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2003 J. Phys.: Condens. Matter 15 S2843

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J. Phys.: Condens. Matter **15** (2003) S2843–S2850 PII: S0953-8984(03)67298-X

The origin of the 0.78 eV luminescence band in dislocated silicon

A J Kenyon[1], E A Steinman[2], C W Pitt[1], D E Hole[3] and V I Vdovin[4]

[1] Department of Electronic and Electrical Engineering, University College London, Torrington Place, London WC1E 7JE, UK
[2] Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow District 142432, Russia
[3] Ion Implantation Laboratory, School of Engineering and IT, University of Sussex, Falmer, Brighton BN1 9QH, UK
[4] Institute for Chemical Problems of Microelectronics, B Tolmachevsky per. 5, 109017 Moscow, Russia

Received 7 August 2003
Published 19 September 2003
Online at stacks.iop.org/JPhysCM/15/S2843

Abstract
We report the results of a study into the influence of implanted impurities on luminescence in the region of the well-known D1 luminescence band that is associated with dislocations in silicon. A photoluminescence band at around 0.78 eV, which is sometimes seen in silicon containing a high density of dislocations, has been attributed to the presence of oxygen complexes. In this study we have deposited layers of $Si_{0.9}Ge_{0.1}$ onto single-crystal Si substrates by MBE in order to induce dislocations in the silicon substrate. The samples have subsequently been implanted with iron, erbium or oxygen in order to study the effect of implanted impurities on D-band photoluminescence at around 800 meV. Following implantation with oxygen, two luminescence bands appear at around 0.85 and 0.78 eV, respectively. These bands are not present in either the unimplanted sample or those subject to Er or Fe implantation. The correlation between oxygen doping and the appearance of these bands supports the conjecture that they are associated with oxygen complexes.

1. Introduction

Plastic deformation of crystalline silicon as a result of strain produced either by compression or the growth of an epilayer of material with a lattice parameter mismatch, such as $Si_{1-x}Ge_x$, gives rise to a number of broad luminescence bands in the near infra-red that are associated with dislocations in the silicon bulk [1, 2]. The bands are conventionally labelled D1, D2, D3 and D4 and occur at energies between 1.0 eV and 800 meV, dependent on the nature of the sample (p or n doped, float zone (FZ) or Czochralski material), the degree of deformation,

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and the thermal history of the sample. Of these luminescence bands, the D1 line, which occurs at energies of around 800–820 meV is of particular technological interest because it coincides with the principal low-loss window in silica optical fibres. Although the D bands suffer from strong temperature quenching, the promise of a silicon-based source operating at these energies is very attractive and, for that reason, much research has been directed at understanding the source of this luminescence band.

Despite much research, the origin of the D1 band remains difficult to assign unambiguously. It is generally thought that this band arises from misfit dislocations in the silicon bulk; suggestions for the precise nature of the dislocation responsible for this line range from Lomer–Cottrell dislocations to dislocation kinks and jogs as well as the presence of self-interstitial or vacancy clusters at dislocation cores. It has also been suggested that it may be due to a point defect on a dislocation line that corresponds to the intersection of two dislocations, though cathodoluminescence experiments have suggested an association of both the D1 and D2 lines with regions between dislocations [3]. Such dislocations may be produced readily by compressive strain at elevated temperatures, by the growth of a fully relaxed epilayer of SiGe on a single-crystal silicon substrate [1] or, in some cases, by ion implantation [4]. However, uncertainty remains over the role of impurities in D-band luminescence, and there have been suggestions that the presence of transition metal impurities around the dislocation centres is a prerequisite for luminescence; the picture is confused by the observation that, whilst D1 luminescence is associated with the presence of trace contamination with Ni, Fe or Cu, high levels of transition metal impurities result in quenching of the D1 and D2 lines through the formation of silicide aggregates such as $NiSi_2$ or $FeSi_2$. To further confuse the issue, iron silicide is itself luminescent at around 800 meV in its semiconducting β-phase [5, 6]; at annealing temperatures above 1000 °C it converts to the non-luminescent α-phase. A further particular problem in erbium-implanted silicon is the correspondence between the D1 band and the $^4I_{13/2} \rightarrow {}^4I_{15/2}$ intra-4f transition of the Er^{3+} ion, making the assignment of photoluminescence from such material in this region problematic [7, 8].

