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## Defect-related Auger excitation of erbium ions in amorphous silicon

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**Abstract.** The transition probability for defect-related Auger excitation (DRAE) of a rare-earth ion inserted into an amorphous matrix is calculated. The result is applied to excitation of an erbium ion in amorphous silicon occurring via capture of an electron by the dangling bond (D) defect. We have demonstrated high efficiency of the DRAE process which ensures strong photoluminescence and electroluminescence of erbium ions in an amorphous silicon matrix. It is shown that the temperature quenching of erbium luminescence in amorphous silicon is controlled by competition of the DRAE and the multiphonon nonradiative transitions.

### 1. Introduction

Photoluminescence and electroluminescence of rare earth (RE) elements which are embedded in a solid state matrix are of great interest because of possible optoelectronic applications [1]. RE ions exhibit luminescence arising from transitions in the inner 4f shell at photon energies which are almost independent of the host matrix. Of particular interest is Er, which in its 3+ state emits at a wavelength of about 1.54  $\mu\text{m}$ , very close to the minimum absorption of optical fibres. This emission arises from transitions from the excited state  $^4\text{I}_{13/2}$  to the ground state  $^4\text{I}_{15/2}$  of the 4f shell. It is well known that f–f transitions are dipole forbidden but become partially allowed when RE ions are incorporated into a solid matrix due to an admixture of other orbital momentum states to the f-wave functions. The interaction of the erbium ion with the neighbouring atoms is weak due to screening of the f electrons by the external 5s and 5p electrons. Thus, the energy position of deep f-electron multiple states of the  $\text{Er}^{3+}$  ion lying below the valence band of the semiconductor (by  $\sim 10$  eV) is practically independent of the host matrix. On the other hand, the mechanism of electronic excitation of RE ions is usually specific for each particular host matrix and it is the excitation mechanism that determines the temperature quenching of erbium luminescence in different matrices.

Recently strong photoluminescence and electroluminescence were observed at room temperature in erbium-doped amorphous hydrogenated silicon, a-Si:H(Er) [2–6]. Based on experimental results obtained, a defect-related Auger excitation DRAE mechanism was suggested in which a  $\text{D}^0 + \text{e} \rightarrow \text{D}^-$  transition for a dangling-bond D defect is accompanied by an excitation of the f electron of an erbium ion from the  $^4\text{I}_{15/2}$  to the  $^4\text{I}_{13/2}$  state. However, the explanation of results in [2–5] was purely qualitative since no estimates of the efficiency of the DRAE mechanism were available. In this work we present calculations of the probability of the DRAE process and compare it with that of the radiative transition between the same states. The calculations support the assumption of efficiency of the

DRAE mechanism. We shall also demonstrate that temperature quenching of erbium luminescence in amorphous silicon is controlled by competition between the DRAE process and multiphonon transitions.

## 2. The probability of defect-related Auger excitation in the Condon approximation

Experimental results [4, 5] show that introduction of erbium into amorphous hydrogenated silicon, a-Si:H(Er), leads to rupture of the silicon bonds and formation of D defects at a concentration of the order of  $10^{18} \text{ cm}^{-3}$ . In an amorphous matrix the mobile carriers excited into the conduction or valence band are rapidly thermalized into band tails; therefore, their capture by defects occurs from localized rather than extended electronic states. The configuration-coordinate diagram demonstrating three types of transition from the initial state *i*, which corresponds to the existence of the  $D^0$  centre and an electron in the conduction band tail while the final state *f* corresponds to an additional electron on the D centre (i.e. to a  $D^-$  centre), is displayed in figure 1.

Here we shall calculate the probability of a transition of an electron from the tail state of the conduction band to a  $D^-$  defect state with a simultaneous excitation of the *f* electron of the erbium ion from the ground to one of the upper *f* states (process 1 in figure 1). This is an Auger process, the probability of which is favoured by the fact that the D defect is situated in the close vicinity of the erbium ion inserted into the amorphous silicon matrix. The energy transferred to the *f* shell of the  $\text{Er}^{3+}$  ion in the process of electron capture by a defect is well determined and does not coincide in general with the binding energy of an electron on the defect. Therefore, in the Auger process some energy should be released or acquired in the capture transition. Since deep centres are usually characterized by stronger electron-phonon interaction than band electrons, this energy can be provided or accepted by local phonons. It should be noted that Coulomb interaction inducing the DRAE transition does not act directly on the vibration modes. However, local phonons are absorbed or emitted since the free and bound states of the electron correspond to displaced adiabatic potentials. The  $D^-$  defect after the Auger excitation can occur in the excited vibration state. Then local vibration excitation relaxes very fast to equilibrium due to decay into lattice phonons (see figure 1).

