

УДК 621.315.592

Erbium doped silicon epilayers grown by liquid phase epitaxy

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(Получена 12 января 1999 г. Принята к печати 12 января 1999 г.)

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 Er and oxygen. This 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 dislocation and is enforced by the presence of erbium-oxygen complexes.

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 alternative to the intrinsic Er³⁺ 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 quite larger temperatures.

Incidentally, also on Er-free samples the band at 0.8 eV was observed, in addition to the band edge luminescence. As the band at 0.8 eV in Er-doped samples does not exhibit the fine structure associated to the Er³⁺ multiplet and both band fall in the energy range of the D1 and D2 bands of dislocations, these PL effects were 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 of the order of 10¹⁷ cm⁻³ for Er and 10¹⁶ 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 on the dislocation luminescence was found.

Aim of this paper is to add some further insights of 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 saturated in silicon and containing variable amounts of Er onto Czochralski (CZ) or float zone (FZ) silicon substrates. The growth temperature was held at 950°C. Other details about the growth conditions are reported in [2]. The indium concentration in the epilayer was found reasonably close to the saturation at the growth temperature, while that of Er ranged between 10¹⁷ and 10¹⁸ cm⁻³. The average thickness of the layers ranged 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 are reported in [3].

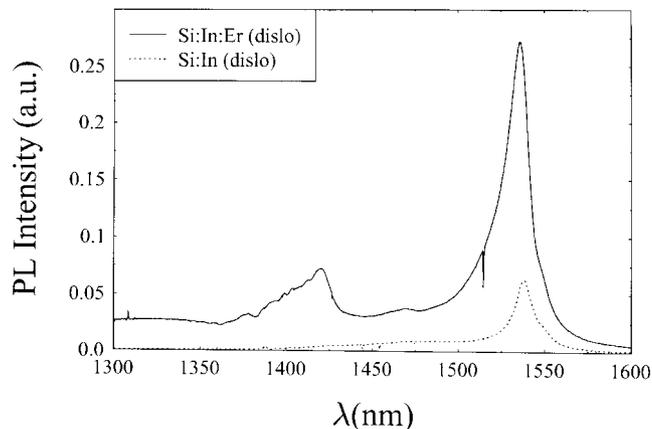
Photoluminescence measurements were performed in the 2–300 K range using the multiline emission of an Ar ion laser as the exciting sources, as already described in [1].

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, independently 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 co-



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/cm².

ordination of Er, which present, in fact, the typical features of Er in a matrix of erbium oxide. The same Er coordination could be observed in Er–O co-implanted samples. As in the case of LPE samples grown onto 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 the formation of Er–O clusters occurs during the growth process, dislocations acting as heterogeneous nucleation centres of the erbium oxide.

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

The comparison of the PL spectra of a reference LPE grown Er-free sample and of a Er-doped sample is reported in the Figure. It is quite evident that the PL intensity, at the same exciting power (1.7 W/cm^2), is larger by a factor 5 in the case of Er-doped silicon and that in the case of reference sample only the *D1* band is perceptible. 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, in good agreement with the Kveder results on plastically deformed silicon [5], at the temperatures close to 250 K.

DLTS results

Deep level transient spectroscopy and optical DLTS measurements were performed on the same samples studied by EXAFS and PL experiments. The main results of these experiments are reported in the Table, where we have also displayed the results obtained on a reference Er-free sample also presenting 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} [6].

Summary of the results concerning the majority (*H*) and minority (*E*) trap centres

Level	Energy, eV	Reference sample	Er-doped sample	Remarks
<i>H0</i>	$E_v + 0.18$		✓	
<i>HX</i>	$E_v + 0.45$	✓	✓	<i>D</i>
<i>H4</i>	$E_v + 0.65$	✓	✓	<i>D</i>
<i>E1</i>	$E_c - 0.18$	✓		
<i>E2</i>	$E_c - 0.20$		✓	Er

The traps labelled *HX* and *H4* are dislocation related, thus marked with *D*. As no dislocation related trap was observed by 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 of those present in the Kveder's [5] samples. Of these traps, the *H4* one, which is only present in Er-doped dislocated samples, apparently

works as a non-radiative recombination centre. From the Table one can further recognize the presence of the *E2* level at $E = E_c - 0.20 \text{ eV}$ in the luminescent Er-doped sample.

It closely corresponds to a level at $E_c - 0.18 \text{ eV}$, assigned in literature to an Er–O centre [7] as it is only present in Er–O co-implanted samples. Finally, a shallow level at $E_c - 0.18 \text{ eV}$ is only present in the reference sample.

Discussion and conclusions

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

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

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

In fact, the permanence of the dislocations-related PL at Er concentrations much larger than those at which transition metals kill the PL is certainly associated to the enhancement of Er solubility associated to the presence of oxygen and/or of Er–O centres. Work is in progress to get more details of the Er–O centres in dislocated and undislocated samples from recent results of EXAFS experiments, which could give a further support our present conclusion.

Acknowledgments

This work was presented in the annual INTAS–RFBR Meeting, held in St.Petersburg, 24–29 October, 1998, in the frame of the INTAS–RFBR 95-531 Program. INTAS is acknowledged for the financial support of the entire Project.

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Редактор В.В. Чалдышев