Optical properties of isoelectronic centers in crystalline silicon
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Chapter 7

Optical Properties of the Er-1 Center: A Candidate for Realization of Optical Gain in Si:Er

In Chapters 5 and 6 we have investigated microscopic structure of the Er-1 center formed in Si/Si:Er nanolayers grown by a modified SMBE technique. In this Chapter we examine specific optical properties of this center in order to evaluate its potential for photonic applications. In particular, we determine its effective excitation cross section and estimate the percentage of Er dopants involved in formation of Er-1.

7.1 Introduction

While crystalline silicon continues to dominate the mainstream integrated circuit device manufacturing, applications of this most important semiconductor material remain electronic rather than photonic. Due to the relatively small and indirect bandgap, silicon is a poor light emitter. Although various approaches to silicon photonics, such as quantum confinement in nanostructures [71] and inhomogeneous Si-based media [110], or optical doping with rare-earth ions [70,111], have been actively explored, lasing action still has not been demonstrated, and reports on optical gain [112] and intense room temperature emission [113] from Si structures remain controversial. In Chapters 5 and 6, we have confirmed preferential production of a single type of an optically active Er-related center in silicon [95,114,115]. High concentration of a specific center (labeled Er-1) was found in Er-doped Si
nanolayers grown by sublimation MBE. We have also established the ultra-small linewidth characteristic of emission related to the Er-1 center which indicates a possibility of a $10^3 - 10^4$ increase of the expected gain coefficient, when compared to the implanted Si:Er materials used so far. Therefore the Er-1 center emerges as a plausible candidate for achieving population inversion and stimulated emission in Si based materials: a long sought after goal of semiconductor science and technology.

The research on optical properties of silicon continues to be spurred by prospects of a full integration of electronic and photonic components (also on-chip) and by almost unlimited possibilities of the highly developed silicon technology. While an efficient band-to-band recombination is not possible, crystalline silicon shows some typical features of optical materials, such as afterglow and optical memory [116,117], and has properties that are potentially very attractive for optical applications. The most prominent of these is the possibility to suppress nonradiative recombinations, offered by a superior level of impurity control.

Quantum confinement effect can influence the energy band structure. In deed, following this approach optical gain in nanocrystalline silicon [112] and efficient room-temperature (RT) emission from boron inclusions were reported [113]. An alternative approach to improve the photonic properties of silicon is offered by optical doping, i.e. by introduction of efficient radiative recombination centers. Rare-earth ions are especially suited for optical doping as their (core) structure is well screened from external influence. Erbium has become the optical dopant of choice, in view of the fact that its emission wavelength of $\sim 1.5 \mu m$ is suitable for telecommunication applications.

In the past decade Si:Er has been intensively investigated for emission optimization [72]. The research revealed several disadvantages of this system, which could not be fully eliminated: a strong emission reduction at higher temperatures, and a low percentage of optically active Er-related centers. Thermal quenching is absent for photoluminescence (PL) of Er ions embedded in a SiO$_2$ matrix, but this system, in turn, is characterized by a very small cross section of (direct) excitation. In view of that, a nonhomogeneous medium of Si nanocrystals (nc-Si) dispersed in a SiO$_2$ matrix is recently investigated as an alternative host for Er doping. In this case, the large bandgap of SiO$_2$ provides thermal stability for the Er emission, while Si nanocrystals facilitate efficient excitation. Following this approach, development of RT-operating LED's was proven to be possible. However, recent results indicate that population inversion might be difficult to reach in this system [118,119].

In view of a low optical activity of Er ions in Si, a high concentration in range of $10^{19} - 10^{20} \text{ cm}^{-3}$ is necessary. Such high impurity levels exceed by far the
solubility limits, and can only be realized by nonequilibrium methods. For that purpose implantation [70, 71] and MBE [120] are commonly used. The currently obtained quantum efficiencies of RT photo- and electroluminescence from Si:Er are rather low — typically $10^{-5} - 10^{-4}$.