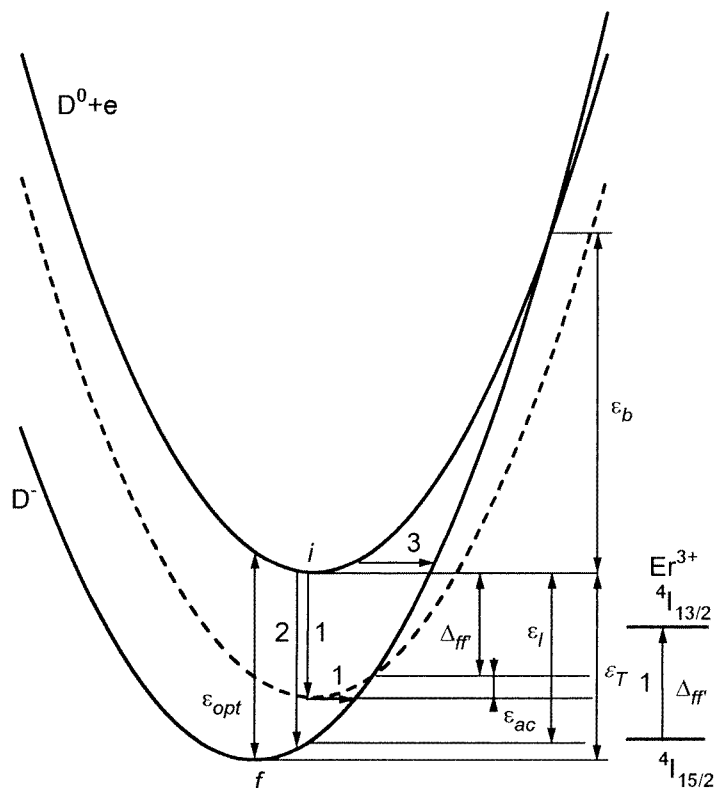
The probability of a transition involving the reorganization of the lattice in the vicinity of the erbium-defect complex is

$$W = \frac{2\pi}{\hbar} |\langle f | \hat{V} | i \rangle|^2 \delta(E_i - E_f - \Delta_{ff'}) \quad (1)$$

where *i* and *f* denote the initial and the final state of the electron transition,  $E_i$  and  $E_f$  are the corresponding energy of the electron-plus-defect system,  $\Delta_{ff'}$  is the energy difference between the excited and ground states of the erbium ion, and  $\hat{V}$  is the Coulomb interaction leading to the Auger process.

For simplicity we shall consider a one-mode approximation for interaction of  $D^-$  defects with local vibrations. The role of this mode can be played by the so-called breathing mode which induces maximal shift of the electronic level.

While applying the one-mode approximation we are using a simple model in the sense of a minimal number of unknown parameters to be adjusted to the experimental results. We should like to stress also that the one-mode approximation gives usually quite satisfactory results for crystalline semiconductors and since short order is preserved in the amorphous matrix and the properties of local phonons are determined by the close vicinity of the defect we can expect the one-mode approximation to be satisfactory also in the case of amorphous



**Figure 1.** A configuration-coordinate diagram for  $D^0 + e \rightarrow D^-$  transitions.  $i$  and  $f$  are initial and final states;  $\varepsilon_{opt}$ ,  $\varepsilon_l$  and  $\varepsilon_T$  are the energies of optical absorption, luminescence and thermal excitation, respectively. 1, The process of defect-related Auger excitation of the  $Er^{3+}$  ion (DRAE). The dashed curve corresponds to the adiabatic potential for virtual state;  $\varepsilon_{ff'}$  is the energy of excitation of the  $^4I_{15/2} \rightarrow ^4I_{13/2}$  transition of the  $Er^{3+}$  ion;  $\varepsilon_{ac}$  is the activation energy of the DRAE process. 2, the radiative transition. 3, the multiphonon nonradiative capture due to thermally activated tunnelling;  $\varepsilon_b = \varepsilon_l^2/2(\varepsilon_{opt} - \varepsilon_l)$  is the activation energy for multiphonon capture.

material. As concerns the role of the breathing mode, the values of the deformation potential point usually to its predominance though the specificity of the phonon mode is not used anywhere in our calculations.

