Influence of Er and O concentrations on the microstructure and luminescence of Si:Er/O LEDs

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Abstract. Erbium(Er)/Oxygen(O) doped Silicon (Si) layers grown by molecular beam epitaxy (MBE), can be used for fabricating Si-based light emitting diodes. The electroluminescence intensity from these layers depends sensitively on the formation of specific types of Er/O precipitates inside the Si host. We have performed a detailed microstructure analysis of MBE-grown Er/O doped Si layers using electron microscopy and combined it with secondary ion mass spectrometry (SIMS) measurements as well as electroluminescence studies. Two types of microstructures are observed in different samples with specific Er and O concentrations and grown using Er and Si co-evaporation in O ambient. The first type of microstructure consists of planar precipitates along (311) planes mostly initiated at the onset of the growth of the Si:Er/O layer. The second characteristic type of microstructure observed contain round precipitates of Er/O. Using analytical microscopy techniques it was revealed that the round precipitates contain a higher ratio of Er to O as compared to the planar precipitates of the first type. The planar precipitates normally result in structures with high electroluminescence intensity while the structures with round precipitates have low intensity.

1. Introduction

Due to mature processing technology and low cost, silicon (Si) is the dominant material of electronic industry. As a result of the increasing communication demands there is a continuous decrease of geometrical dimensions of electronic devices, which imply limitations on inter- and intra-chip interconnects [1]. A possible solution for that is to take advantage of optical communication for faster and larger amount of data transfer, which certainly would benefit from a fully Si based efficient light emitter. Being an indirect bandgap semiconductor, Si is unfortunately not a very efficient optical material. However there have been several approaches to try to solve this problem including the efforts to achieve a direct bandgap transition in Si by alloying with other direct bandgap semiconductors [2, 3] and searching for possibilities to dope Si with some optically active dopants [4, 5, 6]. The rare earth element erbium (Er) is a very promising optical dopant which can give 1.54 $\mu$m wavelength radiation from the 4f shell of Er$^{3+}$ ions in a transition from the first excited state $^4I_{13/2}$ to the ground state $^4I_{15/2}$, when doped in Si [7, 8].
Co-doping of Er doped single crystal Si layers with O has been used to fabricate light emitting diodes (LEDs) for a long time, with O playing important roles in enhancing the Er incorporation limit in Si and increasing the electroluminescence (EL) intensity of these devices [9, 10, 11].

In this paper we present the characterization of the microstructure of Si:Er/O LEDs for optimization of the Er and O concentrations with respect to the EL intensity of these devices. This study consists of work related to the growth of Si:Er/O layers, device processing to fabricate LEDs, optical characterization, concentration measurements, and microstructure analysis.

2. Experimental details

The technique used to grow all the samples included in this report was ultra high vacuum Molecular Beam Epitaxy (MBE) using a VG manufactured V80 MBE system. This system is equipped with e-gun evaporators for deposition of Si and germanium (Ge) and thermal effusion cells for Boron (B), antimony (Sb) and Er dopants. For all LED structures the growth was performed on p-doped Si(100) substrates with B concentration of about $1 \times 10^{15}$ cm$^{-3}$.

Initially, after the in-situ thermal cleaning of a 3 inch Si(100) substrate wafer, a 70 nm thick p$^+$-buffer layer followed by a 130 nm p$^+$-Si$_{0.8}$Ge$_{0.2}$ layer was grown. After that, a 30 nm layer of intrinsic Si was grown before the 150 nm thick active layer of Er/O doped Si. At the end a 250 nm thick n$^+$-Si layer was grown for having a good ohmic contact, see figure 1(a). The importance of each layer is clearly understandable from the energy band diagram of figure 1(b), which is a simulated plot obtained using the program “Simwin32” for a Si:Er/O LED under reverse bias of 5 V and an estimated n-doping level of $7 \times 10^{17}$ cm$^{-3}$ for the Er/O doped layer.

![Figure 1](image.png)

Figure 1: (a) The layer structure of the Si:Er/O LEDs and (b) Energy band diagram of a Si:Er/O PIN diode under reverse bias of 5 V.

The energy band diagram of these devices is engineered in such a way that on the p-side the edge of the narrower bandgap of the p$^+$-Si$_{0.8}$Ge$_{0.2}$ lies at the top of the potential barrier, providing the shortest distance for tunneling, as is seen in the band diagram of figure 1(b). This narrow part of the bandgap is further reduced under reverse bias by the Franz-Keldysh effect. These tunneled electrons then get accelerated in the 30 nm intrinsic region due to the reverse field and eventually excite the Er$^{3+}$-ions via the well-known hot electron excitation mechanism. Hence the operating region for these devices is the tunneling breakdown regime.

To determine the composition of grown layers we have performed secondary ion mass spectrometry (SIMS). For measurements of the Er concentration a primary beam of O$_2^+$ was used and for determining the O concentration Cs$^+$ ions were used as the primary beam. The structural characterization studies were performed using cross-section transmission electron microscopy (TEM), which was done using an analytical FEI Tecnai G$^2$ UT 200 kV FEG (Field-effect Electron Gun).
microscope, equipped with an energy-dispersive x-ray (EDX) spectrometer for chemical analysis. The grown wafers were cut into 2×2 cm\(^2\) pieces for device fabrication. The LED devices were fabricated as 600×600 \(\mu\)m\(^2\) mesa structures using photolithography, RIE, and metallization steps.