It is clear that oxygen plays a key role in dislocation luminescence from silicon in the 0.8 eV region [9, 10]. There is evidence that the presence of oxygen can stabilize D-band luminescence so that it may be observed at higher temperatures, and photoluminescence at around 0.8 eV has been attributed to interstitial carbon–oxygen complexes [11, 12], oxygen precipitates [10], and thermal donors [13]. The generation of oxygen clusters is a complex process and may be influenced by a number of factors, including gettering by fixed dislocations, aggregation of oxygen atoms around dislocations propagating through the lattice during deformation [14], and formation of clusters around impurity ions. The formation of thermal donors can lead to the appearance of a luminescence line at 767 meV (the so-called P line), which is attributed to the interaction between an interstitial carbon atom and a di-oxygen molecule [12]. The P line may be suppressed by the formation of oxygen aggregates [15], which themselves are responsible for lines at around 780 meV. However, the picture is further complicated by the observation that one of the possible first stages in the formation of dislocations is the generation of self-interstitials by the aggregation of oxygen to form clusters [16]. Nevertheless, there is unambiguous evidence that such clusters are responsible for luminescence bands at around 800 meV and that this luminescence may coexist with that from the D1 band [16]. In particular, it has been reported that there is an association between the appearance of luminescence bands at 778 and 850 meV and oxygen precipitates [10].

In this study, we undertook to investigate the influence of implanted impurities on D1-band luminescence from strained-layer SiGe/Si samples. Specifically, the influence of oxygen on the intensity and lineshape of the luminescence band at around 800 meV was investigated.

2. Experiment

Samples were produced by MBE growth of 1400 nm thick layers of $Si_{0.9}Ge_{0.1}$ onto p-type (10^{15} cm^{-2}) single-crystal (111) FZ silicon substrates. Films were grown at temperatures between 700 and 800 °C, which ensured that the substrate was sufficiently relaxed that a high density of misfit dislocations was produced below the $Si_{0.9}Ge_{0.1}$ epilayer.

After deposition, the samples were divided into two sets, labelled SG1E*n* and SG1AE*n*. In each set, the $n = 1$ sample was unimplanted, $n = 2$ implanted with erbium, $n = 3$ implanted with iron, and $n = 4$ implanted with oxygen (see below). Both sets were etched using a $SiCl_4$ plasma; the former set to a depth of 1300 nm and the latter to 1400 nm (i.e. the entire $Si_{0.9}Ge_{0.1}$ layer was removed). The latter set (SG1AE*n*) was further annealed at 900 °C in argon prior to etching. Samples were then implanted with implantation energies that were chosen to give an ion penetration depth of 160 nm in each case. This corresponded to 60 keV for oxygen, 190 keV for iron, and 380 keV for erbium. Fluxes were 10^{15} cm^{-2} for each species. Following implantation, all samples were annealed at 900 °C in argon for 90 min to remove implantation-induced damage.

A further set of anneals were undertaken to investigate the effect of rapidly quenching the temperature of the sample. Selected samples were annealed at 900 or 1100 °C, and then removed from the annealing furnace rapidly in order that they should cool to room temperature in a few seconds. Such treatment is known both to produce a high density of misfit dislocations and to quench the D2 luminescence band [10].

Photoluminescence spectra were measured for each sample using an argon-ion laser operating at 488 or 514 nm as an excitation source. The samples were placed in a continuous-flow liquid nitrogen cryostat. Luminescence was dispersed through a Bentham M300 monochromator and detected using either an InGaAs PIN diode or a Hamamatsu InGaAs photocathode photomultiplier tube. Standard lock-in techniques were employed.

Selected samples were studied by transmission electron microscopy (TEM) to confirm the presence of dislocations and oxygen complexes.