In the adiabatic approximation we can express the initial state as

$$|i\rangle = |i_e\rangle |i_L\rangle \quad (2)$$

where  $|i_e\rangle$  is the electron wave function of the initial state and  $|i_L\rangle$  is the oscillator wave function corresponding to the defect vibration state. In a general case  $|i_e\rangle$  is a function of the oscillator coordinate but to the first order it is not (Condon approximation). The Condon approximation allows us to separate the matrix element into purely electronic and purely vibration components involving nothing more than the overlap of the oscillator wave functions

$$\langle f | \hat{V} | i \rangle = \langle f_e | \hat{V} | i_e \rangle \langle f_L | i_L \rangle. \quad (3)$$

Here  $\langle f_e |$  refers to the final electron state and  $\langle f_L |$  to the final vibration state of the defect. If the oscillator is displaced when an electron is captured by the D defect, the factor  $\langle f_L | i_L \rangle$  should be less than unity even if no phonons are absorbed or emitted, and it contributes a nonzero factor if phonons are absorbed or emitted. Taking into account a possible change of the phonon number, we can write for the energy conservation in the DRAE process

$$E_i - E_f - \Delta_{ff'} = \varepsilon_T - \Delta_{ff'} - N\hbar\omega_p$$

where  $\varepsilon_T$  is the energy difference between free and bound electron states including the polarization of the defect in equilibrium (the energy of thermal ionization of the  $D^-$  centre (see figure 1)),  $\Delta_{ff'}$  is the energy change of the f-electron system corresponding to the  ${}^4I_{15/2} \rightarrow {}^4I_{13/2}$  transition,  $N = N_f - N_i$  is the difference between the phonon numbers of final and initial states, and  $\omega_p$  is the local phonon frequency.

Now we can write the probability of the DRAE process,

$$W_A = \frac{2\pi}{\hbar} |\langle f_e | \hat{V} | i_e \rangle|^2 \sum_{N_i, N} P(N_i) |\langle f_L, N_i + N | i_L, N_i \rangle|^2 \delta(\varepsilon_T - \Delta_{ff'} - N\hbar\omega_p) \quad (4)$$

where  $P(N_i)$  is the probability for the phonon number to be  $N_i$  in the initial state. In the case of two displaced oscillators with the same frequency the factor

$$\mathcal{I}(N) = \sum_{N_i} P(N_i) |\langle f_L, N_i + N | i_L, N_i \rangle|^2 \quad (5)$$

was calculated in the theory of radiative transitions [7] and we have

$$\mathcal{I}(N) = \exp[-2S(N_T + \frac{1}{2})] \exp(N\hbar\omega_p/2k_B T) I_N\{2S[N_T(N_T + 1)]^{1/2}\} \quad (6)$$

where  $S$  is the Huang–Rhys factor, which is determined by the difference between the optical excitation energy  $\varepsilon_{opt}$  and the energy  $\varepsilon_l$  of luminescence from the minimum of the  $(D^0 + e)$  adiabatic potential (see figure 1)

$$2\hbar\omega_p S = \varepsilon_{opt} - \varepsilon_l. \quad (7)$$

In (6),  $N_T$  is the Bose–Einstein factor

$$N_T = \frac{1}{\exp(\hbar\omega_p/k_B T) - 1}$$

and  $I_N(z) = I_{-N}(z)$  is the modified Bessel function of order  $N$  where  $N$  for the DRAE process is determined by the  $\delta$  function from equation (4)

$$N = \frac{\varepsilon_T - \Delta_{ff'}}{\hbar\omega_p} \equiv N_{ff'}. \quad (8)$$

At low temperatures, when the argument of the Bessel function is small, we can use the following approximation:

$$I_N(z) \cong \left(\frac{z}{2}\right)^N \frac{1}{N!}. \quad (9)$$

In this case we have

$$\mathcal{I}(N) \approx S^N \frac{\exp(-S)}{N!} \quad (10)$$

which is the Poisson distribution around a mean value at  $N = S$  corresponding to an overlap of the wave functions of two displaced oscillators.