Finally, we note that although the Si:Er system exhibits a long excited state lifetime, due to the forbidden character of the intra-4f-electron shell transitions, population inversion and laser action have not been achieved in crystalline Si:Er (while optical amplifiers based on Er-doped insulators are routinely manufactured). Realization of lasing action would provide a major boost for optoelectronic applications of Si. In order to achieve gain, the absorption by Er$^{3+}$ ions should be maximized and losses minimized. The latter include absorption of the 1.5 $\mu$m radiation in the host and nonradiative recombinations of excited Er$^{3+}$ ions. For reliable gain estimation, the value of the absorption cross section $\sigma$ at 1.5 $\mu$m for Er$^{3+}$ ions embedded in Si substrate is necessary. This is not known and has to be derived from the linewidth $\Delta E$ and decay time $\tau$ of the 1.5 $\mu$m Er-related emission band. For the presently used implanted Si:Er materials these are typically $\Delta E \approx 5$ meV and $\tau \approx 1$ ms. Using these values and assuming that the $\tau \approx 1$ ms time constant represents the purely radiative lifetime, the Er$^{3+}$ ion excitation cross section can be estimated as $\sigma \approx 2.5 \times 10^{-19}$ cm$^2$. In order to calculate the gain $\alpha$, the excitation cross section has to be multiplied by the available concentration of excited Er$^{3+}$ ions:

$$\alpha_{\lambda=1.5\mu m} = \sigma_{\lambda=1.5\mu m} N(Er^{3+}).$$  \hspace{1cm} (7.1)

Assuming a typical concentration of Er$^{3+}$ ions in the implanted layer to be $N(Er^{3+}) \approx 10^{20}$ cm$^{-3}$ and taking into account that usually only 1% of them is optically active, we obtain the gain coefficient of $\alpha \approx 0.25$ cm$^{-1}$. On the other hand, losses due to free-carrier absorption at 1.5 $\mu$m, non-radiative recombination of Er$^{3+}$ ions (Auger effect, upconversion, etc.), are usually estimated as at least 1 cm$^{-1}$. Therefore realization of a Si laser based on Er doping is usually considered unlikely.

Recently a new type of Si:Er optical structures has been proposed [79]. The idea follows from a notion that since the most efficient low temperature excitation mechanism of Er proceeds via excitons, the generation conditions for excitons should be optimized. The requirements of a high Er$^{3+}$ ions concentration and efficient exciton generation cannot be met simultaneously. Therefore for heavily Er-doped layers excitons are generated in the substrate rather than in the layer itself. This is evidenced by the fact that PL intensity does not increase above certain thickness of a Si:Er layer. It does increase, however, when a "spacer" of undoped Si is inserted into the Si:Er layer. Therefore, a sandwich structure of interchanged Si/Si:Er nanolayers exhibits superior optical properties. Upon illumination with
a laser beam, excitons generated in spacer regions diffuse into doped layers and provide excitation of Er\textsuperscript{3+} ions. Such an "spatially-separated" excitation scheme is in its concept somewhat similar to that utilized in the earlier mentioned inhomogeneous \text{SiO}_2/\text{nc-Si:Er} samples, where processes of photon absorption (\text{nc-Si}) and emission (Er\textsuperscript{3+} ions in the \text{SiO}_2 matrix) also take place in different parts of the sample. In addition to the more efficient exciton formation, spatial separation reduces Auger quenching by free carriers generated during the excitation process.

![PL spectra measured at 4.2 K for (a) sample of Si:Er and (b) SiO\textsubscript{2}:Er under excitation wavelength $\lambda_{\text{exc}}=520$ nm. The inset shows a PLE spectrum SiO\textsubscript{2}:Er sample — see text for details.]

In Chapters 5 and 6, we have conclusively showed that Er-related 1.5 $\mu$m emission in such structures is dominated by a single center, the Er-1 center, which is characterized by a homogeneous and ultranarrow bandwidth of $\Delta E < 10 \mu$eV. In this Chapter we investigate potential of the multilayer structures for realization of optical amplification. To this end, we attempt to measure excitation cross section and percentage of Er dopants participating in the optically active centers.

