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The photoluminescence mechanism of erbium in silicon: intensity dependence on excitation power and temperature

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Abstract

The photoluminescence intensity of erbium in silicon was measured as a function of laser excitation power and temperature. Results of these measurements are described on the basis of a physical model which includes the formation of free excitons, the binding of excitons to erbium ions, excitation of 4f-shell electrons of erbium ions and decay of excited erbium ions by light emission. An Auger energy transfer to free carriers by both erbium-bound excitons and excited erbium ions must be included in the model in order to obtain a quantitative agreement with experiment. From the temperature dependence two activation energies are derived, which are associated with the binding of excitons to erbium centers and with an energy transfer process from excited erbium ions back to erbium-bound excitons, respectively. The luminescence properties of the different types of Er-doped crystalline silicon are remarkably similar.

Keywords: Silicon; Erbium; Photonics; Photoluminescence

1. Introduction

The luminescence of erbium in silicon has triggered considerable research activity in recent years. From a fundamental point of view, the chain of processes through which the energy imparted to s and p electrons of the host crystal is transferred to the final step of light emission in the $^4I_{13/2}$ to $^4I_{15/2}$ transitions of 4f inner-shell electrons is a challenging topic. The particular emission wavelength of 1.54 μm, as a wide-band carrier for long-distance signal transport via glass fibers, stimulated application-oriented research. In particular, the efficiency of the light generation and its dependence on temperature are important topics.

In the present experiments, the photoluminescence (PL) from erbium in silicon was measured in crystalline float-zoned and Czochralski-grown samples and in a sample grown by a sublimation MBE method. The characteristic luminescence spectra, in the wavelength range between 1.5 and 1.6 μm, were observed. The different line structures of the spectra, which reflect the crystal-field effect, revealed the presence of optically active centers of different symmetry and/or atomic structure, in individual samples. The dependence of the photoluminescence intensity on Ar^+ laser excitation power and on the temperature was measured and analyzed on the basis of the excitonic luminescence model with the aim of achieving quantitative agreement.

2. Experimental

In the experiments three different kinds of samples were used. The first sample was prepared from

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Czochralski-grown silicon by erbium and oxygen implantation (Cz-Si:Er,O), followed by annealing for 30 min at the temperature of 900°C. The peak Er concentration was $10^{17}\,cm^{-3}$. The second sample was prepared from float-zoned silicon implanted with Er (Fz-Si:Er) at an elevated temperature of 500°C to a peak concentration of $4\times10^{17}\,cm^{-3}$. No co-implants were done and no further heat treatment was applied. The third sample was a crystalline silicon layer of 2 μm thickness, which was grown by a sublimation MBE method at 500°C on top of a p-type silicon wafer, followed by annealing at 700°C for 30 min (MBE-Si:Er). The sample had an Er concentration of $10^{18}\,cm^{-3}$.

Luminescence was excited by the 514.5 nm line of an Ar^+-ion laser. The laser power could be varied in the range of 1 μW to 10 mW and was focused on a spot of about 1 mm diameter measured in front of the sample dewar. The temperature of samples was measured by a RhFe metallic resistor in a four-point-probe configuration to an accuracy of 0.1 K. Temperature measurements were performed in the range of 4–200 K. The PL signal was detected by a Ge-detector cooled by liquid nitrogen.