The result (10) for  $N$  given by (8) includes the probability of tunnelling through the barrier arising near the crossing point of two adiabatic potentials (a virtual one for the DRAE and that for the final state (figure 1)). The barrier for the DRAE process is given by

$$\varepsilon_{ac} = \frac{(\varepsilon_T - \Delta_{ff'} - S\hbar\omega_p)^2}{4S\hbar\omega_p} = \frac{(N_{ff'} - S)^2\hbar\omega_p}{4S}. \quad (11)$$

Calculations of tunnelling under the barrier  $\varepsilon_{ac}$  in the semiclassical approximation lead according to Markvart to the result equivalent to equation (10) (see [8] and [9]).

It should be noted that semiclassical calculations give good agreement with the experimental data in a large majority of cases and the difference from more elaborate methods is limited mostly to the difference in coefficients of the order of unity (see p 145 of [9]).

In the case of high temperatures we can use the approximation

$$I_N(z) \cong (2\pi z)^{-1/2} \exp[-(z - N)^2/2z] \quad (12)$$

and we obtain

$$\mathcal{I}(N) \approx (\hbar\omega_p/4\pi Sk_B T)^{1/2} \exp[-(N - S)^2\hbar\omega_p/4Sk_B T]. \quad (13)$$

Here we used the condition  $2Sk_B T/\hbar\omega_p \gg N$ . This result for  $N = N_{ff'}$  contains the exponential dependence on the barrier hindering the transition  $\varepsilon_{ac}$  (11).

Now we shall calculate the matrix element  $\langle f_e | \hat{V} | i_e \rangle$  by taking into account the Coulomb interaction between a free electron localized by the fluctuation potential of an amorphous matrix in an energy state belonging to the conduction band tail at the distance  $R_0$  from the D defect and an f electron of the  $Er^{3+}$  ion associated with the D defect (their exchange interaction is neglected since as a rule it is less than direct interaction [10]). We shall describe the conduction band tail state by a wave function of Bohr type with the radius  $a$  and the bound electron state on the D defect by the model of zero-radius potential with the characteristic localization length  $\kappa^{-1}$ ,  $\kappa$  being determined by the electron binding energy for the defect in equilibrium, i.e. by the energy of optical ionization (see figure 1)

$$\kappa \approx \sqrt{2m\varepsilon_{opt}}/\hbar. \quad (14)$$

As concerns the f electron functions we shall not need their explicit form if we assume that their localization radius is less than the localization radius of the electron state on defect.

The matrix element of the Auger process for an electron localized at distance  $R_0$  from the D defect created by an erbium ion is given by

$$\langle f_e | \hat{V} | i_e \rangle = \int d^3r_1 \int d^3r_2 \frac{1}{\sqrt{\pi}a^{3/2}} \exp\left(-\frac{|\mathbf{r}_1 - \mathbf{R}_0|}{a}\right) \sqrt{\frac{\kappa}{2\pi}} \frac{\exp(-\kappa r_1)}{r_1} \frac{e^2}{\varepsilon_\infty |\mathbf{r}_1 - \mathbf{r}_2|} \times \Psi_{f'}^*(\mathbf{r}_2) \Psi_f(\mathbf{r}_2). \quad (15)$$

Strongly localized wave functions  $\Psi_f$  and  $\Psi_{f'}$  correspond to the initial ( $^4I_{15/2}$ ) and final ( $^4I_{13/2}$ ) states of the  $Er^{3+}$  ion;  $\varepsilon_\infty$  is the high-frequency dielectric constant (the problem of polarization in Auger processes is discussed in [9]).

Calculations of integrals in (15) can be readily fulfilled by taking into account the relation  $\kappa^{-1} \ll a \ll R_0$ . As the result we have

$$\langle f_e | \hat{V} | i_e \rangle = \frac{2\sqrt{2}e^2(\mathbf{R}_0 \cdot \mathbf{d}_{f'f})}{3\varepsilon_\infty R_0(\kappa a)^{1/2}a^2} \exp\left(-\frac{R_0}{a}\right) \quad (16)$$

where

$$\mathbf{d}_{f'f} = \int d^3r_2 \Psi_{f'}^*(\mathbf{r}_2) \mathbf{r}_2 \Psi_f(\mathbf{r}_2) \quad (17)$$