### 7.2 Experimental details

The experiments were performed on two samples: Er-doped silicon grown by sublimation MBE (Si:Er - #51) and Er-doped silica (SiO\textsubscript{2}:Er). The sample #51 has
been investigated in Chapter 6 and comprises 400 interchanged Si and Si:Er layers of a few nanometers thickness stacked along the <100> growth direction. The total Er density is found to be $2 \times 10^{14}$ cm$^{-2}$. The SiO$_2$:Er sample has been prepared by a triple Er-implantation: $1.5 \times 10^{14}$ cm$^{-2}$ at 200 keV; $2.8 \times 10^{14}$ cm$^{-2}$ at 500 keV and $5.6 \times 10^{14}$ cm$^{-2}$ at 1000 keV and followed by 30 min. at 1000 °C annealing in nitrogen. The total Er implantation dose was then $9.9 \times 10^{14}$ cm$^{-2}$.

For comparison, data obtained for an implanted sample (labeled J900) have been also included in the study. This sample has been prepared by Er (energy 320 keV, dose $3 \times 10^{12}$ cm$^{-2}$) and O (energy 40 keV, dose $3 \times 10^{13}$ cm$^{-2}$) implantations followed by 900 °C/30 min. anneal in nitrogen.

The PL experiments were carried out in a variable temperature continuous-flow cryostat accessing the 1.5 – 300 K range (Oxford Instruments Optistat CF). The samples were excited using a cw argon-ion laser operating at 514.5 nm or a tunable Optical Parametric Oscillator (OPO) laser. producing pulses of 5 ns duration at 20 Hz repetition rate. The luminescence was resolved with a 1 m F/8 monochromator (Jobin-Yvon THR-1000) equipped with a 900 grooves/mm grating blazed at 1.5 μm and detected by an infrared photomultiplier with a 35 μs response time. Figure 7.1 shows the PL spectra of the Si:Er (#51) and SiO$_2$:Er samples in the 1.5 μm range at 4.2 K under excitation with OPO set to a wavelength of $\lambda_{exc} = 520$ nm. In this excitation wavelength, the SiO$_2$:Er sample was excited resonantly corresponding to the $^4I_{15/2} \rightarrow ^2H_{11/2}$ transition. The inset shows a photoluminescence excitation (PLE) measurement for SiO$_2$:Er sample obtained by scanning the OPO wavelength.

### 7.3 Results and discussion

For determination of the excitation cross section, the excitation power dependence of the PL intensity was measured at 4.2 K - see Fig. 7.2. for all four major components of Er-1 center: line $L_1^1$ (6502.85 cm$^{-1}$) - trace a; $L_2^1$ (6443.72 cm$^{-1}$) - trace b; $L_2^2$ (6433.59 cm$^{-1}$) - trace c and $L_3^2$ (6393.17 cm$^{-1}$) - trace d, under cw argon-ion laser excitation - see Chapter 6 for line labelling. All the measurements were performed with the same experimental settings, so that the PL intensity scale is common for all the data points. As can be seen, the behavior of these lines is similar. Results were fitted by a formula [72] [121]:

$$I_{PL} = \frac{A\sigma\tau\Phi}{1 + \beta\sqrt{\sigma\tau\Phi} + \sigma\tau\Phi},$$

(7.2)

where $\beta$ is an adjustable parameter representing the physical elements of the luminescence process, $\sigma$ is an effective excitation cross section of Er$^{3+}$ ion, $\tau$ is the
effective lifetime of erbium in the excited state and $\Phi$ is the flux of photons. The appearance of the $\beta \sqrt{\sigma \tau \Phi}$ term is a fingerprint of the Auger effect hindering the luminescent process [72] [121]. The solid curves are best fits to the experimental data using Eq. 7.2 with parameter $\beta = 1.9 \pm 0.1$. In that way, the excitation cross section parameters of Er-1 center are determined as: $\sigma(\lambda_{exc} = 514.5 \text{ nm}) = 4.9 \times 10^{-15}$, $5.7 \times 10^{-15}$, $8.5 \times 10^{-15}$ and $5.9 \times 10^{-15}$ cm$^2$ for line $L_1$, $L_2$, $L_3$ and $L_4$, respectively. With the experimental error of $\Delta \sigma = \pm 2 \times 10^{-15}$ cm$^2$, the excitation cross sections are identical for all the emission lines. This is consistent with the results of Chapter 6 where we have showed that these lines originate from the same Er-related center.

