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Mechanisms of excitation of the $f-f$ emission in silicon codoped with erbium and oxygen

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The problem of energy transfer from photo- and electrogenerated carriers to f-electrons of a rare earth center is a primary consideration in physics of rare earth doped semiconductors. It is a complicated problem, especially in the case of complex centers involving rare earth ions and other impurity atoms. In spite of numerous papers on this subject [1,2], the nature of the excitation mechanisms of rare earth centers in semiconductors has not been yet clarified. In this paper we propose the simple model describing the excitation of the Er-related emission in Er_2O_3 clusters in silicon through the photo- and electrogeneration of carriers. The high efficiency of excitation is connected with the presence of the discrete and quasi-discrete electron states localized on Er_2O_3 clusters in silicon. In the case of photoluminescence and electroluminescence under forward bias the excitation of Er ions occurs via the Auger recombination of excitons localized on Er–O complexes. In the case of electroluminescence under reverse bias the electron capture of hot carriers in the conduction band of silicon into the quasi-bound states of the Er_2O_3 clusters leads to the large value of the impact excitation cross section.

Complexes Er–O in Si

Silicon codoped with erbium and oxygen is a best studied material due to the high intensity of the Er-related emission. Numerous studies [1,2] have shown that the optically active center in erbium-doped silicon is a complex formed as a result of interaction between erbium and oxygen atoms. The authors of [3] used the EXAFS method to identify the optically active complex in CZ-silicon. The EXAFS analysis indicates that $> 80\%$ of the Er atoms are coordinated with the oxygen atoms. The first shell around the Er atom resemles the 6 oxygen coordination in Er_2O_3 [4]. The value 2.25 Å of the Er–O bond length is, however, somewhat smaller than the mean value 2.27 Å of the bond length in the oxide.

The authors of [5] have obtained by EXAFS data analyses almost the same result for silicon coimplanted by Er and O after annealing of the sample at 900°C. In this case the coordination number of oxygen atoms is equal to 5, and the value $2.26 \div 2.27$ Å of the Er–O bond length is quite close to the mean value 2.27 Å in Er_2O_3.

Masterov et al. [6,7] using $^{169}Er(^{169}Tm)$ Emission Mössbauer Spectroscopy (EMS) established correlation between the Er–O clusters and the $f-f$ photoluminescence intensity in amorphous (a-Si:H) and crystalline (c-Si) silicon. The Mössbauer spectra of the silicon samples codoped with erbium and oxygen have been compared with the spectrum of Er_2O_3.

The Mössbauer spectrum is a superpositions of a quadrupole doublet (spectrum I) and a singlet (spectrum II). Spectrum I belongs to the erbium centers with low symmetry, whereas spectrum II to the centers with cubic or almost cubic surrounding. As far as the relative intensity of spectrum I correlates with the intensity of Er-related emission, the corresponding erbium centers should be responsible for the Er-doped Si photoluminescence at the wavelength of 1.54 μm. It is believed that spectrum I corresponds to the complex consisting of the Er^{3+}-ion with the six-oxygen environment. Spectrum II might be ascribed to the erbium ion surrounded by silicon atoms only in $ErSi_2$ configuration.

Electron paramagnetic resonance (EPR) has been used to examine the structure of the Er–O complexes formed in silicon codoped with Er and O by Carey et al. [8]. In order to observe EPR sharp lines for Er concentration of 10^{19} Er/cm^3 it is necessary to have O concentration in excess of $3 \cdot 10^{19}$ O/cm^3. At oxygen concentrations below or equal to this value, only broad resonance lines are observed. Accordingly to [8] in samples of silicon containing Er and O in ratio 1:10 sharp EPR lines were observed. The principal g-values and the paramagnetic center concentration are shown to be extremely sensitive to post-regrowth processes. The angular dependence of the several lines measured on the sample codoped with 10^{20} O/cm^3 and annealed at 900°C for 30 s, allowed authors of [8] to attribute the spectra observed to Er^{3+} in the sites of both monoclinic (C_{1h}) and trigonal symmetry. The principal g-values for the monoclinic center are $g_1 = 0.80$, $g_2 = 5.45$, $g_3 = 12.60$ and for the trigonal center $g_\perp = 0.69$, $g_\| = 3.24$. The authors suggest that the monoclinic center consists of an Er^{3+} ion surrounded by six oxygen ions in configuration characteristic for the monoclinic center in Er_2O_3. Really, cubic erbium oxide occurs in two forms each with one Er atom surrounded by six O atoms: the monoclinic C_2 center and the trigonal C_{3i} center [3]. However, the EPR studies of Er^{3+} in Y_2O_3 having the crystal structure similar to Er_2O_3 have shown that the monoclinic and trigonal centers have g-values $g_x = 1.645$, $g_y = 4.892$, $g_z = 12.314$ and $g_\| = 12.176$, $g_\perp = 3.318$, respectively [9]. It should be noted that erbium oxide is an antiferromagnetic material with the Neel temperature

