Erbium-doped silicon epilayers grown by liquid-phase epitaxy

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A careful analysis of the features of the spectroscopic properties of Er-doped and undoped epitaxial silicon films grown by liquid-phase epitaxy at 950 °C in silicon-saturated indium melts shows that threading dislocations work as effective gettering sites for erbium and oxygen. The last impurity is incorporated in the epitaxial film by back diffusion from the Czochralski substrate during the growth. The photoluminescence emitted by these films appears to be related to the dislocation and is enforced by the presence of erbium-oxygen complexes. © *1999 American Institute of Physics.* [S1063-7826(99)00206-9]

INTRODUCTION

We have already shown in previous papers[1,2] that Er:Si epilayers grown by liquid-phase epitaxy (LPE) in indium melts present, in the alternative to the intrinsic Er^{3+} photoluminescence (PL) band at 0.8 eV, two intense PL bands at 0.807 and 0.873 eV (at 10 K), of which the first falls within few meV in the same energy range of the Er band but quenches out at higher temperatures.

In addition to the band edge luminescence, the band at 0.8 eV was also observed in the Er-free samples. Since the band at 0.8 eV in Er-doped samples does not exhibit the fine structure associated with the Er^{3+} multiplet and since both bands fall in the energy range of the $D1$ and $D2$ bands of the dislocations, these PL effects are attributed to dislocations generated by strain-release effects at the interface between the epilayer, which incorporates Er and In as dopants at a concentration level on the order of $10^{17}\,cm^{-3}$ for Er and $10^{16}\,cm^{-3}$ for In, and the substrate. Dislocations were, in fact, clearly identified by selective etching, but no clear indication about a possible role of the erbium dopant at the dislocation luminescence was found.

Our aim in this paper is to add further insights into these effects, which might help in the future development of silicon-based optoelectronics.

EXPERIMENTAL DETAILS

The LPE Si:Er epilayers were grown from 99.99% pure indium melts which are saturated in silicon and which contain variable amounts of Er deposited on the Czochralski (CZ) or float-zone (FZ) silicon substrates. The growth temperature was held at 950 °C. Other details about the growth conditions were reported in Ref. 2. The indium concentration in the epilayer was found to be reasonably close to the saturation at the growth temperature, while that of Er ranged between 10^{17} and $10^{18}\,cm^{-3}$. The average thickness of the layers was close to 4 μm, as measured by spreading resistance measurements.

EXAFS measurements, addressed at the study of the local structure of the Er^{+3} ion in the silicon matrix, were carried out at the European Synchrotron Radiation Facility in Grenoble (France) using the Italian GILDA beam line. Details about the measurement conditions were reported in Ref. 3.

Photoluminescence measurements were performed in the 2 to 300-K range using the multiline emission of an Ar ion laser as the exciting sources, as was described in Ref. 1.

Deep level transient spectroscopy (DLTS) and optical DLTS measurements were carried out with a SULA Tech. Inc. system in the 80 to 350-K temperature range.[4]

EXPERIMENTAL RESULTS

Local structure of erbium in LPE-grown epilayers

The results of EXAFS measurements showed that the local structure of Er ions in a dislocation-free LPE-grown Si:Er epilayer is that of the erbium silicide, regardless of the nature of the substrate, which could be either FZ or CZ silicon. In the case of epilayers grown onto CZ silicon substrates, the presence of threading dislocations in the epilayer causes instead a strong change in the local coordination of Er, which gives the typical features of Er in a matrix of erbium oxide. The same Er coordination could be observed in Er-O coimplanted samples. As in the case of LPE samples grown on CZ substrates, oxygen back diffuses from the substrates, which acts as an oxygen source. It can be concluded that only in the presence of dislocations does the formation of Er-O clusters occur during the growth process, where dislocations act as heterogeneous nucleation centers of the erbium oxide.