We have also examined decay characteristics of the $L_1$, $L_2$ and $L_3$ lines at 4.2 K under OPO excitation with a wavelength of $\lambda_{exc} = 520 \text{ nm}$ and $\Phi = 3 \times 10^{22} \text{ cm}^{-2}\text{s}^{-1}$. Figure 7.3 shows that under these conditions the decay kinetics is composed of a fast and a slow component. Fitting two exponentials to the measured profiles, we obtained $1/e$ decay times of $\tau_F = 150 \mu\text{s}$ and $\tau_S = 900 \mu\text{s}$ contributing to the signal for all the four lines. The intensity ratio of the fast and the slow component is found to be 1:1, the same for all the lines.

Presence of two components in decay kinetics could indicate the presence of two different centers [122]. To examine this possibility we separated PL spectra for the fast and the slow components by integrating the signal over time windows.
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Figure 7.3: PL decay at 4.2 K for lines $L_1$, $L_2$ and $L_3$ under $\lambda_{exc} = 520$ nm of pulse laser and $\Phi = 3 \times 10^{22}$ cm$^{-2}$s$^{-1}$. The inset shows the power dependence of these lines with pulse laser.

t $\in [0, 100 \mu s]$ for the fast and $t \in [100 \mu s, 4 \text{ ms}]$ for the slow component. The spectra are found to be identical, regardless of the different decay time constants. Taking into account the very small linewidth of the investigated PL lines, we conclude that a possibility of a co-existence of two different Er-related centers is not consistent with our findings. The PL intensity of these prominent emission lines as a function of excitation density up to $3 \times 10^{23}$ cm$^{-2}$s$^{-1}$ is shown in the inset of the Fig. 7.3. By looking at the decay kinetics at different excitation densities, we find that the intensity ratio of the fast to the slow component increases with the laser power. While this issue is still under investigation, this suggests that two different de-excitation processes take place for the same center. The slow component is likely to represent the radiative decay time of Er ion in silicon which is generally assumed to be around 1 ms. The fast component could be induced by an Auger process with free carriers generated by the excitation pulse.

To obtain quantitative information from the pulsed laser measurements, we use the following rate equation, involving the carrier density $n$, the density of exciton $n_{ex}$, and the concentration of excited Er center $N_{Er}^*$:

\[
\frac{dN_{Er}^*}{dt} = \sigma \Phi (N_{Er}^* - N_{Er}^*) - N_{Er}^* \frac{1}{\tau}, \quad (7.3a) \\
\sigma = \alpha \ c_A \ \tau_{ex}, \quad (7.3b)
\]
\( N_{Er}^{ex} \) is the total concentration of excitable \( \text{Er}^{3+} \) ions present in the sample, \( \alpha \) is the absorption coefficient of silicon, \( c_A \) is the capture coefficient of free excitons by erbium-related centers with erbium excitation, \( \tau_x \) and \( \tau \) are the effective lifetime of exciton and \( \text{Er}^{3+} \) in the excited state. The exciton lifetime, \( \tau_x \), is controlled mainly by nonradiative Auger processes associated with presence of Er-related donors or other impurities. We assume that the binding of free carriers into free excitons dominates at low temperatures (for more details see Appendices). The decay time \( \tau \) corresponds to an effective lifetime of \( \text{Er}^{3+} \) ions in the excited state due to both radiative and nonradiative recombinations:

\[
\frac{1}{\tau} = \frac{1}{\tau_{rad}} + c_{A,Er} \mu.
\]  (7.4)

where \( \tau_{rad} \) is the decay time of excited Er centers by radiative transitions and \( c_{A,Er} \) is the coefficient of the Auger process of nonradiative recombination of excited \( \text{Er}^{3+} \) ions. Eq. [7.3a] concerns concentration of excited Er centers with two possible de-excitation paths: radiative emission with spontaneous emission time \( \tau_{rad} \) and Auger quenching process which is proportional to the density of free carriers. In the present experiment, the duration of the OPO pulse (\( \Delta t = 5 \) ns) is much shorter than the characteristic lifetime \( \tau \) of \( \text{Er}^{3+} \) in the excited state (\( \Delta t \ll \tau \)). We assume that recombination does not take place during illumination, and the population \( N_{Er}^{ex} \) reaches the level of:

\[
N_{Er}^{ex}(t = \Delta t) = N_{Er}^{ex}[1 - exp(-\sigma \Phi \Delta t)].
\]  (7.5)