3. Model and discussion

3.1. Excitonic luminescence model

In the model the overall process of energy transfer in the Er-doped Si is considered. The process starts with the formation of electron–hole pairs by the incident light, at the rate G, followed by free-exciton creation with the rate $\gamma_x n^2$. Free excitons can be bound at erbium-related traps, which will occur proportional to their concentration n_{Er} and the available unoccupied fraction $[(n_{Er}-n_{xb})/n_{Er}]$, where n_{xb} denotes the concentration of excitons trapped at Er-related centers. Er-bound excitons can transfer their energies in an Auger process with a transfer time τ^* to the 4f electrons of a Er ion in the ground state, i.e., proportional to fraction $[(n_{Er}-n^*_{Er})/n_{Er}]$. Finally, the Er PL follows from decay of the excited Er ions with a temperature-stable radiative decay time τ_d: $I\propto n^*_{Er}/\tau_d$. Competing recombination paths included in the model are the alternative electron–hole recombinations with the rate γn^2, the direct recombination of free excitons or their recombination via alternative centers with the lifetime τ_x and the thermally induced dissociation of Er-bound excitons into free excitons. Apart from these, two Auger processes, which remove energy from the PL path, should be accounted for in the competition paths. They are related to Er-bound excitons and excited Er ions and dissipate energy to free electrons in the conduction band. Based on the above description the following balance equations can be written for free electrons (n), free excitons (n_x), Er-bound excitons (n_{xb}) and excited Er ions (n^*_{Er}), respectively:

$$G+fn_x=\gamma n^2+\gamma_x n^2, \tag{1}$$

$$\gamma_x n^2+cf_{xb}n_{xb}N_x=cn_x n_{Er}\frac{n_{Er}-n_{xb}}{n_{Er}}+fn_x+\frac{n_x}{\tau_x}, \tag{2}$$

$$cn_x n_{Er}\frac{n_{Er}-n_{xb}}{n_{Er}}+n^*_{Er}f_1\frac{1}{\tau^*}=n_{xb}\frac{n_{Er}-n^*_{Er}}{n_{Er}}\frac{1}{\tau^*}+cf_{xb}n_{xb}N_x+c_{Ax}nn_{xb} \tag{3}$$

and

$$n_{xb}\frac{n_{Er}-n^*_{Er}}{n_{Er}}\frac{1}{\tau^*}=\frac{n^*_{Er}}{\tau_d}+n^*_{Er}f_1\frac{1}{\tau^*}+c_{AEr}nn^*_{Er}, \tag{4}$$

where $f=\gamma_x(N_cN_v/N_x)e^{-E_x/kT}$, $f_{xb}=e^{-E_{xb}/kT}$ and $f_1=e^{-E_A/kT}$; E_x, E_{xb} and E_A are the binding energy of electron and hole in a free exciton, the exciton binding energy on the Er-related trap and the energy dissipated in the creation of an excited Er ion from the bound exciton situation, respectively. N_c, N_v and N_x are temperature-dependent densities of states in conduction, valence and exciton bands, respectively. Similar set of rate equations, but without Auger processes, has been developed earlier [1].

3.2. Excitation power dependence

The power dependence of the PL intensity was measured at low temperature. In this case, we can simplify the equations by putting $f=f_{xb}=f_1=0$. Solving Eqs. (1)–(4), an approximate solution for n^*_{Er}/n_{Er} is derived as

$$n^*_{Er}/n_{Er}=c_2G/(b_0+b_1G^{1/2}+b_2G+b_3G^{3/2}), \tag{5}$$

where b_0, b_1, b_2, b_3 and c_2 are temperature-independent factors. In the high-power limit this result yields $n^*_{Er}\sim 1/G^{1/2}$ or $n^*_{Er}\sim 1/n$ resulting in a decrease of PL intensity. This decrease of Er PL has not been observed in the present experiments, nor has it been reported in the literature. A numerical estimate [2] shows that such an effect corresponds to a high value of G, about $10^{26}\,cm^{-3}\,s^{-1}$, which is not reached in actual experiments. For this reason, under the usual experimental conditions linear increase at low power with $(c_2/b_0)G$ is observed, followed by saturation at the level c_2/b_2. Using the normalized units for power $P\equiv G/G_1$ with $G_1=b_0/b_2$ and for PL intensity $I\equiv(n^*_{Er}/n_{Er})/(c_2/b_2)$, Eq. (5), for the case of strong Auger processes, will read

$$I=\frac{P}{1+\beta\sqrt{P}+P} \tag{6}$$

with

$$\beta=\left(\frac{c_{AEr}\tau_d}{c_{Ax}\tau^*}\right)^{1/2}+\left(\frac{c_{Ax}\tau^*}{c_{AEr}\tau_d}\right)^{1/2}. \tag{7}$$

