Influence of p-n junction formation at a Si/Si:Er interface on low-temperature excitation of Er^{3+} ions in crystalline silicon

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(Received 26 March 2001; published 12 September 2001)

The characteristic $\lambda = 1.54$ μm emission of Er^{3+} ions implanted into a silicon wafer is excited by an Ar laser pointed at the nonimplanted side of the sample. In this experimental configuration energy has to be transferred across the bulk of the crystal, of approximately 350 μm thickness, before reaching the Er-doped layer. Effects related to the presence of a p-n junction formed by Er doping at the Si/Si:Er interface are consistently explained assuming that excitons are responsible for $4f$-electron core excitation of the Er^{3+} ions in crystalline silicon at low temperatures.

DOI: 10.1103/PhysRevB.64.132202 PACS number(s): 78.60.Fi, 78.55.Ap, 71.55.Cn

I. INTRODUCTION

The properties of erbium-doped silicon receive much attention due to the photonic potential of this material. As a result of intensive research, room-temperature electroluminescence from crystalline silicon has been reported by a number of groups.[1–3] However, intense room-temperature photoluminescence (PL) has so far been demonstrated only for amorphous silicon[4] and silicon/silicon oxide mixtures (SIPOS)[5,6] but not for crystalline silicon. Therefore, a thorough understanding of the microscopic process responsible for the energy transfer between the crystalline silicon matrix and the $4f$-electron core of Er ions is of prime importance.

While impact with hot carriers is responsible for generation of efficient electroluminescence in reverse-biased diodes,[7] localization or collisions with excitons at Er-related donor centers is a generally accepted mechanism of low-temperature photoluminescence in crystalline Si:Er.[8] The Auger process of exciton recombination with a simultaneous energy transfer to the $4f$-electron shell of the Er^{3+} ions has been modeled theoretically,[9,10] but it has not been unambiguously supported by experiment, all evidence in its favor being of an indirect nature. In this contribution we present data on exciton transport in an Er-doped Si wafer and show that it governs the Er^{3+} excitation. The evidence confirms the prominent role of excitons in the low-temperature photoluminescence mechanism of Er in Si.

In the past, it has been reported that Er PL generated by band-to-band excitation of the matrix can be observed also when the laser-beam illuminates the nonimplanted side of the wafer, i.e., typically at a distance of 350–500 μm from the Er-doped layer.[11] In the case of band-to-band absorption at low temperature in Si with low concentration of defects/doping, practically all created electron-hole pairs couple very fast into free excitons. Since energy transfer in the silicon matrix by emission and reabsorption of infrared photons is highly improbable, the observation of the backside excitation of Er PL was interpreted as evidence of exciton participation in the excitation process, and provided the main experimental support of an exciton-mediated excitation mechanism for Er in crystalline silicon.

Some time ago we have reported that Er PL generated from the nonimplanted side of a wafer appears with a considerable time delay with respect to the excitation laser pulse.[12] In the current research we investigate more closely Si:Er PL generated under conditions of backside excitation, and compare the results with those obtained under standard conditions, when the Er-related emission is obtained by illumination of the Er-implanted wafer side.

II. EXPERIMENTAL DETAILS

The experimental set-up permitted an easy change between two configurations of excitation: with the laser-beam directed either on the implanted side or on the nonimplanted side of the sample. In both cases PL was collected from the Er-implanted side. The experiments were performed in a closed-cycle cryostat in the temperature range between $T \approx 15$ K and $T = 150$ K. An on-off modulated (25 Hz) argon laser operating at $\lambda = 514.5$ nm was used as an excitation source. The emerging PL signal was monitored with a high-sensitivity germanium detector (Edinburgh Instruments).

The possibility of Er excitation from the nonimplanted side was tested for differently prepared materials. We have found that for almost all the samples PL emission could be detected in that configuration. A sample with the strongest intensity of Er PL (for excitation of the nonimplanted side) was selected for further studies. Detailed investigation was then conducted for a low-energy (300 keV, 3×10^{12} cm^{-2} dose) Er implanted oxygen-rich p-type (B-doped) Cz-Si wafer of approximately 350 μm thickness. The sample was also coimplanted with oxygen (40 keV, 3×10^{13} cm^{-2} dose) and annealed at 900 °C in a nitrogen atmosphere for 30 min.