3. Results and discussion

Because of the strain induced by the $Si_{0.9}Ge_{0.1}$ layer, a considerable degree of relaxation can be expected in the silicon substrate, resulting in a very dense network of extended dislocations. Figure 1 shows a TEM image of the dislocated layer of an oxygen-implanted sample that confirms the presence of a dislocation network. The plane of the image is (001). The lines correspond to misfit dislocations introduced due to the strain field and the arrows indicate the position of oxygen precipitates. However, a puzzling observation is that the observed dislocations have a different appearance to those commonly associated with D-band luminescence [4]. Specifically, they have a more complex structure than expected. The conventional picture of dislocations associated with D-band luminescence is of a 'tram-line' pattern of extended linear dislocations, which can extend for several microns. However, figure 1 shows short dislocations with more random orientations and half-formed loop structures. A possible explanation for this is the damage caused by ion implantation, or perhaps redistribution of strain due to the removal of the majority of the $Si_{0.9}Ge_{0.1}$ epilayer. However, this remains conjecture until further structural studies have been performed. Nevertheless, the presence of both oxygen precipitates and dislocations in both oxygen-implanted samples (SG1E4 and SG1AE4: etched and non-etched) has been confirmed by the TEM results. In all cases these dislocations appeared to be different from the misfit dislocations induced by the $Si_{0.9}Ge_{0.1}$

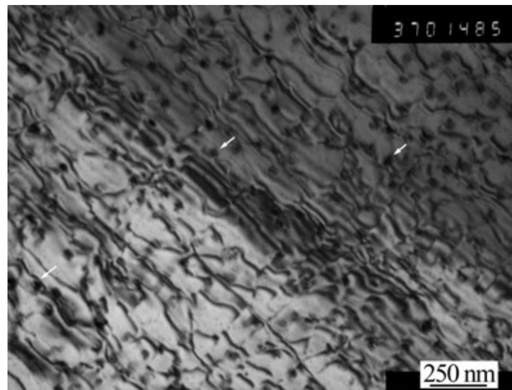

Figure 1. A TEM image of a dislocated layer in an oxygen-implanted sample.

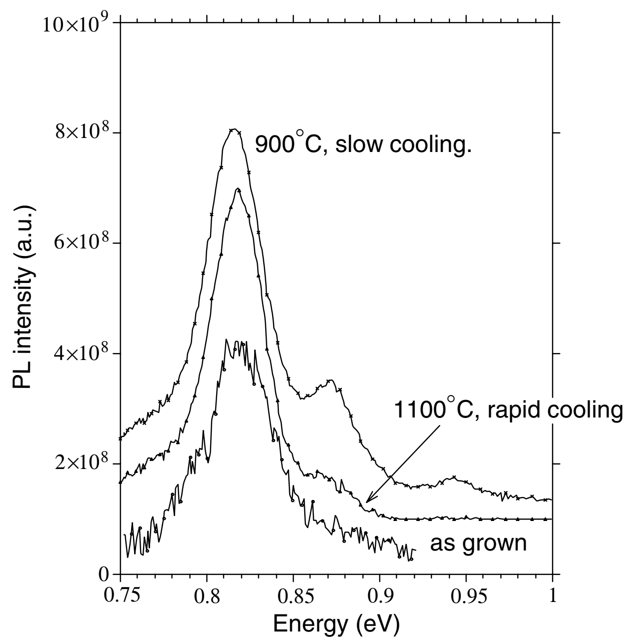

Figure 2. The effect of annealing and rapid cooling on an unimplanted sample.

layer, and we must therefore surmise that implantation has introduced these defects and that annealing at 900 °C is not sufficient to remove them.

The dislocation-related luminescence (DRL) spectrum of the unimplanted sample (SG1E1) is shown in figure 2; it consists of only a D1 line (820 meV) of low intensity. It is known that dislocations that are introduced at temperatures below 800 °C generate a great number of non-radiative recombination centres, which decrease the efficiency of radiative recombination. The other two spectra in figure 2 illustrate the effect of different annealing procedures. On annealing at 900 °C for 30 min and cooling slowly to room temperature, the degree of substrate relaxation becomes much higher, the dislocation network develops further into the substrate, and a considerable proportion of non-radiative centres are annealed. The PL intensity becomes larger and the spectrum now consists of the two lines D1 (812 meV) and D2

