

Erbium Related Centres in Silicon

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The intra-4f transition of Er as a dopant in Si at 1.54 μm is investigated in view of possible applications for optical data communication. In order to clarify the widely discussed influence of codoping with light elements on the efficiency, we investigate Si implanted with Er by means of high-resolution photoluminescence. We find at least 5 different, optically active Er centres whose abundance depends strongly on the annealing procedure. DLTS investigations show some electrical activity due to Er and defect complexes which are stable up to annealing temperatures of 900 C.

1. Introduction

The 4f shell of rare earth elements is well shielded by the outer shell electrons. Therefore these elements exhibit sharp and almost atom-like spectra when incorporated as dopants in semiconductors and insulators. The emitted wavelengths practically coincide with those observed for isolated atoms and depend only little on the host material. The host crystal and other nearby defects manifest themselves in weak crystal field effects causing rather small line splittings which become visible only because of the exceedingly narrow lines if high resolution spectroscopy is available.

Erbium implanted into Si thus produces rich spectra of sharp lines in photo- (PL) and also in electroluminescence in a narrow spectral region close to 1.54 μm . This wavelength stimulates interest in Si:Er as a candidate for light emitting devices for fibre-optic communication systems and also for on-chip and inter-chip optical data transfer. Attempts to increase the rather low yield led to the discovery of a strong influence of codoping with light elements by Michel *et al.* [1].

In order to shed light onto the underlying mechanisms, we have investigated high resolution PL and deep level transient spectroscopy (DLTS) of Er-implanted Czochralski (CZ)- and float-zone (FZ) silicon subjected to different implantation and annealing conditions [2]. From the influence of temperature, excitation power and preparation conditions, we are able to sort most of the observed lines into groups corresponding to five different centres, whose symmetry was investigated by comparison of their line patterns to crystal field theory [2], [3].

2. Photoluminescence Investigations

Studies of the Si:Er system reported so far have been directed towards obtaining a higher luminescence yield and therefore they have concentrated mostly on CZ grown material since the latter was shown to exhibit one or two orders of magnitude higher PL yield. In particular, because of the much lower PL yield of Er implanted into FZ Si, no systematic comparison of the kind of emitting Er centres has been done so far, possibly also since Fourier spectroscopy, which allows high resolution also at low intensity, has not been invoked in this problem. Therefore the higher PL yield was attributed to oxygen-related complexes since the oxygen concentration is much higher in CZ material.

For an explanation, a complex of Er with 6 oxygen atoms as nearest neighbours was postulated with lower than cubic symmetry [4]. The lower symmetry was held responsible for a breaking of selection rules which, in turn, should increase the transition rate (in the free Er atom, the transition is parity forbidden). In our first investigations we were not able to substantiate these conclusions as we will show in the following.

Fig. 1 shows a comparison of PL spectra obtained at 4.2 K on an FZ sample (a) and on two CZ samples (b and c) implanted with different dose and energy. The arrows denoted with „C“ in Fig. 1a indicate a quintet of PL lines which can be attributed to an Er centre with cubic surrounding. This type of spectra is also observed in Er-implanted CZ-Si after annealing at 900°C for 30 min, especially for implantation with higher dose and higher energy.

In Fig. 1b, the PL spectrum of a CZ sample implanted, annealed and measured under the same conditions as the sample of Fig. 1a is given. The same quintet due to the cubic centre is still visible at comparable intensity (arrows marked C. The main line is not indicated since it overlaps with another more intense line in such samples). The dominant emission in Fig. 1b originates, however, from a centre with close to axial symmetry. The seven PL lines (out of eight expected, the eighth one is outside the spectral range of our Ge detector) due to this centre are indicated by dashed lines. High resolution spectra show, that there are actually two such centres with almost identical crystal field. These do not occur in FZ material and therefore we attribute them to oxygen related Erbium complexes and denote them as O1 and O2.

In Fig. 1c, PL spectra are shown of a CZ sample implanted at higher energy (2 MeV) with a dose of $3 \cdot 10^{13} \text{ cm}^{-2}$ which gives a peak Er concentration of about 10^{18} cm^{-3} . Like the other samples, it was also annealed at 900 °C for 30 min. Here the cubic centre emission is 500 times stronger. The lines due to O1 and O2 (their positions are indicated in Fig. 2) are still visible but an order of magnitude less intense than the cubic ones.

With increasing Er dose, additional low symmetry centres appear in the PL of both FZ and CZ material, inhomogeneously broadened in the latter though, because of additional modifications of the impurity surrounding. Here we can distinguish at least 3 different types of centres, which are independent of the oxygen content of the sample and thus we attribute them to low symmetry complexes with other defects („D-lines“).

Increasing the Er concentration from $3\text{-}7 \cdot 10^{17} \text{ cm}^{-3}$ at an implantation energy of 320 keV, the cubic centre PL first increases and shows a maximum around $5 \cdot 10^{17} \text{ cm}^{-3}$, whereas the oxygen related centres, which occur only in CZ-Si decrease already in intensity at lower concentration relative to the C and D lines (Fig. 2).