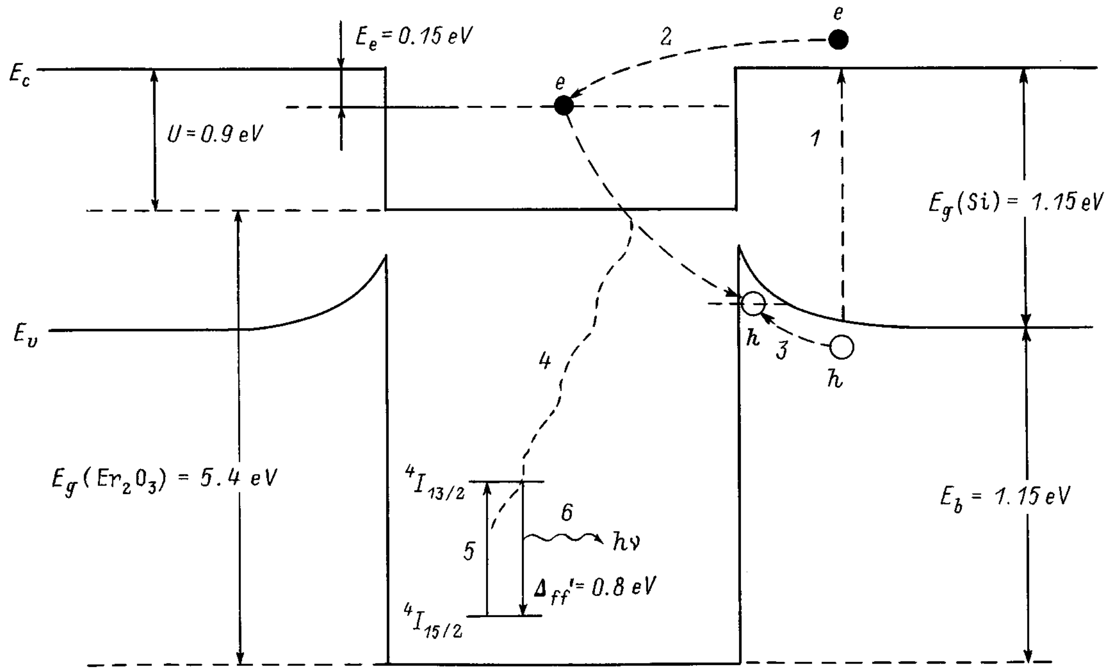

Figure 1. The schematic illustration of the quantum well Er_2O_3 in silicon: *1* — photogeneration of the electron-hole pair; *2* — capture of the electron on the level within the quantum well; *3* — capture of the hole, forming of the exciton; *4* — Auger process; *5* — Er^{3+}-ion excitation; *6* — $f-f$-emission.

equal to 3.4 K [3]. That is why in Er_2O_3 clusters in silicon the Er–O–Er exchange bonded pairs of Er^{3+} ions must be exist and these are responsible for considerable distinctions between g-values of Er^{3+} ions in silicon and those in Y_2O_3, where erbium atoms are distributed in the crystal lattice randomly. It should be also noted that in the unit cell of erbium oxide twenty-four rare-earth ions are on the sites with twofold rotational symmetry (C_2) and eight ones are on the sites with threefold rotary inversion symmetry (C_{3i}) [4].