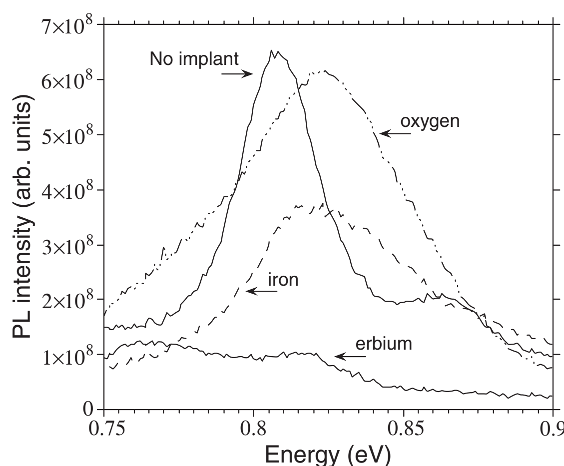

Figure 3. PL spectra taken at 77 K of the sample series SG1E*n*, implanted with ions as labelled.

(870 meV). There is also a weak line at 940 meV, which is possibly related to the D4 centre in the strained lattice. However, a further anneal at 1100 °C followed by rapid quenching to room temperature quenches the D2 photoluminescence line.

Figure 3 shows a set of photoluminescence spectra, taken at 77 K, of the SG1E*n* series samples. Clearly evident in the un-implanted case (SG1E1) is a strong peak at around 805–810 meV with a weaker side-band at around 860 meV. These correspond to the D1 and D2 lines, respectively. Implantation with erbium (SG1E2) strongly quenches the luminescence; iron (SG1E3) and oxygen (SG1E4) produce a shift in the peak energy to around 820–830 meV, though the latter produces considerable quenching. Of particular note is the enhancement of the low-energy side of the luminescence band evident in SG1E4 (oxygen implanted).

Figure 4 shows the excitation power dependence of the 70 K luminescence from the oxygen-implanted sample SG1E4. There is a clear increase in the peak energy with increasing excitation power. Such behaviour could be associated with donor–acceptor radiative transitions.

Figure 5 shows the effect of the rapid quenching of a 900 °C anneal of the same oxygen-doped sample. The main effect is the quenching of the low-energy side of the luminescence peak. Similar results were obtained from an anneal at 1100 °C followed by a rapid thermal quench. This behaviour is associated with dissolution and 'freezing-out' of oxygen complexes as a result of rapid quenching; slow cooling allows them to nucleate and stabilize.

Figure 6 shows PL spectra of the sample SG1AE4. Recall that this sample has had the SiGe epilayer removed; note the absence of characteristic D1 luminescence. The most striking observation is the appearance of new luminescence bands at 780 and 850 meV. TEM results confirmed that the SiGe layer had been removed from the SG1AE*n* series. No photoluminescence was detectable from the unimplanted sample (SG1AE1) in this region; the iron-implanted sample showed a very weak band at around 820 meV that may be the D1 line due to residual dislocations still present in the silicon; the Er-implanted sample SG1AE3 showed very weak photoluminescence at around 780 meV.

Figure 7 shows the 70 K photoluminescence spectrum of sample SG1E4 fitted using three Gaussian peaks, centred at 778, 820 and 850 meV, respectively. The first and last energies correspond to the positions of the peaks induced in sample SG1AE4 by oxygen implantation, and have been observed in previous work and identified with the presence of oxygen precipitates in FZ silicon [10]. This implies that the observed luminescence in this sample is a combination

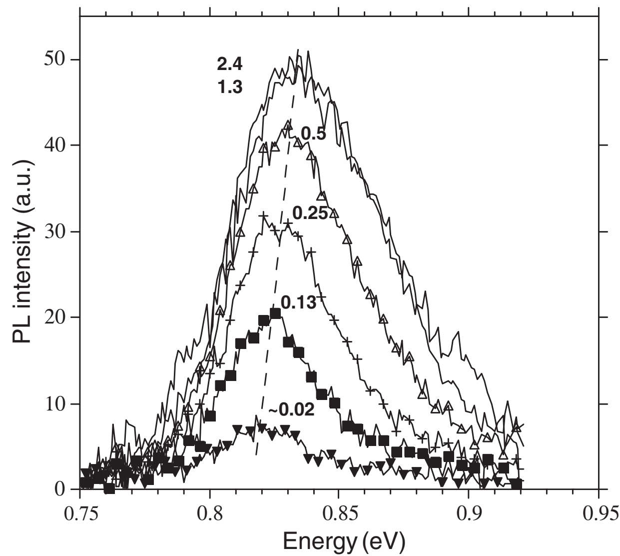

Figure 4. The excitation power dependence of luminescence from the oxygen-implanted sample SG1E4. Curves are labelled with excitation power densities in MW cm^{-2}. Spectra are taken at 70 K.