is the same integral that determines the magnitude of optical dipole transition between  $^4I_{13/2}$  and  $^4I_{15/2}$  states [10]. This integral is not equal to zero only due to the admixture of the orbital states with the opposite parity to the f states induced by interaction of the  $Er^{3+}$  ion with the atoms of its close environment in amorphous silicon. From (4), (5) and (16) we get

$$W_A(R_0) = \frac{16\pi}{9} \left( \frac{e^2}{\varepsilon_\infty} \right)^2 \frac{(\mathbf{R}_0 \cdot \mathbf{d}_{f'f})^2}{R_0^2(\kappa a)a^4\hbar} \exp\left(-\frac{2R_0}{a}\right) \sum_N \mathcal{I}(N) \delta(\varepsilon_T - \Delta_{ff'} - N\hbar\omega_p). \quad (18)$$

If we replace the sum over  $N$  by integration over the phonon energy  $E = N\hbar\omega_p$ , and use the  $\delta$  function, the probability of DRAE by an electron at distance  $R_0$  from the defect will be

$$W_A(R_0) = \frac{16\pi}{9} \left( \frac{e^2}{\varepsilon_\infty} \right)^2 \frac{(\mathbf{R}_0 \cdot \mathbf{d}_{f'f})^2}{R_0^2(\kappa a)a^4\hbar^2\omega_p} \mathcal{I}(N_{ff'}) \exp\left(-\frac{2R_0}{a}\right) \quad (19)$$

where  $\mathcal{I}(N)$  is given by (6) in general case, by (10) in the limit of low temperatures, and by (13) in the limit of high temperatures. If we average (19) over various angle positions of the initial electron states we obtain

$$\langle W_A(R_0) \rangle = \frac{16\pi}{27} \frac{e^4 d_{f'f}^2}{\varepsilon_\infty^2 (\kappa a) a^4 \hbar^2 \omega_p} \mathcal{I}(N_{ff'}) \exp\left(-\frac{2R_0}{a}\right). \quad (20)$$

(20) with (6), (10), (13) and (8) gives the probability of the DRAE process if the conduction band electron is localized at distance  $R_0$  from the defect, and the energy difference of free and bound electron states is equal to  $\varepsilon_T$  in the case of equilibrium positions of the D defect (see figure 1). The parameter  $\kappa$  is determined by (14).

### 3. The probabilities of radiative and multiphonon transitions

There are two other paths of  $D^0 + e \rightarrow D^-$  transition: (i) radiative and (ii) multiphonon ones (processes 2 and 3, respectively, in figure 1). It is specially interesting to compare the probability of DRAE process with that of radiative transition. The total probability of photon emission assisted by multiphonon transitions in the  $D^0 + e \rightarrow D^-$  transition is given by [7]

$$W_{em} = \sum_{N=-\infty}^{\infty} \frac{4e^2\omega_v^3}{3\varepsilon_\infty\hbar c_v^3} |x_{if}|^2 \mathcal{I}(N) \quad (21)$$

where the spectrum of energies of photons emitted is determined by the relation  $\hbar\omega_v = E_f - E_i - N\hbar\omega_p$  and  $x_{if}$  is the dipole matrix element between the initial and the final electron states.

Using the fact that  $\mathcal{I}(N)$  depends exponentially on  $N$  while all the other factors are weaker functions of  $N$ , we have taken them out of the sum over  $N$  at the  $N$  value corresponding to the maximum of  $\mathcal{I}(N)$  :  $N = S$ . Then we applied the relation [7]

$$\sum_{N=-\infty}^{\infty} \mathcal{I}(N) = 1. \quad (22)$$

Thus, we obtained for the probability of radiative transition

$$W_{em} \approx \frac{4e^2\omega_m^3}{3\varepsilon_\infty\hbar c_m^3} |x_{if}|^2 \quad (23)$$

where  $\omega_m$  and  $c_m$  correspond to the photon frequency and light velocity for the maximum transition probability (determined by the condition  $N = S$ ). For calculation of the dipole matrix element  $x_{if}$  we used the same approximations as applied in section 2 and obtained

$$|x_{if}|^2 = \frac{32 \exp(-2R_0/a) \cos^2 \phi}{(a\kappa)^5 \kappa^2} \quad (24)$$

where  $\phi$  is the angle between the vector of electrical polarization and  $\mathbf{R}_0$ . Inserting the result (24) into the expression for the radiative emission probability we arrive at

$$W_{em} \approx \frac{128e^2 \omega_m^3 \exp(-2R_0/a) \cos^2 \phi}{3\varepsilon_\infty c_m^3 \hbar (a\kappa)^5 \kappa^2}. \quad (25)$$