Quantum dot model for Er_2O_3 cluster in silicon

In our model we consider the Er_2O_3 cluster in silicon as a quantum dot (nanoplatelet in [10]) with the size close to the lattice parameter in silicon $a(\mathrm{Er_2O_3}) \approx 1.05$ nm [11]. It is necessary to add to this size the correction length d which represents an adaptation or transition length needed to change the cation coordination number from $N_c = 6$ in Er_2O_3 to $N_c = 4$ in silicon. According to [10] this length is about 0.12 nm. Hence, the characteristic diameter of the Er_2O_3 quantum dot is about 1.2 nm. As a first approximation, we assume that this quantum dot represents a spherical quantum well with the radius $R \approx 0.6$ nm in the energy scheme of Si:Er, O. The depth of the well may be obtained from the band gaps of erbium oxide and silicon $E_g(\mathrm{Er_2O_3}) = 5.4$ eV, $E_g(\mathrm{Si}) = 1.17$ eV (at $T = 0$ K), and the energy parameters of oxygen and silicon atoms. The top of the valence band is formed by $2p$ states of oxygen in Er_2O_3 and by $3p$ states in silicon. That is why we should estimate the energies of p states (E_p) in free O and Si atoms. Using the method of determination of atomic parameters, proposed previously [12], we obtained $E_p(\mathrm{O}) = -13.6$ eV and $E_p(\mathrm{Si}) = -8.15$ eV. Thus the valence band edge in the Er–O complex $E_v(\mathrm{Er_2O_3})$ lies about 5 eV below that in the bulk silicon $E_v(\mathrm{Si})$. The complex constitutes a weakly transparent barrier of 5 eV high for holes while for electrons it acts as the quantum well $U = 0.9$ eV in depth with the discrete electron level with binding energy 0.15 eV observed experimentally in DLTS measurements [13]. The f-levels lie close to the bottom of the quantum well according to the notion band structure of rare-earth metal oxides. Fig. 1 shows the energy scheme described.

The electron level localized in the quantum well (QW) plays the role of an electron trap. The trapped electron attracts through the Coulomb interaction the hole in the valence band of silicon forming an "indirect" (in space) exciton. Then the Auger recombination of the electron and the hole takes place leading to the excitation of the f-shell electrons of the Er^{3+} ion in the Er_2O_3 cluster.

Now we estimate the energy E_e of an electron bound to the Er–O complex using the proposed model. The electron effective mass should be different inside and outside the QW. Inside the QW we put the effective mass equal to the free electron mass m_0 and in the bulk semiconductor we take the average mass m_c in the conduction band of silicon. There is a single spherical symmetric electronic state with the energy

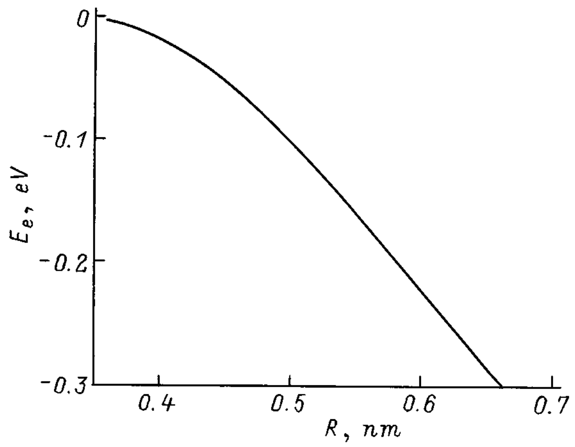

Figure 2. The energy of the Er–O cluster localized electron level as a function of the Er–O complex radius R.

determined by the transcendental equation

$$\tan(kR) = -\frac{km_c}{\kappa}, \tag{1}$$

where $k = \sqrt{2m_0(U - E_e)}/\hbar$ is the electron wave vector in the QW region, $\kappa = \sqrt{2m_c(-E_e)}/\hbar$ is the wave function decrement in the bulk, the electron energy E_e is measured from the conduction band edge in silicon E_c. The result of solution Eq. (1), the energy of the electron level as a function of the quantum dot radius is shown in Fig. 2. Certainly, the proposed model is very rough. The aim of this simulation is to demonstrate that the electron localized within the Er–O complex with the characteristic radius $R \approx 0.6$ nm has energy which corresponds to the position of the real electron level $E_e = -0.15$ eV.