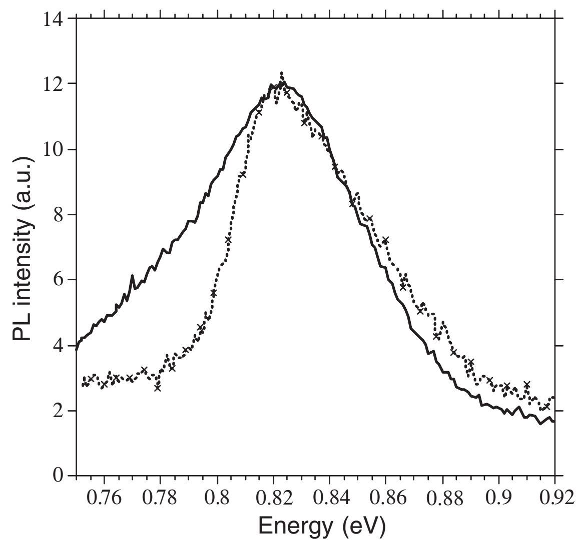

Figure 5. PL spectra taken at 70 K for the oxygen-implanted sample SG1E4—black curve: before annealing; dotted curve: after annealing and rapid quenching.

of that due to misfit dislocations and that from oxygen complexes. Note that the data could not be fitted with two Gaussian peaks.

4. Conclusions

Dislocations may be introduced into single-crystal silicon by the growth of a SiGe layer of sufficient thickness. Characteristic D-band luminescence is readily seen from such samples; the spectral shape and intensity of this emission is strongly influenced by the presence of

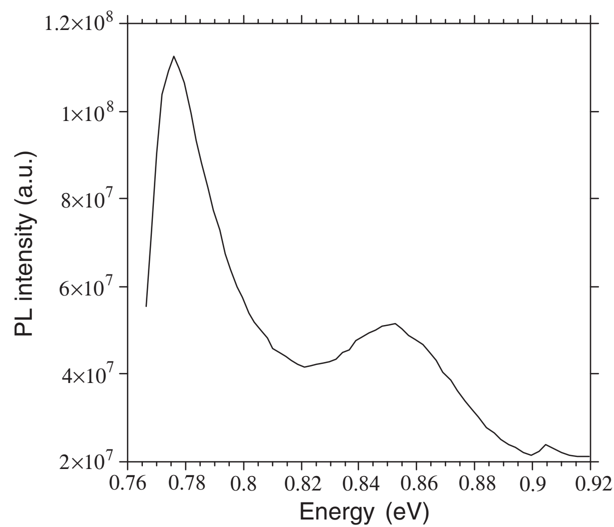

Figure 6. The PL spectrum of sample SG1AE4: $Si_{0.9}Ge_{0.1}$ epilayer removed, then implanted with oxygen. Note the absence of D1 luminescence and the appearance of new PL bands centred at 780 and 850 meV, respectively.

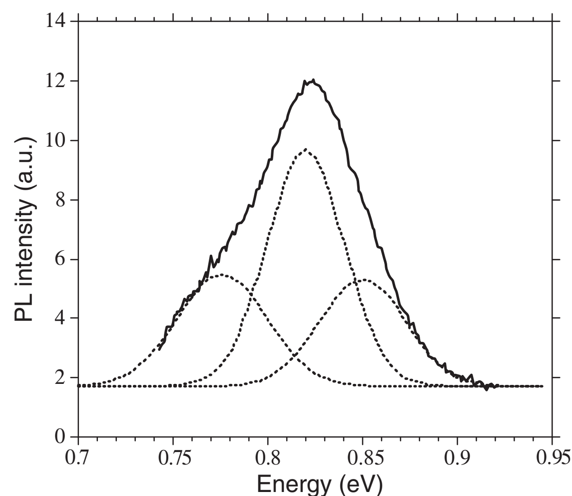

Figure 7. A fitting of the PL spectrum of sample SG1E4 using three Gaussian peaks. Experimental data are shown by solid curve.