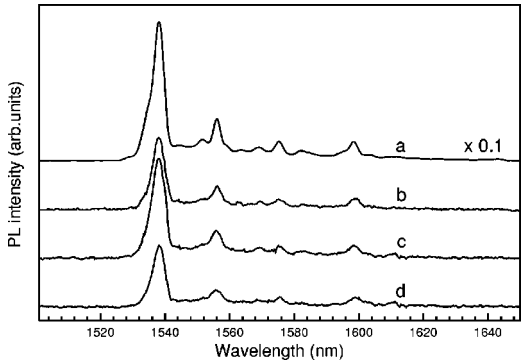

FIG. 1. PL spectra obtained for implanted (a) and nonimplanted side excitation (b,c,d): (b) without electrical bias, (c) under forward, and (d) reverse bias. Note that the intensity scale is adjusted for (a).

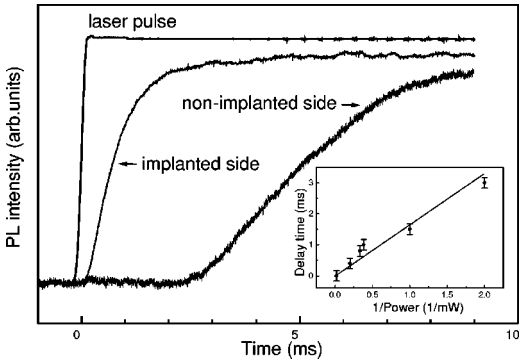

FIG. 2. Time dependence of the intensity of Er-related PL under implanted and nonimplanted side excitation. The laser pulse is also shown. In the inset, the delay time observed for the nonimplanted side excitation is plotted as a function of (inverse) laser power.

The PL spectrum of the sample was dominated by the *so-called* cubic Er center.

III. EXPERIMENTAL RESULTS

It has been frequently reported that Er implantation into crystalline silicon produces a variety of Er-related optically active centers.[13] These individual centers, which might differ by, e.g., details of their microstructure, could possess their own excitation mechanisms. Consequently, it seems plausible to imagine that the two different excitation regimes explored here could lead to activation of different Er-related centers. In order to check that possibility PL spectra obtained under implanted and nonimplanted side excitation were carefully compared. The result is depicted in Fig. 1, as can be seen both spectra differ in magnitude but are identical in their structure. We conclude therefore that the same optically active centers are excited in both experimental configurations, i.e., excitation diffusion across the bulk of the material does not influence the ''final'' excitation mechanism responsible for the energy transfer to the rare-earth ion core. We note that emission due to both free and (boron) bound excitons was also present in the observed PL spectrum.

Figure 2 compares the time development of the Er-related PL signal observed in the two experimental configurations. For reference, the laser signal is also shown. We notice that for illumination of the nonimplanted side, the PL signal appears with some delay with respect to the excitation pulse. In the experiment we have concluded that this delay is of the order of a few milliseconds, and that its actual magnitude depends on the laser power. This dependence is depicted in the inset of the figure. By extrapolation, one expects an infinite rise time of the signal at a zero power level.

IV. DISCUSSION

We will first consider the case of excitation by a green-laser pointed at the wafer side opposite to the Er-implanted layer. In that case the relevant parameters are as follows: photon energy $h\nu=2.4$ eV, absorption coefficient $\alpha=10^4\ \mathrm{cm}^{-1}$, and pumping intensity $I=3\times10^{16}\ \mathrm{cm}^{-2}\mathrm{s}^{-1}$ for 0.4 mW, and a spot diameter of 2.2 mm. At low temperatures, for such a pumping-level excitonic-recombination dominates, and practically all created electron-hole pairs transform into excitons. As a result we have an exciton source $S(x,t)$ near the surface (at $x=0$): $S(x,t)=\alpha I g(t)\exp(-\alpha x)$, where α is the absorption coefficient, and $g(t)$ describes the temporal evolution of the pump: $g(t)=1$ for $0<t\leqslant t_0$, and $g(t)=0$ for $t>t_0$, where the excitation laser is switched off at $t=t_0$. Due to a concentration gradient the excitons created near the nonimplanted surface diffuse into the bulk and toward the Er-doped layer near the opposite side of the sample. In what follows we will consider the exciton diffusion process in detail.