The localized electron attracts via Coulomb field the hole in the valence band of silicon. We use the system of differential equations [14] to describe the hole motion in the bulk semiconductor with the degenerated valence band in the presence of the electric field of the localized electron. We assume that this equations describe also the hole in the Er–O complex. Since the Er–O complex represents a weakly permeable barrier for holes, the parameters of the valence band in the quantum well region are not very essential for the hole binding energy. So we take the same heavy hole mass value m_{hh} in the quantum well and in the bulk. For light holes we take into acoount the nonparabolisity in the Kane model [15] of the energy spectrum caused by mixing of the valence states and the states of the bottom of the quantum well which lies quite close to the hole energies. The details of these calculations were published in our previous work [12] and we do not present them here. The boundary conditions were obtained by integration of the differential equations for the hole radial wave functions through the quantum well border. The numerical calculations give the following results for the hole binding energies of the upper hole states localized by the Er–O cluster: $E_h - E_v(\mathrm{Si}) = 0.021$ eV for the even state with angular momentum $J = 3/2$ and $E_h - E_v(\mathrm{Si}) = 0.011$ eV for the odd state with angular momentum $J = 1/2$. Due to the selection rules the latest state plays the main role in the Auger excitation of the Er ion in the Er–O cluster. This state has the light hole nature and the characteristic size of the hole orbit is a few times larger than the Er–O complex radius.

Auger excitation

In the case of photoluminescence and electroluminescence under forward bias when there are not enough hot carriers in silicon the excitation of Er f-shell electrons proceeds via the Auger recombination of the exciton localized on the Er–O cluster. As indicated above the exciton bond energy to the Er–O complex $E_{\mathrm{Ex}} = E_e - E_h = 0.96$ eV is larger than the transition energy $\Delta_{ff'} = 0.8$ eV between the first excited state $^4I_{13/2}$ and the ground state $^4I_{15/2}$ of Er^{3+} ion. Thus the energy excess $\Delta E = E_{\mathrm{Ex}} - \Delta_{ff'} \approx 0.2$ eV should be transferred to a "third body". Usually (see, for example, [16]) this difference is ascribed to electron–phonon interaction, but the rate of this process is too small to describe the real energy transfer from the carriers in silicon to the Er ions. That is why we shall discuss another Auger excitation process when the energy excess ΔE is transferred to the free carriers (electrons or holes) in the host semiconductor.

Fig. 3 shows the Feynman diagram of this process. Note that the electron energy in intermediate state is quite close to the discrete level energy E_e. It differs from E_e by the energy ΔE only. Since the value $\Delta E \approx 0.16$ eV is much smaller than the electron quantum size energy $\hbar^2/m_0R^2 \approx 1$ eV, the main contribution to the Auger recombination amplitude is given by the term in which the intermediate state is the electron level bound to the Er–O

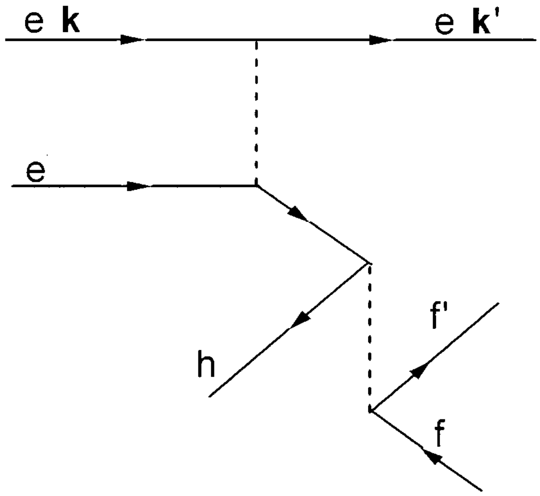

Figure 3. The Feynman diagrams of the Auger recombination processes when ΔE is transferred to the free carrier. Indexes f and f' denote f-shell states of Er, e and h denote the electron and hole states bound to the Er–O complex, $\mathbf{k}$ and $\mathbf{k}'$ denote the initial and final states of the free carrier in silicon.