impurities. We have specifically investigated the effect of oxygen on D1 luminescence. Our results indicate that the implantation of oxygen into the dislocated silicon substrate broadens the D1 band, particularly to the low-energy side. The resultant luminescence band appears to be a convolution of three lines: that due to dislocations, centred around 820 meV, and two 'new' bands centred at 778 and 850 meV, respectively. When the silicon layer containing the dislocations is removed by etching, although the D1 luminescence band is quenched, implantation with oxygen again produces the two new luminescence bands. We therefore conclude that these bands are related to the formation of oxygen precipitates, though it should be borne in mind that the TEM results indicate the presence of some residual or implantation-

related dislocations in this sample that may also contribute to the observed photoluminescence. Nevertheless, our conclusion is supported by the observation that the low-energy side of the broadened luminescence band seen in un-etched samples is strongly reduced by rapid thermal quenching; this is behaviour that is consistent with the dissociation and 'freezing-out' of oxygen clusters. It is tempting to conclude that the observation of a weak luminescence band in the erbium-doped sample at around 780 meV may possibly be attributed to the gettering effect of erbium on oxygen, leading to the formation of oxygen complexes around erbium ions [17, 18], although this is speculation until further work has been performed.

Acknowledgments

The authors are grateful to the Engineering and Physical Sciences Research Council for funding provided under grant no GR/R69501. One of the authors (EAS) would like to acknowledge the support of INTAS, grant no 01-0194. The authors are grateful to the Royal Society for the provision of funding to allow EAS to visit UCL.

References

[1] Fitzgerald E A, Currie M T, Samavedam S B, Langdo T A, Taraschi G, Yang V, Leitz C W and Bulsara M T 1999 *Phys. Status Solidi* a **171** 227
[2] Higgs V, Lightowlers E C, Fitzgerald E A, Xie Y H and Silverman P J 1993 *J. Appl. Phys.* **73** 1952
[3] Higgs V, Chin F, Wang X, Mosalski J and Beanland R 2000 *J. Phys.: Condens. Matter* **12** 10105
[4] Vdovin V I 1999 *Phys. Status Solidi* a **171** 239
[5] Bost M C and Mahan J E 1985 *J. Appl. Phys.* **58** 2696
[6] Schuller B, Carius R, Lenk S and Mantl S 2001 *Opt. Mater.* **17** 121
[7] Sobolev N A, Gusev O B, Shek E I, Vdovin V I, Yugova T G and Emel'yanov A M 1998 *J. Lumin.* **80** 357
[8] Vernon-Parry K D, Evans-Freeman J H, Hawkins I D, Dawson P and Peaker A R 2001 *J. Appl. Phys.* **89** 2715
[9] Feklisova O V, Mariani-Regula G, Pichaud B and Yakimov E B 1999 *Phys. Status Solidi* a **171** 341
[10] Steinman E A and Grimmeiss H G 1998 *Semicond. Sci. Technol.* **13** 124
[11] Davies G 1989 *Phys. Rep.* **17** 683
[12] Kürner W, Sauer R, Dörnen A and Thonke K 1989 *Phys. Rev.* B **39** 13327
[13] Pizzini S, Acciarri M, Leoni E and LeDone A 2000 *Phys. Status Solidi* b **222** 141
[14] Giri P K, Coffa S, Raineri V, Privitera V, Galvagno G, LaFerla A and Rimini E 2001 *J. Appl. Phys.* **89** 4310
[15] Tajima M, Warashina M, Takeno H and Abe T 1994 *Appl. Phys. Lett.* **65** 222
[16] Pizzini S, Guzzi M, Grilli E and Borionetti G 2000 *J. Phys.: Condens. Matter* **12** 10131
[17] Cavallini A, Fraboni B, Binetti S, Pizzini S, Lazzarini L and Salviati G 1999 *Phys. Status Solidi* a **171** 347
[18] Pizzini S, Binetti S, Calcina D, Morgante N and Cavallini A 2000 *Mater. Sci. Eng.* B **72** 173