A. Exciton diffusion

To analyze the exciton diffusion at distance s, we should find the solution on a semi-infinite straight line to the diffusion equation with a source of excitons near $x=0$

$$\frac{\partial N_{ex}}{\partial t}=D\frac{\partial^2 N_{ex}}{\partial x^2}-\frac{N_{ex}}{\tau_{ex}}+\alpha I g(t)\exp(-\alpha x), \tag{1}$$

with boundary condition

$$\frac{\partial N_{ex}}{\partial x}=0 \quad \text{at } x=0. \tag{2}$$

Here N_{ex}, D, and τ_{ex} are the exciton concentration, diffusion coefficient, and the exciton lifetime, respectively. The solution of this problem is given by:[14]

$$N_{ex}(x,t)=\int_0^t d\tau\int_{-\infty}^{\infty}d\xi\frac{\alpha I g(\tau)}{2\sqrt{\pi D(t-\tau)}}\exp\left[-\frac{(x-\xi)^2}{4D(t-\tau)}-\alpha\left|\xi\right|-\frac{t-\tau}{\tau_{ex}}\right]. \tag{3}$$

From Eq. (3), we can get the exciton density flux $j_{ex}(x,t)=-D\partial N_{ex}/\partial x$ at the distance $x=s\gg\alpha^{-1}$ and for time $t<t_0$,

$$j_{ex}(s,t)=\frac{I}{\sqrt{\pi}}\int_0^{t/\Delta t}dz\frac{1}{z^{3/2}}\exp\left[-\left(\frac{1}{z}+\frac{s^2}{4L^2}z\right)\right]. \tag{4}$$

In Eq. (4) we introduce parameter $\Delta t = s^2/4D$ and the diffusion length of the excitons $L = \sqrt{D\tau_{ex}}$. The parameter Δt determines the diffusion-related time delay, i.e. the time necessary for an exciton to arrive at distance s due to diffusion. For $t \gg \Delta t$, the exciton density flux becomes independent of time: $j_{ex}(s,t) \rightarrow j_{ex}(s)$. From Eq. (4) at $t/\Delta t \rightarrow \infty$ (using the saddle approximation technique) we get

$$j_{ex}(s) \simeq I\sqrt{\frac{\pi}{8}}\exp(-s/L). \tag{5}$$

After switching off the pump, for $t > t_0$, the exciton density flux at $x = s \gg \alpha^{-1}$ is given by

$$j_{ex}(s,t) = \frac{I}{\sqrt{\pi}}\int_{(t-t_0)/\Delta t}^{t/\Delta t} dz\,\frac{1}{z^{3/2}}\exp\left[-\left(\frac{1}{z}+\frac{s^2}{4L^2}z\right)\right]. \tag{6}$$

For a reasonable parameter value of $D = 90\ \mathrm{cm^2 s^{-1}}$ Ref. 15, the time delay $\Delta t = s^2/4D$ due to diffusion for the distance of $s \cong 350\ \mu$m is about 3.5 μs. Although the exciton diffusion constant $D = 90\ \mathrm{cm^2 s^{-1}}$ was obtained for a high-purity material and should therefore be taken as an upper limit, we note that the experimentally measured delay (see Fig. 2) exceeds the estimated value by 3 orders of magnitude. Therefore we conclude that the exciton diffusion itself cannot lead to such a long delay, and that another explanation has to be considered. As a possible mechanism we suppose that the long delay time could be induced by destruction of the depletion region associated with a *p-n* junction that could appear in the silicon substrate due to Er doping.