complex. So the given Auger recombination has a resonance character. It proceeds mostly via the discrete electron level E_e. In the resonance approximation we can write the Auger recombination amplitude as

$$M = \frac{M_A M_{\mathrm{Ex}}}{\Delta E}, \tag{2}$$

where

$$M_A = \int \Psi_e^*(\mathbf{r})\Psi_e(\mathbf{r}) \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \Psi_{\mathbf{k}'}^*(\mathbf{r}')\Psi_{\mathbf{k}}(\mathbf{r}') d\mathbf{r} d\mathbf{r}' \tag{3}$$

is the Auger amplitude which corresponds to the upper part of the Feynman diagram (Fig. 3), Ψ_e is the wave functions of the discrete electron level and $\Psi_{\mathbf{k}}$, $\Psi_{\mathbf{k}'}$ are the free carrier wave functions of the initial and final states with wave vectors $\mathbf{k}$ and $\mathbf{k}'$ respectively. This part of the Auger amplitude describes the energy transfer of the excess energy to the free carriers. The amplitude M_{Ex} which corresponds to the lower part of the Feynman diagram (Fig. 3)

$$M_{\mathrm{Ex}} = \int V(\mathbf{r})\Psi_h^*(\mathbf{r})\Psi_e(\mathbf{r}) d\mathbf{r},$$

$$V(\mathbf{r}) = \int \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \Psi_{f'}^*(\mathbf{r}')\Psi_f(\mathbf{r}') d\mathbf{r}', \tag{4}$$

describes the Auger recombination of the electron and hole bound to the Er–O complex and excitation of the Er f-electron from the ground level f to the exited level f' [16]; Ψ_h, Ψ_e are the wave functions of the hole and electron bound to the Er–O complex; $\Psi_{f'}$, Ψ_f are the wave functions of the Er f-electrons. Since the characteristic value of the f-shell radius $r' \approx r_f \approx 0.08\,\mathrm{nm}$ is much smaller than the radius of the electron and hole motion the multipolar expansion for $V(\mathbf{r})$ can be used:

$$V(\mathbf{r}) = \frac{e d_{ff'}}{r^2} P_1(\cos\theta) + \frac{e Q_{ff'}}{r^3} P_2(\cos\theta), \tag{5}$$

where P_1 are Legendre polynomials, $d_{ff'}$ and $Q_{ff'}$ are the dipole and quadrupole Er matrix elements. The zero term of the expansion $\propto 1/r$ does not contribute to the Eq. (5) due to orthogonality of the Er wave functions $\Psi_{f'}$, Ψ_f. Since the $f-f'$ optical transition is forbidden the dipole matrix element is small $d_{ff'}/er_f \approx 10^{-3}$ while $Q_{ff'}/er_f^2 \approx 1$ [16]. So the quadrupole transitions turns out to be more effective in the Auger excitation processes [12,16] and we will consider below only the second term in Eq. (5).

We use the effective mass approximation to calculate the Auger amplitudes (3), (4). Thus, the wave functions of the electron and hole states we write as a composition of distinct components corresponding to the different energy bands $\Psi_{e,h} = \sum\limits_i \Psi_i^{(e,h)} u_i$, where u_i are the Bloch functions of the i-band and $\Psi_i^{(e,h)}$ are the envelope wave functions obtained by solution of the corresponding eigen value problem for the electron and hole states localized on the Er–O complex, described in the previous section. The silicon conduction band is the nearest to the electron level and might have the largest wave function component for the electron state. But as it was shown [3] the overlapping integral of the valence and conduction band Bloch functions gives zero contribution to M_{Ex}. Thus the main contribution to the amplitude M_{Ex} provides the overlapping of the valence components of the electron ($\Psi_\nu^{(e)}$) and hole ($\Psi_\nu^{(h)}$) functions, namely the light hole component. This components can be easily written down if we again use the assumption concerning the mixing of the conduction and valence band states in the Er–O complex according to the Kane model. The details of such calculations have been described in our previous work [12]. Here we present the final result:

$$M_{\mathrm{Ex}} = 6 \cdot 10^{-2} Q_{ff'}/er_f^2\ \mathrm{meV}. \tag{6}$$

Note that in our estimations we put $Q_{ff'}/er_f^2 \approx 1$. The main contribution to the Auger matrix element M_{Ex} (6) is given by the area of the bulk semiconductor close to the Er–O complex.