After averaging over the angle  $\phi$  we obtain for the total probability of radiative  $D^0 + e \rightarrow D^-$  transition

$$\langle W_{em}(R_0) \rangle \approx \frac{128e^2 \omega_m^3 \exp(-2R_0/a)}{9\varepsilon_\infty c_m^3 \hbar (a\kappa)^5 \kappa^2}. \quad (26)$$

For the probability of nonradiative multiphonon process we shall use the results of [8] and [9]. At nonzero temperature this transition occurs as a thermally activated multiphonon tunnel process (designated by 3 in figure 1). Its probability is given by the formula

$$w_{mp} = w_{mp}^0 \exp(-\phi) \quad (27)$$

where

$$\phi = \left\{ -\frac{\theta}{2} + \ln \frac{1 + \sqrt{1 + \xi^2}}{\xi} - \sqrt{1 + \xi^2} + \xi \cosh\left(\frac{\theta}{2}\right) \right\} \frac{\varepsilon_T}{\hbar\omega_p} \quad (28)$$

$$\theta = \frac{\hbar\omega_p}{k_B T} \quad \xi = \frac{S\hbar\omega_p}{\varepsilon_T \sinh(\theta/2)} \quad (29)$$

which is valid for the Huang–Rhys model of two displaced parabolas. (Note that (28) is valid in a large temperature interval and has nothing to do with the low-temperature limit, (9).) In this model the energy of thermal excitation is

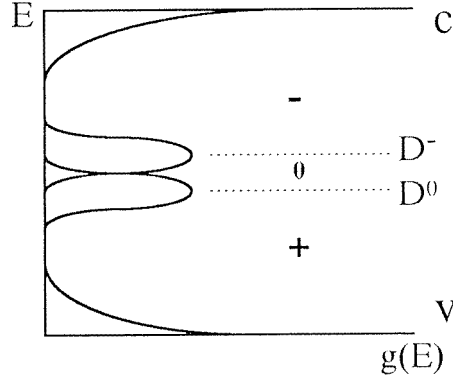
$$\varepsilon_T = (\varepsilon_{opt} + \varepsilon_l)/2. \quad (30)$$

The pre-exponential factor  $w_{mp}^0$  in (27) is highly sensitive to the behaviour of the electron wave function in the vicinity of the crossing point of two adiabatic potentials. Thus, for estimation of  $w_{mp}^0$  a specific model is necessary. We shall limit ourselves to the exponential approximation and will not calculate  $w_{mp}$  explicitly.

#### 4. Discussion

The introduction of erbium into amorphous silicon leads to formation of a large concentration of defects of the dangling bond type (D defects) in the silicon matrix. These defects can exist in three charged states ( $D^+$ ,  $D^0$ , and  $D^-$ ) which induce characteristic narrow bands near the middle of the bandgap. In figure 2 the density of electronic states is presented for amorphous silicon with a sufficiently large concentration of D defects. The fluctuations of potential in the amorphous matrix produce tails of localized states at the edges of the conduction and the valence bands, the extended electronic states in the bands being separated from these by the energy of mobility edge. The same fluctuations of potential broaden the levels of  $D^0$  and  $D^-$  states into two narrow bands. Usually photoconductivity measurements give the width of the gap as about 1.9 eV. The mobile carriers excited into the conduction





**Figure 2.** The effective density of states for amorphous silicon with dangling bond defects (D defects). The possibility for a defect to occur in a particular charge state is determined by the position of the Fermi level. +, 0, - show the D defect charge which an electron 'sees' before its capture on the corresponding level.

or valence band thermalize into localized states of the band tails and recombine from these states. The presence of D defects is detected by the defect luminescence band at 0.8–0.9 eV and the absorption band at 1.0–1.2 eV. Thus, in amorphous silicon an advantageous situation is realized when the energy released at capture of an electron by the  $D^0$  state (a D defect in the neutral state) is close to the excitation energy of the  $^4I_{15/2} \rightarrow ^4I_{13/2}$  transition in the f shell of  $Er^{3+}$  equal to  $\approx 0.8$  eV. The corresponding activation energy of the Auger process is small (see figure 1).