For low excitation density, when \( \sigma \Phi \Delta t \ll 1 \), this formula gives a linear dependence on flux: \( N_{Er}^{ex} = \sigma \Phi \Delta t \). When \( \sigma \Phi \Delta t \gg 1 \), the saturation regime can be obtained: \( N_{Er}^{ex} = N_{Er}^{ex} \). Since in the experiment the PL signal is integrated in time, and the PL intensity is proportional to \( N_{Er}^{ex}/\tau_{rad} \), the result of the experiment is given by \( N_{Er}^{ex}/\tau_{rad} \). By fitting all the data for \( L_1 \), \( L_2 \) and \( L_3 \) in the inset of Fig. 7.3 with Eq. 7.5 we obtain the excitation cross section of \( \text{Er}^{3+} \) ions for all these emission lines as \( \sigma = (6 \pm 2) \times 10^{-15} \text{ cm}^2 \) of the Er-1 center. This value is in a good agreement with that obtained for cw laser measurements - Fig. 7.2, and close to previous reports for Er-implanted silicon [123]. While physical interpretation of this experimentally determined “effective” excitation cross section is cumbersome, this suggests that, in general, the Er-1 center could have a similar excitation mechanism to that of other Er-related optically active centers in Si, e.g. in samples prepared by ion implantation.

Figure 7.4 shows the dependence of PL intensity at \( \lambda = 1.538 \mu \text{m} \) (\( L_1 \)) as a function of excitation density for photon flux up to \( 3 \times 10^5 \) at \( \lambda_{exc} = 520.855, 1035 \) nm. For \( \lambda_{exc} = 520 \) nm the PL intensity increases rapidly with the flux of photons.
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Figure 7.4: PL intensity at $\lambda = 1.538 \mu m$ ($L_1^3$) as function of the pulsed excitation density for three difference excitation wavelength $\lambda_{exc} = 520, 855$ and 1035 nm

reaches a maximum, and then quenches for a still higher flux of photons. For $\lambda_{exc} = 855$ nm excitation, the PL intensity goes up to a saturation level. The saturation level in this case is lower than for $\lambda_{exc} = 520$ nm excitation, and roughly equal to its level reduced at the high photon flux. For the $\lambda_{exc} = 1035$ nm, the PL intensity slowly increases with the flux of photons to the saturation level equal to the maximum found for $\lambda_{exc} = 520$ nm. By fitting the latter curve with Eq. 7.5, we find the excitation cross section for Er ion at $\lambda_{exc} = 1035$ nm as $\sigma = (5 \pm 1) \times 10^{-17}$ cm$^2$. In this case, the excitation cross section is lower by two orders of magnitude than the value at $\lambda_{exc} = 520$ nm. This can be fully accounted for by the fact that the excitation of erbium ions proceeds via Si lattice whose absorption coefficient decreases sharply at longer wavelengths.