The estimation for the amplitude M_A can be obtained taking into account that characteristic value of the bound electron coordinates is $r \approx R$ while the radius vector for free carriers in silicon is $r' \approx \lambdabar = 1/k' > R$ and also that $\Psi_e \approx R^{-3/2}$, $\Psi_{\mathbf{k}} \approx 1$. We have the following estimation:

$$M_A = \frac{e^2}{\lambdabar} \lambdabar^3. \tag{7}$$

According to the Fermi golden rule the probability of the Auger processes for n-Si is given by

$$W = \frac{2\pi}{\hbar} \int |M|^2 f_e(k) \times \delta\left(\frac{\hbar^2\mathbf{k}'^2}{2m_c} - \frac{\hbar^2\mathbf{k}^2}{2m_c} - \Delta E\right) \frac{d\mathbf{k}}{(2\pi)^3} \frac{d\mathbf{k}'}{(2\pi)^3}, \tag{8}$$

where $f_e(k)$ is the free electron distribution function. After integration over $\mathbf{k}'$ and $\mathbf{k}$ and substituting Eq. (2), (6), (7) for the Auger amplitude we obtain

$$W \approx \frac{|M_{\mathrm{Ex}}|^2 e^4 m_c}{\pi\hbar^3 \Delta E^2} (n_e \lambdabar^3). \tag{9}$$

Here $\lambdabar = \hbar/\sqrt{2m_c\Delta E}$ is the wavelength of the outgoing electron, n_c is the electron concentration. Thus the rate of this Auger process is concentration dependent. Expression (9) is proportional to the number of electrons in the reaction area $(n_e \lambdabar^3)$. According to Eq. (9) the Auger pumping time is $\tau_{\mathrm{Ex}} = 1/W \approx 10^{12} n_e^{-1}$.

In the p-type semiconductor the energy excess is transferred to the free hole. In this case we obtained the results described by Eq. (9) with changing n_e by n_h and m_c by m_{hh}. The factor $(n\lambdabar^3)$ is the same for heavy and light holes. So the energy excess is transferred mostly to the heavy holes. Thus in the both cases the efficiency of Auger pumping is determined by the concentration n of the major carriers. If $n \geqslant 10^{18}$ the time of the Auger recombination turns out to be small enough ($\tau_A \leqslant 10^{-6}\,\mathrm{s}$) to excite the major part of the Er ions in the Er–O complex.

The photoluminescence intensity is determined by the two pairs of forward and reverse processes: Auger excitation of the Er ion in the Er–O cluster and Er deexcitation; formation and dissociation of the exciton localized on the Er–O complex [19]. The time scale of the first two processes is much larger than of the last two. This fact allows to separate their influence on the photoluminescence intensity I_{PL}. Indeed, the photoluminescence intensity I_{PL} in the steady state far from saturation can be written as [13]

$$I_{\text{PL}} = \frac{1}{\tau_{\text{rad}}} N^*_{\text{Er}} = \frac{\tau}{\tau_{\text{rad}}\tau_{\text{Ex}}} N_{\text{Ex}}, \tag{10}$$

where N^*_{Er} is the concentration of excited Er ions, τ_{rad} is the radiative lifetime of the excitation, $\tau_{\text{Ex}} = 1/W$ is the time of Auger excitation of Er ion described by Eq. (9), τ is the deexcitation time and N_{Ex} is the concentration of excitons localized on the Er–O clusters. N_{Ex} is determined by the processes of formation and dissociation of bound excitons [13]:

$$N_{\text{Ex}} = \frac{N_{\text{Er-O}}}{1 + \sigma_e \nu_e n_c e^{E_e/kT}/\sigma_p \nu_p G \tau_c}, \tag{11}$$

where $N_{\text{Er-O}}$ is the concentration of Er–O clusters, $\sigma_{e,h}$ are the cross sections of the electron and hole capture by the Er–O cluster, $\nu_{e,h}$ are the electron and hole thermal velocities, n_c is the effective density of states in the bottom of the conduction band, G is the optical generation rate of electron–hole pairs and τ_c is the carrier lifetime. The dissociation of the bound exciton is connected with the thermal activation of the captured electron back to the conduction band of silicon. Thus the number of bound excitons N_{Ex} has the strong temperature dependence (11), which leads to the trivial temperature quenching of photoluminescence.

The deexcitation of the Er ions was comprehensively studied in the recent work by F. Priolo et al. [18]. It was shown that the main contribution to the deexcitation of the Er ions at temperatures above 15 K is given by the Auger processes with participation of free carriers. Thus the deexcitation time has the same strong carrier concentration dependence $\tau = 4.4 \cdot 10^{-13}/n$ [18] as the excitation time τ_{Ex} — see Eq. (9). Therefore the resulting photoluminescence intensity I_{PL} (10) should have much more weak dependence upon the concentration of the free carriers than the times of Auger processes. Note that Eq. (10) obviously valid in the case of electroluminescence under forward bias when excitation of Er ion also occurs via the recombination of the bound exciton described here.