The PL has linear increase at low power with $I = P$ and saturates at high power at $I = 1$. Therefore, characteristic features of the luminescence process are only revealed at intermediate power, e.g. at $P = 1$, where $I = 1/(2 + \beta)$. In Fig. 1 theoretical curves for $\beta = 0$ and 2 are presented. The experimentally obtained power dependence of the PL intensity of sample Cz-Si:Er,O is plotted in the inset. The solid line is the best fit to the data with Eq. (6), yielding $\beta = 2.25$. Similar fits made for samples Fz-Si:Er and MBE-Si:Er gave $\beta = 2.63$ and 3.3, respectively. With Eq. (7) this result is converted to $(c_{AEr}\tau_d/c_{Ax}\tau^*)^{\pm 1} \approx 4$ for implantation samples and ≈ 9 for the MBE sample. This can be compared with the published data for $c_{AEr} = 10^{-12}\,\mathrm{cm^3\,s^{-1}}$, $\tau_d = 10^{-3}\,\mathrm{s}$, $c_{Ax} = 10^{-10}\,\mathrm{cm^3\,s^{-1}}$ and $\tau^* = 4 \times 10^{-6}\,\mathrm{s}$ [3]. One concludes that $c_{AEr}\tau_d/c_{Ax}\tau^*$ is very similar in the three kinds of investigated material. Although this can be due to an accidental combination of parameters, one is tempted to believe that all process parameters, i.e., c_{AEr}, τ_d, c_{Ax} and τ^*, have similar, material-independent values. In such a case the differences in structure of the luminescent centers in the three materials, as evidenced by their PL spectra, have very little influence on the efficiency of the Er PL process.

3.3. Temperature dependence

For an analysis of the Er PL temperature dependence, the set of Eqs. (1)–(4) is considered in its complete form. The solution of n^*_{Er}/n_{Er} is obtained also in the form of Eq. (5), but in this case the coefficients are temperature dependent as they include the state densities in conduction, valence and exciton bands and the functions f, f_{xb} and f_1. At low temperatures, Eq. (5) will give the solution $(n^*_{Er}/n_{Er})_{T=0}$. For the practical purpose of comparing model predictions with experimental results it is useful to express measured intensities normalized to the low-temperature value, i.e., $(n^*_{Er})_T/(n^*_{Er})_{T=0}$. After some approximations one can obtain a final solution

$$(n^*_{Er})_T/(n^*_{Er})_{T=0} = 1/[1 + AN_x\tau^* e^{-E_{xb}/kT} + BN_x\tau_d e^{-(E_{xb}+E_A)/kT}]. \quad (8)$$

Eq. (8) can be rewritten as

$$[(n^*_{Er})_{T=0}/(n^*_{Er})_T - 1]/T^{3/2} = N_x/T^{3/2}[A\tau^* e^{-E_{xb}/kT} + B\tau_d e^{-(E_{xb}+E_A)/kT}] \quad (9)$$

with $A \approx B$. Note that the binding energy of an electron–hole pair in a free exciton E_x does not appear in the solution. The ratio between the two pre-exponential factors is about equal to τ_d/τ^*. Fig. 2 represents experimental data for the sample Cz-Si:Er,O with the solid line as the best fit to Eq. (8). Two activation energies, which are necessary to fit the measured data, are represented in the inset by two straight lines. Results for the three samples measured at an intermediate power are given in Table 1. Fits are performed using a $T^{3/2}$ term in the pre-exponential factors. In the literature, however, analyses with temperature-independent pre-exponential factors prevail. The first activation energy is identified as the binding energy E_{xb} of an exciton at the Er-related trap. At temperatures above 100 K a second energy of about 110 meV becomes significant. At high temperatures the PL intensity has already decreased; this energy therefore cannot be determined with high accuracy. An error limit of at least 10 meV has to be accepted. Following our analysis, this energy corresponds to $E_{xb} + E_A$, leading to the experimental result $E_A \approx 100$ meV. By the physical model E_A is given as $E_A = E_g - E_x - E_{xb} - E_{PL} - E_d$. With estimates for silicon band gap energy $E_g =$