The decrease in the yield of the C-line might be interpreted in terms of an increased number of radiation defects competing in the carrier recombination. On the other hand, Er precipitate formation might be also inferred, although for the latter a higher onset of $2 \cdot 10^{18} \text{ cm}^{-3}$ was given by Eaglesham [5]. A maximum yield due to the cubic centre at a very close concentration of $4 \cdot 10^{17} \text{ cm}^{-3}$ was reported also for 5 MeV implantations which should give higher damage [5]. We conclude thus in agreement with our DLTS results (see below) that the residual damage after annealing cannot account for the decreasing yield and precipitations occur already at somewhat lower concentration. The observed drastic increase in the c-yield at higher implantation energy (higher than expected from the total number of Er in the sample, see Figs. 1b and c) is rather due to the higher implantation depth of 500 nm at 2 MeV as compared to 100 nm for 320 keV. In the latter case, obviously surface recombination plays an important role.

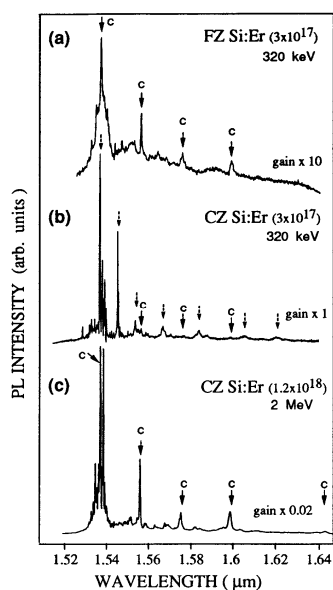


Fig. 1: Photoluminescence spectra of Er-implanted FZ-Si (a) and two CZ-Si samples. The implantation energies and the maximum Er concentrations are indicated together with gain factors

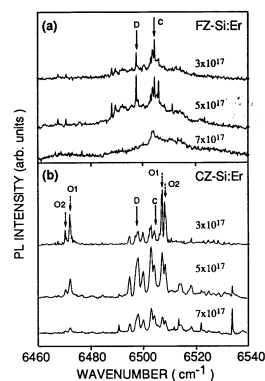


Fig. 2: Photo luminescence of FZ- and CZ-Si:Er implanted at 320 keV with different doses. All samples were annealed at 900 $^{\circ}\text{C}$ for 30 min.

In samples annealed at lower temperature (600 $^{\circ}\text{C}$) two additional types of low symmetry defects, D1 and D2, occur. Their intensities increase after nitrogen- or oxygen co-implantation. We attribute these two types of centres to complexes of Er and implantation induced defects. Their PL yield is lower than that of the O1 and O2 centres. At 4.2 K, the PL intensities of the C centre are comparable to those of the O1 and O2 centres, respectively, but with increasing temperature, they fade away much earlier whereas the C-centre PL can be seen up to 300K. We conclude thus, that under the preparation conditions investigated, the optically most effective Er centre in Si is the isolated interstitial Er but not the oxygen complex postulated earlier. The beneficial role of codoping can be understood rather in terms of the energy transfer mechanism and passivation of implantation induced recombination centres. This conclusion is supported by the observation of almost the same life time for all centres under investigation, only that of the cubic centre is somewhat shorter at low temperature.

3. Investigations by DLTS

In order to gain insight into the influence of annealing conditions, substrate material and the electrical behaviour of Er implanted in silicon we investigate also the doping and defect properties by capacitance-voltage (C-V) profiling and deep-level transient spectroscopy (DLTS). C-V profiling revealed donor behaviour of some fraction of the incorporated Er. The increase in donor concentration is only about 3 % of the implanted Er (for FZ n-type Si). The details of the donor formation are not yet understood.

DLTS measurements (Fig. 3) show that Er implantation introduces both radiation defects and Er-related defects. Radiation defects which are observed after bombardment with any ion species have deep levels at $E_c - 0.17$ eV (O-V pair), $E_c - 0.21$ eV (divacancy) and $E_c - 0.41$ eV (divacancy and P-V pair). These defects anneal out in the

temperature range up to 500 °C. A set of deep level defects is observed after annealing at 600 - 900 °C ($E_c - 0.18, 0.26, 0.32, 0.35, 0.48, 0.59$ and 0.78 eV). All these levels are related to the implanted Er. The profiles of most of them obtained from measurements in the double correlation technique (DDLTS) coincide with the Er implantation profile calculated with the TRIM code. The concentrations of these levels increase in general first with the annealing temperature up to 700 - 800 °C and decrease strongly at higher annealing temperatures. At 900 °C only three levels are observed ($E_c - 0.59$ eV, $E_c - 0.78$ eV and $E_c - 0.15$ eV) with rather low concentrations (about 0.1% of the implanted Er dose). The majority of the Er-related defects has to be annealed out to obtain high photoluminescence efficiency which is highest after annealing at 900°C. Whether the remaining levels show a correlation with photoluminescence is under investigation. The answer to this question might give an indication to the energy transfer mechanism in Er doped silicon which might be the key point in the understanding of the increased efficiency of codoped material. First indications for that were found in the PL rise time which differs significantly for different centres.

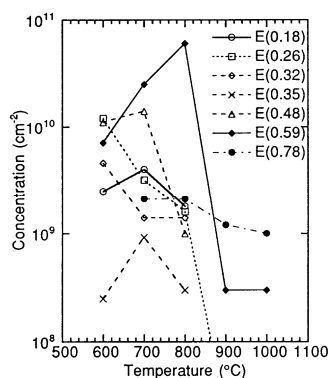


Fig. 3: Concentration of Er implantation induced defect states derived from DLTS spectra of Si:Er (implantation energy: 320 keV, dose: 10^{12} cm⁻²) as a function of the annealing temperature.

Acknowledgements

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