B. Exciton flux across *p-n* junction

It is generally accepted[7] that erbium implantation into silicon leads to the formation of donor centers with ionization energies in the 0.1–0.25 eV range and whose concentration is comparable to that of the Er ions. The sample under investigation was prepared from *p*-type Si doped by boron with a concentration of $N_B = 10^{15}\ \mathrm{cm^{-3}}$. Since the Er concentration in the implanted layer is $\sim 10^{18}\ \mathrm{cm^{-3}}$, even if not all the Er ions form donors, a *p-n* junction should occur in equilibrium at the boundary with the Er-implanted layer. In view of the higher doping level, the width of the depletion region is controlled by boron doping, and at low temperatures is given by

$$W \cong \sqrt{\frac{\varepsilon(E_g - (E_D + E_B)/2)}{2\pi e^2 N_B}}, \tag{7}$$

where E_g is the energy gap, E_D and E_B are the binding energies of the Er-related donors and boron acceptors, respectively, e is the electron charge, and ε is the dielectric constant of silicon. The calculated depletion region of about 1 μm is situated predominantly in the *p*-type layer. In the Er-doped layer, the width of the depletion region is $W_D = W \times (N_B/N_D)$, where N_D is the Er-related donor concentration. The negative charge $(-N_B W)$ is accumulated in the depletion region of the *p*-type layer, and the same positive charge $(+N_D W_D = N_B W)$ is in the *n*-type layer. The resulting maximum electric field in the depletion region reaches approximately 10^4 V/cm. In such a high electric field the excitons are easily destroyed by tunneling enhancement due to the Poole-Frenkel effect. Thus, excitons arriving at the *p-n* junction are divided into electron-hole pairs. Subsequently holes are captured by negatively charged boron ions and electrons become localized at charged donors. Excitons will start to appear in the Er-doped layer and excite Er only after the depletion region has been removed due to charge compensation. The time δt, which is needed for the destruction of the *p-n* junction can be found from the equation:

$$\int_0^{\delta t} dt\, j_{ex}(s,t) = N_B W, \tag{8}$$

where $j_{ex}(s,t)$ is given by Eq. (4). If the diffusion process is fast we soon arrive at stationary conditions, and instead of Eq. (8), we can use the following relation for finding the delay time δt [taking into account Eq. (5)]

$$\delta t\,\frac{\sqrt{\pi}}{2\sqrt{2}}\, I\exp(-s/L) = N_B W. \tag{9}$$

We will now use the above formula to estimate the diffusion length L. With the experimentally obtained value of the delay time δt in the millisecond range, we get $L \approx 60\ \mu$m. Such a diffusion length corresponds to an exciton lifetime of $\tau_{ex} \approx 0.4\ \mu$s. In our experiment the lifetime of the free excitons is controlled by capture at neutral boron acceptors. This assumption is supported by the observation of bound-exciton luminescence for nonimplanted side excitation. In this case we have

$$\frac{1}{\tau_{ex}} = N_B \sigma_{ex} \langle v \rangle, \tag{10}$$

where $\langle v \rangle$ and σ_{ex} are the thermal velocity and capture cross section of free excitons, respectively. The calculated exciton lifetime corresponds to $\sigma_{ex} \approx 1.2 \times 10^{-15}\ \mathrm{cm^2}$, which is a reasonable value. Therefore we conclude that the presence of the *p-n* junction can lead to the observed delay time.

Also we note that from Eq. (9) we get $\delta t \propto 1/I$, which is also supported by experiment, see Fig. 2.

C. Bias effect on delay time

In order to verify the validity of the proposed mechanism and to relate the experimentally observed long onset time of the Er-PL excited in the backside configuration to exciton dissociation at a *p-n* junction, we first tried to observe the effect in a sample prepared in an identical manner but from an *n*-type silicon substrate—P-doped Cz Si [P] $\approx 10^{15}\ \mathrm{cm^{-3}}$. This turned out to be inconclusive, in view of the weaker PL considerably larger laser powers had to be used for excitation. Therefore, while no delay was observed in the experiment, we were not able to unambiguously decide whether that was caused by a reduction of the depletion region or by the increased laser power.