Impact excitation

In the case of electroluminescence under reverse bias when there are enough hot electrons in silicon with energies above 0.8 eV the impact excitation of the Er ions takes place. The impact excitation occurs through the quadrupole interaction between the silicon hot electrons and f-shell electrons of Er [12,16]. The matrix element of this interaction is

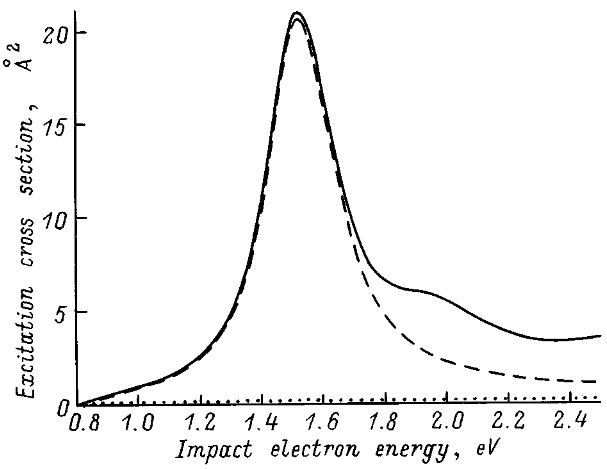

Figure 4. The impact excitation cross section $\sigma(E)$ of Er as a function of the incident electron energy (solid line), the partial cross section for angular momenta of the incident and outgoing electron of unity $\sigma_{1\to1}$ (dash line), the excitation cross section σ_0 of an isolated Er atom (dot line).

$$M_{fLm,fL'm'}(E) = \sqrt{\frac{4\pi}{5}} Q^{2m'-m}_{ff'} \times \int \frac{e}{r^3} \Psi^*_{L'm'}(\mathbf{r}) \Psi_{Lm}(\mathbf{r}) Y_{2m'-m}(\mathbf{n}) d\mathbf{r}. \tag{12}$$

Here e is the electron charge, $Q^{2m'-m}_{ff'}$ is the quadrupole matrix elements between the ground ${}^4I_{13/2}$ and first excited ${}^4I_{15/2}$ states of the Er f-shell, $\Psi_{Lm}(\mathbf{r})$ and $\Psi_{L'm'}(\mathbf{r})$ are the wave functions of the incident and outgoing silicon electrons, E, L, m and E', L', m' are the energy, angular momentum and its projection of the incident and outgoing electrons respectively. The energy of the outgoing electron E' after excitation of Er is smaller than E by the excitation energy $\Delta_{ff'} = 0.8$ eV: $E' = E - \Delta_{ff'}$. The wave functions of the silicon electrons were obtained as the solution of the Schrodinger equation with the electron effective mass and the cluster potential described above.

The impact excitation cross section for the given energy of the incident electron we can calculate using the matrix elements (12) summarizing over all possible angular momenta of the initial and final electron states:

$$\sigma(E) = \frac{\pi}{4\sqrt{E^3 E'}} \sum_{LmL'm'ff'} |M_{fLm,f'L'm'}(E)|^2. \tag{13}$$

Here m is the average effective mass in the silicon conduction band. Fig. 4 shows the energy dependence of the impact excitation cross section. The strong maximum on the $\sigma(E)$ dependence at $E = E_1 + \Delta_{ff'} \approx 1.6$ eV is due to the resonance excitation of Er by the silicon electrons with angular momentum $L = 1$ accompanied by the electron capture into the Er–O cluster resonance state with energy $E_1 = 0.8$ eV and angular momentum $L = 1$ [19]. The partial

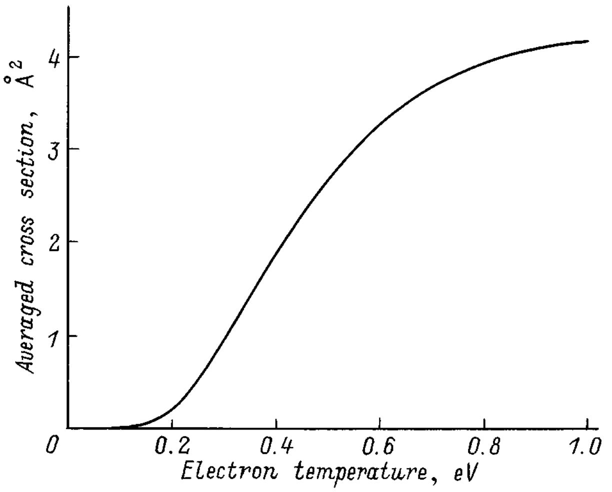

Figure 5. The averaged impact excitation cross section σ as a function of the electron temperature T_e.