Photoluminescence of dislocations in Er-free and Er-doped LPE materials

A comparison of the PL spectra of a reference LPE-grown Er-free sample and of a Er-doped sample is shown in

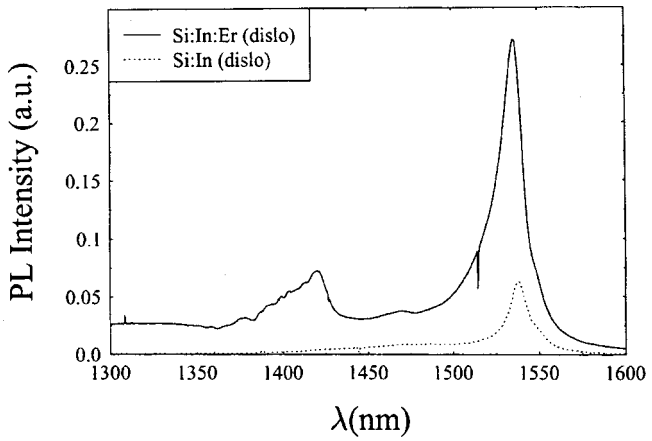

FIG. 1. PL spectra of a reference LPE-grown Er-free sample (dotted line) and of an Er-doped sample at $T=10$ K, $P=1.7$ W/cm^2.

Fig. 1. It is evident that the PL intensity at the same exciting power (1.7 W/cm^2) is larger by a factor of 5 in the case of Er-doped silicon, and that in the case of the reference sample only the $D1$ band is observed. We have then examined the temperature dependence of the intensity of the $D1$ band in Er-doped, dislocated material.

The results showed that the $D1$-PL quenches out at the temperatures close to 250 K, in good agreement with the Kveder results on plastically deformed silicon.[5]

DLTS results

Deep level transient spectroscopy and optical DLTS measurements were performed on the same samples studied in EXAFS and PL experiments. The main results of these experiments are reported in Table I, where we have also presented the results for a reference Er-free sample, also with a dislocation-related PL.

All majority and minority traps were shown to be present at concentrations ranging between 10^{13} and 10^{15} cm^{-3} (Ref. 6).

The traps labeled *HX* and *H*4 are dislocation related, and thus labeled *D*. Since no dislocation-related trap was observed in DLTS measurements by Kveder in single-crystal silicon deformed at 1100 °C under clean conditions, these traps are present in our samples at a concentration at least two orders of magnitude larger than those present in Kveder's[5] samples. Of these traps, the *H*4 trap, which is present only in Er-doped dislocated samples, apparently works as a nonradiative recombination center. From the table one can further recognize the presence of the $E2$ level at $E=E_c-0.20$ eV in the luminescent Er-doped sample.

It closely corresponds to a level at $E_c-0.18$ eV, assigned in the literature to an Er-O center[7] since it is present only in Er-O coimplanted samples. Finally, a shallow level at $E_c-0.18$ eV is present only in the reference sample.

TABLE I. Summary of the results for the majority (*H*) and minority (*E*) trap centers.

Level	Energy, eV	Reference sample	Er-doped sample	Remarks
*H*0	$E_v+0.18$		√	
HX	$E_v+0.45$	√	√	*D*
*H*4	$E_v+0.65$	√	√	*D*
*E*1	$E_c-0.18$	√		
*E*2	$E_c-0.20$		√	Er

DISCUSSION AND CONCLUSIONS

One of the most striking effects of dislocations in LPE-grown epilayers is the drastic change in the local structure of Er, which resembles that of erbium in a cluster of oxygen atoms, while the structure of erbium in erbium silicide in materials without dislocations contains comparable amounts of oxygen.

We could then argue that both oxygen and erbium are gettered at dislocations, which play the role of centers responsible for the $D1$ luminescence band, in agreement with Kveder.

This effect could be unspecific, as for most of the impurities which are called upon to enhance the photoluminescence. We believe, however, that it is peculiar to erbium.

In fact, the permanence of the dislocation-related PL at Er concentrations much larger than those at which transition metals kill the PL is certainly associated with the enhancement of Er solubility associated with the presence of oxygen and/or Er-O centers. Work is in progress to obtain more details on the Er-O centers in dislocated and dislocation-free samples from recent results of EXAFS experiments, which could further support our conclusion.

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