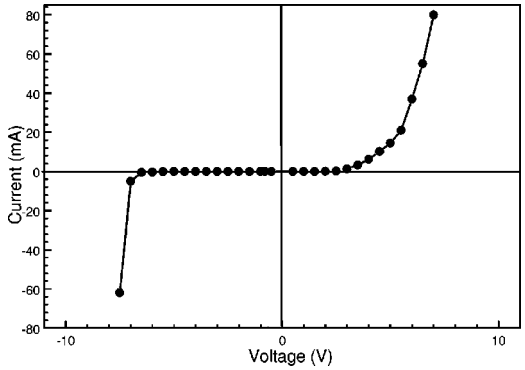

FIG. 3. Low-temperature I-V characteristics of the (p-type) sample used in the experiment.

We then returned to the p-type sample and investigated the delay time as a function of an electric-field bias applied to the sample. For that purpose contacts were made (with silver paste) on the opposing faces of the same sample that was used for the earlier-described measurements. The sample was then placed in the low-temperature experimental set-up allowing for measurements in the two illumination configurations. In addition, dc voltage from a stabilized power supply could now be applied, providing electric field across the thickness of the sample. Prior to the PL experiment we measured the low-temperature I-V characteristics of the sample. The result depicted in Fig. 3 confirms that Er implantation into a p-type silicon substrate results in p-n junction formation. We then proceeded to investigate the PL-signal delay time in the backside illumination configuration and under the applied bias. While the Er-related PL spectrum did not change, see Fig. 1, the kinetics of the signal were clearly influenced by the bias. This is illustrated in Fig. 4 where the PL kinetics measured under electric bias is shown. As can be seen, the PL-onset delay time observed, as before, with low excitation density can now be changed with the voltage applied to the junction. Under conditions of reverse bias the delay time can be increased as the depletion region increases; the delay time can be brought down to zero under forward bias. Following our interpretation, the applied forward bias reduces the depletion region to a level where excitons diffusing towards the Er-implanted layer are no longer destroyed.

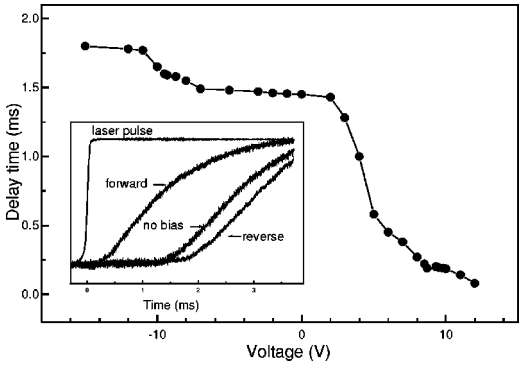

FIG. 4. Delay time of the Er PL observed for nonimplanted side excitation as a function of electrical bias. In the inset, time dependence of the PL signal under electrical-bias conditions is shown.

These findings are in full agreement with the mechanism of exciton dissociation at the p-n junction, as proposed in the preceding section.

V. CONCLUSIONS

We have analyzed the influence of a p-n junction created by Er implantation at a Si/Si:Er interface on the PL kinetics of the Er^{3+} ions. We have shown that dissociation of excitons by the electric-field potential at the junction can explain the delayed onset of Er PL, when excited from the nonimplanted side of the silicon wafer. The particular value of this delay can be tuned by application of a bias voltage to the p-n junction. The current findings confirm that excitons are responsible for the $^4I_{15/2} \rightarrow {}^4I_{13/2}$ excitation of Er^{3+} ions in crystalline silicon at low temperatures.

ACKNOWLEDGMENTS

This work was supported by grants from NATO (Linkage), NWO, ERO, and the Russian Foundation of Basic Research. Si:Er material used in the study was kindly provided by Professor W. Jantsch of Linz University, Austria. Collaboration of Dr. O.B. Gusev of A.F. Ioffe Physico-technical Institute during his stay at the Van der Waals–Zeeman Institute is appreciated.

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