In Fig. 7.5a the decay characteristic of the PL intensity at $\lambda = 1.538 \mu m$ (line $L_1^3$) for $\lambda_{exc} = 520$ nm is shown for selected values of photon flux: $\Phi = 3 \times 10^{22}, 6 \times 10^{22}, 4.5 \times 10^{23}$ and $3 \times 10^{25}$ cm$^{-2}$s$^{-1}$. The ratios of PL intensity of fast and slow components increase with the flux of photons and are determined, respectively, as (1:1), (1.3:1), (1.5:1), (2.2:1). At higher flux of photons the fast component is prominent. This is consistent with a clear quenching PL intensity shown in Fig. 7.4 at high flux values and, again, points to a possible Auger process with free carriers which could become significant at high excitation density, as its origin.
For the $\lambda_{\text{exc}} = 855$ nm excitation, the saturation level is not identical to that for $\lambda_{\text{exc}} = 520$ nm. At this wavelength, the penetration depth is of the same order as the thickness of the optically active layer and larger than the penetration depth of $\lambda_{\text{exc}} = 520$ nm excitation. This could promote the Auger process: with a high concentration of carriers in the optically active layer, the Auger process is more probable. In case of $\lambda_{\text{exc}} = 1035$ nm excitation wavelength, the penetration depth considerably exceeds the thickness of the optically active layer: less carriers are generated in the optically active region and so PL intensity increases slowly with the flux of photons. This scenario is also consistent with the results shown in Fig. 7.5b: the ratio of the fast and the slow components at $\lambda_{\text{exc}} = 855$ nm excitation is higher than at $\lambda_{\text{exc}} = 1035$ nm. We note that the decay kinetics of $\lambda_{\text{exc}} = 520$ nm excitation at maximum intensity is identical to that observed for $\lambda_{\text{exc}} = 1035$ nm at maximum flux of photons.

An estimate of the number of emitting centers can be made by comparing the PL intensity of Si:Er Sample #51 with that of the SiO$_2$:Er sample measured under the same conditions. Figure 7.6 shows the dependence of PL intensity at $\lambda = 1.538$ $\mu$m as a function of excitation density for $\lambda_{\text{exc}} = 520$ nm. From the measurements, we conclude that the intensity of emission from SiO$_2$:Er sample shows a linear dependence over the whole investigated flux range. In this case, the integrated PL intensity is proportional to $N^*_{\text{Er}}(\tau/\tau_{\text{rad}}) = \sigma \Phi N^\text{ex}_{\text{Er(SiO}_2):\text{Er}} \Delta t(\tau/\tau_{\text{rad}})$. For the SiO$_2$:Er system the values of all the parameters are known: $\sigma_{\text{SiO}_2:Er} = 2 \times 10^{-20}$
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Figure 7.6: PL intensity at \( \lambda = 1.538 \mu m \) (\( L_1 \)) as function of the pulsed excitation density for Si:Er and SiO\(_2\):Er samples under excitation wavelength \( \lambda_{exc} = 520 \text{ nm} \). The right hand scale shows the density of Er\(^{3+}\) ions in the excited state in SiO\(_2\):Er sample.

In order to compare emission from the two investigated samples we note that the ratio of time integrated PL intensities is given by:

\[
\frac{I_{Si:Er}}{I_{SiO_2:Er}} = \frac{\eta_{out}^{Si}}{\eta_{out}^{SiO_2}} \frac{N_{Er}^{*} \times (\tau_1/\tau_{rad})}{N_{Er(SiO_2:Er)}^{*} \times (\tau_2/\tau_{rad})},
\]

where \( \tau_1, \tau_{rad} \), \( N_{Er(SiO_2:Er)}^{*} \), \( \eta_{out}^{Si}, \eta_{out}^{SiO_2} \) correspond to the effective and radiative decay times, density of excited Er\(^{3+}\) ions, and the fraction of emitted photons that are collected in the apparatus (extraction efficiency), respectively, for Si:Er and SiO\(_2\):Er sample. \( a \) indicates photon loss due to surface reflection: the Si surface reflection loss reduces the absorbed power by about 70% while reflection loss for SiO\(_2\) can be neglected. The ratio of the extraction loss can be calculated from the refractive indexes of Si and SiO\(_2\):

\[
\frac{\eta_{out}^{Si}}{\eta_{out}^{SiO_2}} = \left( \frac{1}{4} \times \frac{\mu_{out}^{Si}}{n_1^2} \right) / \left( \frac{1}{4} \times \frac{\mu_{out}^{SiO_2}}{n_2^2} \right) \simeq 0.175,
\]

\( n_1 \) and \( n_2 \) are the refractive indexes of Si and SiO\(_2\), respectively.
Figure 7.7: PL intensity at $\lambda = 1.538 \, \mu m$ ($L_1^1$) as function of the pulsed excitation density for sample #51 and sample J900 under cw argon laser $\lambda_{exc} = 514.5 \, nm$.

where $n_1$, $n_2$ are the reflective indexes of 3.49 and 1.46 at 1.5 $\mu m$ emission for Si and SiO$_2$, respectively.

