)}{\frac{1}{\tau_{R,i}^e} + \frac{1}{\tau_{G,i}^e} + \frac{1}{\tau_{R,i}^h} + \frac{1}{\tau_{G,i}^h} + \frac{1}{\tau_{\text{CBT},i}^e} + \frac{1}{\tau_{\text{VBT},i}^h}} D_t^i d\varepsilon \quad (18)$$

$$U_{\text{TAT}}^{h(\text{THER})}(x) = \sum_{i=D,A} \int_{E_V(x)}^{E_C(x)} \frac{\frac{1}{\tau_{R,i}^h} \left( \frac{f_{F_n}(x_{\varepsilon=E_C})}{\tau_{\text{CBT},i}^e} + \frac{1-f_{F_p}(x_{\varepsilon=E_V})}{\tau_{\text{VBT},i}^h} \right) - \frac{1}{\tau_{G,i}^h} \left( \frac{1-f_{F_n}(x_{\varepsilon=E_C})}{\tau_{\text{CBT},i}^e} + \frac{f_{F_p}(x_{\varepsilon=E_V})}{\tau_{\text{VBT},i}^h} \right)}{\frac{1}{\tau_{R,i}^e} + \frac{1}{\tau_{G,i}^e} + \frac{1}{\tau_{R,i}^h} + \frac{1}{\tau_{G,i}^h} + \frac{1}{\tau_{\text{CBT},i}^e} + \frac{1}{\tau_{\text{VBT},i}^h}} D_t^i d\varepsilon \quad (19)$$

$$U_{\text{TAT}}^{e(\text{TUN})}(x_{\varepsilon=E_C}) = \sum_{i=D,A} \left| F_C \right|_{x_{\varepsilon=E_V}}^{x_{\varepsilon=E_C}} \frac{\frac{f_{F_n}(x_{\varepsilon=E_C})}{\tau_{\text{CBT},i}^e} \left( \frac{1}{\tau_{G,i}^e} + \frac{1}{\tau_{R,i}^h} + \frac{1}{\tau_{\text{VBT},i}^h} \right) - \frac{1-f_{F_n}(x_{\varepsilon=E_C})}{\tau_{\text{CBT},i}^e} \left( \frac{1}{\tau_{R,i}^e} + \frac{1}{\tau_{G,i}^h} + \frac{1}{\tau_{\text{VBT},i}^h} \left( \frac{1-f_{F_p}(x_{\varepsilon=E_V})}{1-f_{F_n}(x_{\varepsilon=E_C})} \right) \right)}{\frac{1}{\tau_{R,i}^e} + \frac{1}{\tau_{G,i}^e} + \frac{1}{\tau_{R,i}^h} + \frac{1}{\tau_{G,i}^h} + \frac{1}{\tau_{\text{CBT},i}^e} + \frac{1}{\tau_{\text{VBT},i}^h}} D_t^i dx \quad (20)$$

$$U_{\text{TAT}}^{h(\text{TUN})}(x_{\varepsilon=E_V}) = \sum_{i=D,A} \left| F_V \right|_{x_{\varepsilon=E_V}}^{x_{\varepsilon=E_C}} \frac{\frac{f_{F_p}(x_{\varepsilon=E_V})}{\tau_{\text{VBT},i}^h} \left( \frac{1}{\tau_{R,i}^e} + \frac{1}{\tau_{G,i}^h} + \frac{1}{\tau_{\text{CBT},i}^e} \frac{f_{F_n}(x_{\varepsilon=E_C})}{f_{F_p}(x_{\varepsilon=E_V})} \right) - \frac{1-f_{F_p}(x_{\varepsilon=E_V})}{\tau_{\text{VBT},i}^h} \left( \frac{1}{\tau_{G,i}^e} + \frac{1}{\tau_{R,i}^h} + \frac{1}{\tau_{\text{CBT},i}^e} \right)}{\frac{1}{\tau_{R,i}^e} + \frac{1}{\tau_{G,i}^e} + \frac{1}{\tau_{R,i}^h} + \frac{1}{\tau_{G,i}^h} + \frac{1}{\tau_{\text{CBT},i}^e} + \frac{1}{\tau_{\text{VBT},i}^h}} D_t^i dx \quad (21)$$

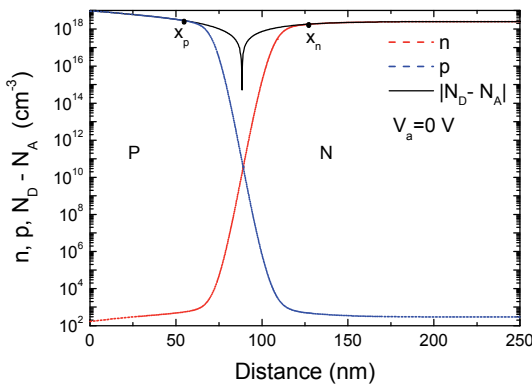
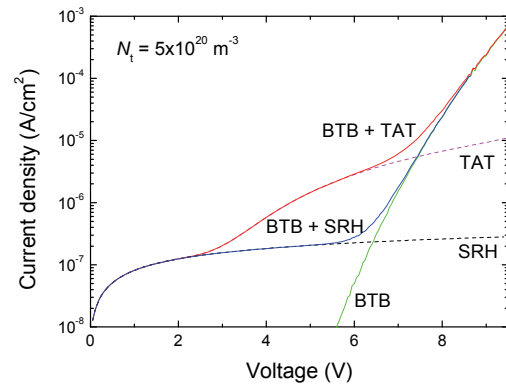

 Fig. 2. Concentration profile of the simulated  $pn$ -diode.