### 3. Results and discussion

Detailed structural analysis of Si:Er/O structures revealed two different precipitate types depending on the Er and O concentrations. Layers with Er/O \(<< 1\) contain planar precipitates mostly along (311) planes and for Er/O \(\geq 1\) round type of precipitates are observed. As examples, two representative microstructures are presented in figure 2, which demonstrates Z-contrast scanning transmission electron microscopy (STEM) micrographs of two Si:Er/O LED device structures with different Er and O concentrations. The micrograph of figure 2 (a) clearly shows lines of contrast along (311) planes in the Er/O doped layer, whereas the micrograph of figure 2 (b) evidently shows very small round precipitates. We believe that the planar precipitates along (311) planes are formed as a consequence of an O-induced growth disturbance starting at the interface to the Si:Er/O layer, which leads to the formation of (311) facets. The Er atoms are preferentially attached to these (311) facets to form the Er and O planar precipitates and eventually these faceted trenches are overgrown in a later growth stage. The role of O in causing faceted growth is also confirmed by growing Si layers doped only with O and performing TEM and atomic force microscopy (AFM) studies, which clearly revealed the presence of lines of contrast along (311) and rectangular faceted trenches in TEM and AFM respectively.

![Figure 2: Z-contrast 130×130 nm\(^2\) STEM micrographs of Si:Er/O LEDs exhibiting (a) planar precipitates and (b) round precipitates.](image)

The SIMS and TEM results for some Si:Er/O LED structures with different Er and O concentrations are summarized in figure 3(a), which is a logarithmic plot of Er and O concentrations. For the sake of simplicity of discussion, the samples are named as A, B, C, D and E. The dashed line is indicating the 1:1 combination of Er and O (i.e. Er/O = 1). Although figure 3(a) shows a few samples mainly below the 1:1 line, there were also samples grown with other Er and O combinations and characterized with TEM, but not shown. The need for a high O level to get the planar precipitates can be seen in a comparison between samples A and B. Both samples have the same Er concentration (2×10\(^{19}\) cm\(^{-3}\)) but sample A, which has lower O concentration (2×10\(^{19}\) cm\(^{-3}\)), revealed only round precipitates (see figure 2(b)) and sample B, which has relatively higher O concentration (1×10\(^{20}\) cm\(^{-3}\)), contains only planar precipitates.

Furthermore, figure 3(a) also exhibits the effect of increasing Er concentration for constant O level. This is evident from a comparison of samples C and D both of which have O concentration of 5×10\(^{20}\) cm\(^{-3}\) but sample D has Er concentration of 2×10\(^{18}\) cm\(^{-3}\) and contain only planar precipitates, while sample C grown with higher Er level (1×10\(^{20}\) cm\(^{-3}\)) contains predominantly round precipitates with some traces of the planar type.

The tendency for creation of round precipitates for a given Er/O ratio seems to be higher at higher Er concentrations. This is indicated by the existence of round precipitates in sample C which has the
same Er/O ratio of 0.2 as sample B (with only planar precipitates). To summarize one can roughly define a region in the Er-O space of figure 3(a), below the dotted line, where one would expect the presence of mainly planar type of precipitates in Er/O doped Si layers.

Figure 3: (a) Diagram showing the relation between Er and O concentrations and the microstructure. Filled circles indicate LED samples that have been analyzed with SIMS. Open circle indicates concentrations estimated from source calibration. (b) Room temperature EL intensity at 1.54 μm versus reverse current, obtained at room temperature, for samples A, B and E. It is evident from figure 3(b) that sample B, which contains the planar type of precipitates in the Er/O doped layer, has a high EL intensity at large currents, while sample A, which only includes round precipitates exhibits only background luminescence at 1.54 μm. Thus it is concluded that Si:Er/O layers with planar precipitates contain optically active Er/O centers, while Si:Er/O layers with round precipitates contain optically inactive Er/O centers.

The saturation of EL intensity is attributed to two mechanisms. Primarily it is associated with the total number of excited Er$^{3+}$ ions, however it can also be due to a rise of competing non-radiative mechanisms with increasing number of free carries at higher currents. Taking into account the enhancement of luminescence signal and the requirement for obtaining gain in these Si:Er/O LEDs it is rational to grow Si:Er/O LEDs with highest possible number of Er atoms incorporated but there are also limitations set by the microstructure type on the Er concentration. The microstructure studies revealed that higher Er concentrations would lead to the formation of the optically inactive round precipitates. Also the O doping level can not be enhanced above a certain level to keep the crystalline quality of grown layers free of detrimental structural defects. An O concentration of less than $10^{21}$ cm$^{-3}$ is observed to be reasonable, and in this range the Er concentration is optimized in order to achieve the highest possible Er doping levels without forming the optically inactive round precipitates. In this regard sample E, with Er concentration of about $4 \times 10^{19}$ cm$^{-3}$ containing weak planar type of precipitates, exhibit the most efficient optical characteristics so far, as seen in figure 3(b).

4. Summary and conclusions
Several Si:Er/O single crystal structures were grown using MBE and processed to fabricate LEDs. Detailed microstructure analysis revealed two types of Er/O precipitates in these layers, planar and

round type precipitates depending on Er and O concentrations. Quantitative composition studies of several Si:Er/O structures were also performed to determine the Er and O concentrations in these structures using SIMS analysis. It is observed that layers with Er/O \(\ll 1\) contain planar precipitates along (311) planes while layers with Er/O \(\geq 1\) contain round precipitates.

EL measurements show that LEDs with planar precipitates exhibit much stronger room-temperature 1.54 \(\mu\)m intensity as compared to the LEDs containing round precipitates. Based on the microstructure and EL studies a preliminary optimization of Er and O concentrations, obtained from SIMS, was performed. These studies present an approximate value of Er about \(4 \times 10^{19}\) cm\(^{-3}\) with Er:O \(\sim 1:10\).

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