For Si, the Er$^{3+}$ excited state population should be corrected due to nonradiative contribution to the effective lifetime. If we assume the slow component in the decay kinetic to represent radiative recombination, the correction of the integrated PL intensities is given by:

$$
\frac{I_{\text{Si:Er}}}{I_{\text{total}}} = \frac{A_F \tau_F + A_S \tau_S}{(A_F + A_S)\tau_S} = \frac{A_F / A_S \tau_F + \tau_S}{(A_F / A_S + 1)\tau_S},
$$

(7.8)

where $A_{F,S}$, $\tau_{F,S}$ correspond to amplitudes and decay time of the fast and the slow components of the signal, respectively. At the saturation level, $A_F / A_S = 1.5/1$, $\tau_F = 0.15 \, ms$, $\tau_S = 0.85 \, ms$, and we get $I_{\text{Si:Er}}/I_{\text{total}} = 1/2$ and $\tau_1/\tau_1^{\text{rad}} = 1/2$. Consequently, under the same excitation conditions the excited state population in Sample #51 has to be 2 times higher in order to give PL intensity equal to that of sample SiO$_2$:Er.

Finally, the different spectral shape of the 1.5 $\mu m$ band in the two samples has to be accounted for: for the same intensity at a selected wavelength, the integrated PL from SiO$_2$:Er sample is about 3 times higher than for Sample #51. Therefore, the PL saturation observed for Si:Er sample under band to band excitation corresponds to an excited Er$^{3+}$ density of:

$$
N_{Er}^{\text{cf}} = 1.5 \times 10^{12} \times \frac{1}{0.175 \times 0.7} \times 2 \times \frac{1}{3} \approx 8.2 \times 10^{12} \, \text{cm}^{-2}.
$$

(7.9)
This implies that the percentage of the optically active Er\(^{3+}\) ions in Sample #51 is: 
\[ P(\%) = \frac{8.2 \times 10^{12}/2 \times 10^{14}}{1} = (4.1 \pm 0.8) \, (\%) \]
This value is comparable to the highest level achieved in Si:Er materials prepared by ion implantation.

To cross-check this estimation, we performed a comparative measurement using the implanted Sample J900. Fig 7.7 shows the power dependence of PL intensity for the #51 and J900 samples measured under cw argon laser excitation. As can be seen, the intensity of Sample #51 is about 25 times higher than that of sample J900. The percentage of the optically active center in this sample is:

\[ P = \frac{N_{\text{Er, J900}}^*}{N_{\text{Er, J900}}} \times \frac{(\tau_1/\tau_{1\text{rad}})}{(\tau_1/\tau_{1\text{rad}})} = \frac{1}{25} \times \frac{1}{2} \times 8.2 \times 10^{12} \times 3 \times 10^{12} \approx 5.5 \, (\%) \] 

which agrees well with an independent measurement based on absolute number of all the photons emitted from Sample J900 [125].

We therefore conclude that about 5\% of all the Er atoms present in Sample #51 are involved in optically active Er-1 centers. That implies that with an optimized sample - see data in Table 6.1, Chapter 6, the maximum percentage of optically active centers which can be realized in Si/Si:Er nanolayers can be estimated as \(\sim 32\%\). This is about an order of magnitude higher than in any other Si:Er materials.

### 7.4 Conclusions

A detailed consideration of excitation mechanisms of the erbium in crystalline silicon prepared by SMBE, the Er-1 center, is carried out under cw and pulse lasers pumping. The overall excitation cross section for Er\(^{3+}\) ions has been evaluated as 
\[ \sigma = (6 \pm 2) \times 10^{-15} \, \text{cm}^2 \]
This value is high suggesting that excitation of the Er-1 center is a very efficient process. Further, by a direct comparison with a calibrated SiO\(_2\):Er sample, we conclude that up to \(\sim 32\%\) of the total number of Er\(^{3+}\) ions present in Si/Si:Er nanolayers can attain optical activity. This represents a considerable improvement over Si:Er prepared by ion implantation and in view of the discussion presented in the introduction paragraph of this Chapter opens new hopes towards realization of optical gain in Si:Er.