Fig. 3. Comparison of our TAT model with classical SRH model.

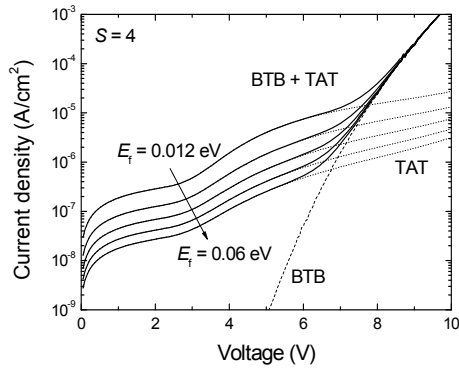


Fig. 4. Reverse  $I$ - $V$  characteristics for a constant Huang-Rhys factor  $S=4$ , for different effective energies  $\hbar\omega_0=12, 24, 36, 48$  and  $60$  meV.

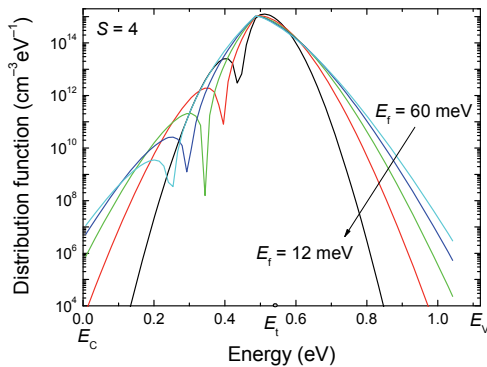


Fig. 5. The distribution function in dependence on the effective energy  $\hbar\omega_0=E_t$ .

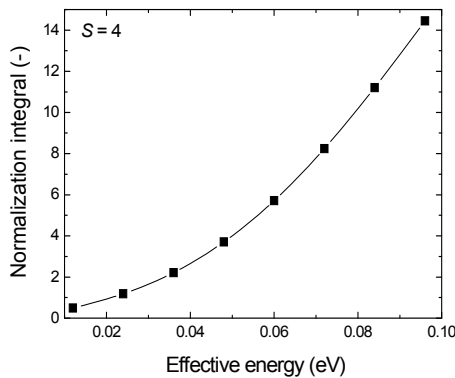


Fig. 6. Normalization integral for different effective energies  $\hbar\omega_0=12, 24, 36, 48$  and  $60$  meV and constant Huang-Rhys factor  $S=4$ .

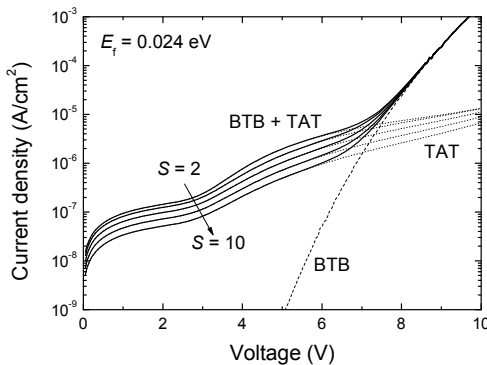


Fig. 7. Reverse  $I$ - $V$  characteristics curves for a constant multiphonon effective energy  $\hbar\omega_0=24$  meV, for different values of the Huang-Rhys factor,  $S=2, 4, 6, 8$  and  $10$ .

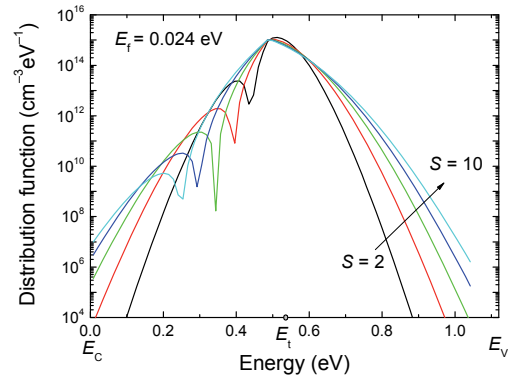


Fig. 8. The distribution  $t$  function for different values of the Huang-Rhys factor,  $S=2, 4, 6, 8$  and  $10$ .

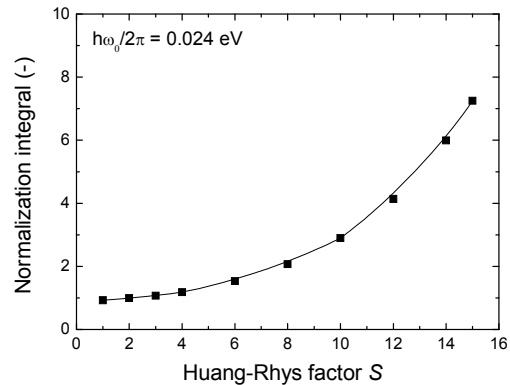


Fig. 9. Normalization integral for different values of the Huang-Rhys factor  $S=2, 4, 6, 8$  and  $10$ , and constant  $\hbar\omega_0=24$  meV.

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