For numerical estimates we shall accept as the energy of the local phonon the energy of the optical phonon in silicon ( $\hbar\omega_p \approx 50$  meV) and the following values of characteristic energies for the  $D^0 + e \rightarrow D^-$  transition: the energy of photon emission (luminescence) is  $\varepsilon_l = 0.85$  eV, while that of optical absorption is  $\varepsilon_{opt} = 1.05$  eV. Then, for the Huang–Rhys model the energy of thermal ionization of the  $D^0$  state is  $\varepsilon_T = 0.95$  eV. Thus, in our case the Huang–Rhys parameter given by (7) is  $S = 2$ , and the activation energy for the DRAE process (see (11)) is  $\varepsilon_{ac} \approx 6$  meV.

The nearly resonant character of the Auger transition leads to the result that the factor  $\mathcal{I}(N_{ff'})$ , which takes into account the probability of emission of phonons assisting the Auger process, reduces only insignificantly the probability of erbium excitation. For the same reason  $\mathcal{I}(N_{ff'})$  is only slightly dependent on the temperature. In figure 3 the temperature dependence of  $\mathcal{I}(N_{ff'})$  is presented calculated with the accepted parameters. We see that  $\mathcal{I}(N_{ff'})$  is  $\approx 0.2$  in the whole temperature range of interest.

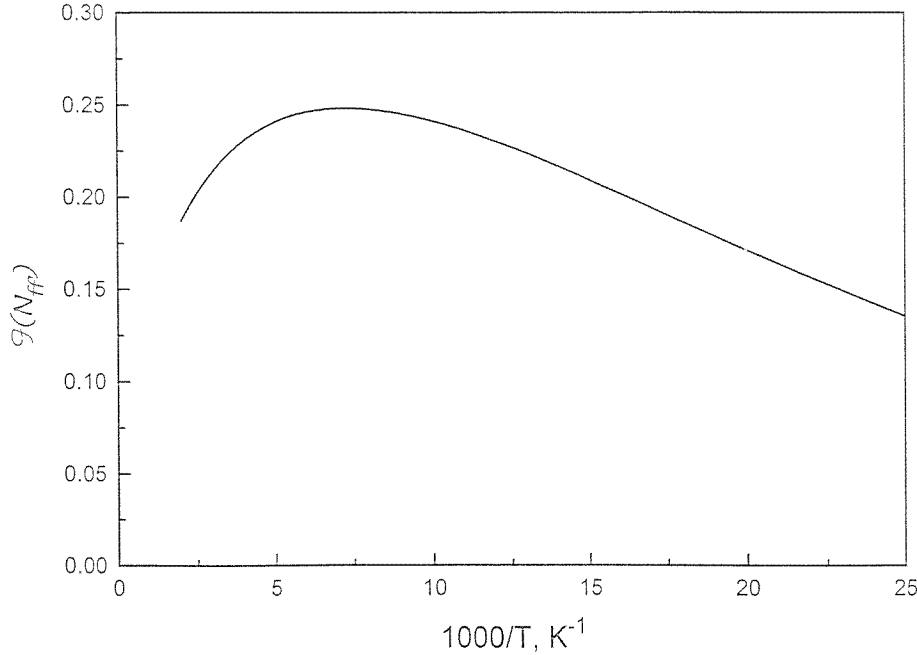
Now we can compare the probabilities of radiative and Auger-excitation processes:

$$\frac{\langle W_A(R_0) \rangle}{\langle W_{em}(R_0) \rangle} \approx \frac{\pi}{24} \frac{e^2 \kappa}{\varepsilon_\infty \hbar \omega_p} (\kappa \lambda)^3 (d_{f'f} \kappa)^2 \mathcal{I}(N_{ff'}) \quad (31)$$

where the wavelength of erbium emission (inside the medium) is

$$\lambda = \frac{2\pi \hbar c_m}{\Delta_{ff'}} \quad (32)$$

and the energy of erbium luminescence  $\Delta_{ff'} = 0.8$  eV. We obtained  $\lambda \approx 4.4 \times 10^{-5}$  cm. Parameter  $\kappa$  was calculated from the formula (14) connecting it with the optical excitation energy of the  $D^-$  level ( $\varepsilon_{opt} = 1.05$  eV) and the effective mass (we used the value



**Figure 3.** The temperature dependence of the factor  $\mathcal{I}(N_{ff'})$  resulting from multiphonon transition involved in the DRAE process in *a*-Si:H(Er).