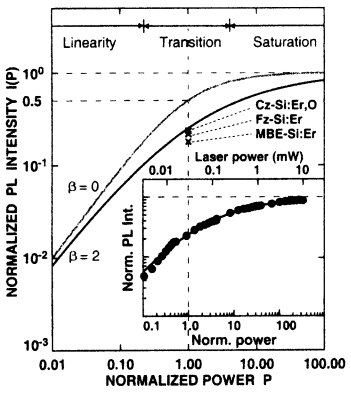

Fig. 1. Normalized luminescence intensity I as a function of normalized laser power P with $\beta = 0$ and 2. The experimental data points (×) at $P = 1$ are given for three samples. The inset shows the Er PL intensity versus excitation power with the solid line as the best fit to Eq. (6) for sample Cz-Si:Er,O.

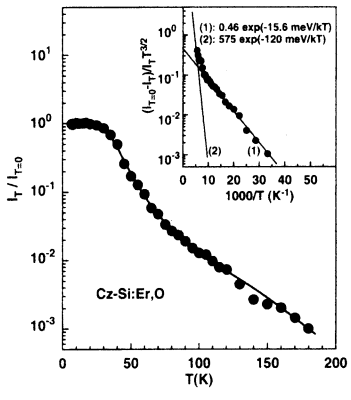

Fig. 2. PL intensity as a function of sample temperature normalized to the yield at low temperature. The solid line is the fit with Eq. (8). The inset plots $(I_{T=0} - I_T)/I_T T^{3/2}$ as a function of reciprocal temperature illustrating the analysis based on Eq. (9) for sample Cz-Si:Er,O.

Table 1
Activation energies and their corresponding pre-exponential factors following from the fits with Eq. (9) for the investigated samples. Notation $A_1 = A\tau^* N_x T^{3/2}$ and $B_1 = B\tau_d N_x T^{3/2}$ is used

Sample	A_1 ($K^{-3/2}$)	E_{xb} (meV)	B_1 ($K^{-3/2}$)	$E_{xb} + E_A$ (meV)
Cz-Si:Er,O	0.46	15.6	575	120
Fz-Si:Er	0.04	12.2	32	92
MBE-Si:Er	0.006	3.6	370	123

1170 meV, electron–hole binding energy $E_x = 15$ meV, exciton binding energy to Er center $E_{xb} = 15$ meV, PL energy $E_{PL} = 800$ meV, a donor ionization energy of $E_d = 240$ meV is required. This is close to the level position at 266 meV as reported in Ref. [4] for the same Fz-Si sample as used in this experiment. The order of magnitude between two pre-exponential factors estimated as $\tau_d/\tau^* \approx 10^3$ is in agreement with time constants found experimentally. The small E_{xb} in the MBE-Si:Er sample and the much larger τ_d/τ^* value may be related to a much larger Er concentration in this material.

4. Conclusion

The dependence of Er PL intensity on excitation power and temperature has been measured and analyzed by a physical model. A satisfactory agreement could be obtained by the consistent use of normalized units for both PL intensity and excitation power. The thermal dependence is governed by the binding energy of excitons to Er centers in the temperature range below 100 K. At higher temperatures, an activation energy about 100 meV becomes more prominent. This energy is associated with the energy back-transfer from an excited Er into an Er-bound exciton. The physical properties are similar for all Er-doped crystalline samples and are consistent with numerical data published in the literature.

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