cross section $\sigma_{1\to 1}$ of this process is shown by dash line. It is clearly seen that this process dominates in the Er excitation below energy 1.7 eV. The maxima in $\sigma(E)$ dependence at higher energies are connented with the resonance states with the higher agular momenta $L > 1$. For comparison we plot by dot line the excitation cross section σ_0 for isolated Er atoms. In the resonance region the impact cross section $\sigma(E)$ of Er in the cluster exceeds the cross section σ_0 of an isolate Er atom by to two orders of magnitude.

Note that in the electroluminescence experiments on Er-doped Si diodes only small part of the hot electrons fall into the resonance region. So one should average $\sigma(E)$ over the energy distribution of the hot electrons in order to obtain the experimentally observed cross section σ. Assuming the energy distribution function to be Maxwellian with the electron temperature T_e we get the following expression for the excitation cross section:

$$\sigma = \frac{1}{T_e^2} \int\limits_{\Delta_{ff'}}^{\infty} \sigma(E)\, e^{-E/T_e} E dE. \tag{14}$$

In Fig. 5 we plot the averaged impact excitation cross section σ as a function of the electron temperature T_e. The actual value of the electron temperature in the experiments [20,21] is estimated as 0.65 eV. The corresponding value of the excitation cross section (14) is $\sigma = 3.5\,\text{Å}^2$, which is quite close to the experimental value $\sigma \approx 4\,\text{Å}^2$ [20,21].

Conclusion

The model of excitation of the Er-related emission in silicon codoped with erbium and oxygen is proposed. This model allows a deeper insight into the energy transfer processes in photoluminescence and electroluminescence occuring from the carriers of the semiconductor host toward the Er^{3+} ions in Er–O clusters. In both cases the discrete and quasi-discrete electron levels localized on the Er–O cluster play the main role.

In the case of photoluminescence and electroluminescence under forward bias, when there are not enough hot carriers in silicon the excitation of Er f-shell electrons occurs via the Auger recombination of the exciton bound on the Er–O cluster. In the present paper the concrete scheme of this process is proposed where the excess energy is transferred to the free carriers. The excitation rate as well as the rate of the reverse process of energy backtransfer are proportional to the concentration of the free carriers in silicon. It results in the rather weak dependence of the luminescence intensity on the carrier concentration.

In the case of electroluminescence under reverse bias the suggested mechanism of the Er impact excitation in Si : Er, O explains the role of O in the enhancement of the Er-doped silicon diode electroluminescence. The proposed mechanism is based on the presence of the resonance levels with non-zero angular momentum formed by the quantum well potential of the Er–O cluster. The resonance scattering of the hot electrons on these quasi-discrete levels enhanced the impact excitation cross section.

Of course the model used by us is rather rough and simple but it reproduces quite well the main features of the excitation processes and explain the high efficiency of Er luminescence in Si : Er, O.

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Mechanisms of excitation of the $f-f$ emission in silicon codoped with erbium and oxygen

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Abstract The Er_2O_3 cluster in silicon is discussed as a possible source of the Er-related emission in Si : Er, O. We propose a mechanism that gives a simple explanation of the high efficiency of Er atom excitation in Er–O clusters. Both the cases of photoluminescence and electroluminescence are considered. In the case of photoluminescence the Er excitation high efficiency is connected with the electron state localized on the Er–O cluster. The excitation of f-shell electrons in Er atoms occurs via the Auger recombination of the exciton bound on the Er–O cluster. We calculate the rate of this Auger process and discuss the dependence of the photoluminescence intensity upon the carrier concentration. In the case of electroluminescence under reverse bias the impact excitation cross section is enhanced due to resonance scattering of the hot electrons on the quasi-discrete levels formed by the Er–O cluster quantum-well potential. The calculated impact excitation cross section is close to the experimental value.

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