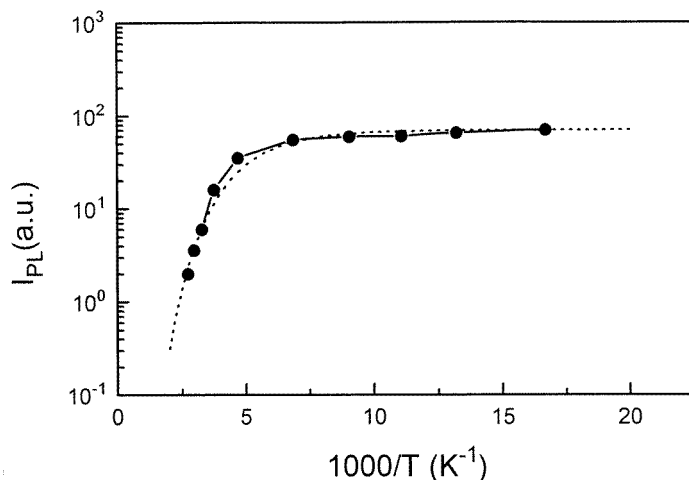
$m \approx 0.2m_0$ ). In this case  $\kappa \approx 2.35 \times 10^7 \text{ cm}^{-1}$ . For the dielectric constant we used the value  $\varepsilon_\infty = 12$ . For  $\mathcal{I}(N_{ff'})$  we accepted the value 0.2. The dipole moment of the transition in the f shell of the erbium ion can be estimated as a product of the radius of the f state ( $\sim 1 \text{ \AA}$ ) by the ratio of the energy of crystal splitting of the f multiplet to the energy distance between the f shell and the upper shells of the free  $\text{Er}^{3+}$  ion ( $\sim 10^{-3}$ ).

As a result we obtain

$$\frac{\langle W_A(R_0) \rangle}{\langle W_{em}(R_0) \rangle} \approx 7 \quad (33)$$

which gives of course only an order of magnitude estimate. However, we can draw a conclusion that the probability of the DRAE process is stronger than that of the defect radiative transition. This result is in agreement with the experimental data demonstrating that in *a*-Si:H(Er) defect luminescence sharply increases at high excitation rates when erbium luminescence saturates [4, 5]. For the value of the DRAE probability we get  $W_A \approx 9 \times 10^4 \text{ s}^{-1}$  from (20) with  $a \approx R_0 \approx 10 \text{ \AA}$ .

As concerns the multiphonon transition, it has a large energy threshold as stated above and in a definite temperature range (at low temperatures) can be weaker than the DRAE process but dominates at higher temperature leading to temperature quenching of erbium luminescence. To check the latter statement we have calculated the temperature dependence of reciprocal capture probability  $w_{mp}^{-1}$  from the formulae (27)–(30) using the accepted parameters and compared it with the experimental dependence of intensity of erbium luminescence in figure 4. The absolute value of the probability was adjusted to the experimental curve at low temperatures where luminescence intensity is nearly temperature independent. It is clear from the comparison of the mentioned plots that there is a close



**Figure 4.** Temperature dependence of erbium luminescence in a-Si:H(Er). Circles correspond to experimental data; the dotted curve is the reciprocal probability of multiphonon thermally activated tunnelling  $w_{mp}^{-1}$  calculated from (27)–(29).

correspondence between them. Thus, we can conclude that the temperature quenching of erbium luminescence is actually controlled by the onset of multiphonon processes. However, comparatively weak electron–phonon interaction for the  $D^-$  defect ( $S = 2$ ) leads to the result that at room temperature multiphonon transitions do not suppress completely the Auger excitation. This fact enables the observation of erbium luminescence in a-Si:H(Er) at room temperature.

In conclusion, we have calculated transition probability of the defect-related Auger excitation of an RE ion inserted into an amorphous matrix. The result obtained was applied to consideration of excitation of erbium ions in amorphous silicon. We have demonstrated that the probability of the DRAE process for the  $D^0 + e \rightarrow D^-$  transition is significantly higher than that of the radiative capture of an electron on the D (dangling bond) defect competing with it. The temperature quenching is controlled by a sharp increase of the probability of multiphonon capture at elevated temperatures.

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