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SCIENCE DIRECT
Nuclear Instruments and Methods in Physics Research B 248 (2006) 127–132
NIM B
Beam Interactions with Materials & Atoms
www.elsevier.com/locate/nimb

Effect of Ge doping on the creation of luminescent radiation defects in MBE Si

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Received 13 February 2006; received in revised form 10 April 2006
Available online 5 June 2006

Abstract

We report on the observation of new luminescence centres in irradiated Ge-doped Si (Si:Ge). Molecular beam epitaxy grown Si:Ge samples with Ge content in the range 0–1.25 at.% were irradiated with protons at room temperature and subjected to post-irradiation heat treatments at temperatures from 100 to 650 °C. For each annealing step, the samples were investigated by means of photoluminescence (PL) spectroscopy at temperatures between 4 and 300 K. We have found that the PL spectra of Ge-containing samples are different from those measured in Ge-free samples and from those previously reported in irradiated bulk Si:Ge. Several new lines have been found in the near band edge (NBE) region of the spectrum, whereas many lines typically measured in Ge-free irradiated Si have not been observed. The dependence of the intensity of the new NBE lines on the measurement temperature has been studied. With increasing Ge content, these lines shift to lower energies following the band gap shrinkage. However, they are broader than expected, when only a purely statistical variation of the band gap energy produced by local fluctuations in the alloy composition is taken into account.

PACS: 78.55.Ap; 81.40.Tv; 81.40.Wx

Keywords: SiGe alloys; Ge-doped Si; Radiation defects; Photoluminescence

1. Introduction

The SiGe technology is finding more and more applications due to its benefits over other electronic materials: speed, high linearity, lower power consumption and ability to combine analog and digital functions on a chip. In certain environments, e.g. in space, the radiation hardness of the devices is a key issue. Despite this, not much is known about radiation defects in Ge-doped Si and $Si_{1-x}Ge_x$ alloys. The only positively identified defect in Si incorporating Ge is the Ge–vacancy pair [1], however, it is stable only up to 200 K. In previous photoluminescence (PL) studies on irradiated bulk silicon doped up to 0.4 at.% of Ge, new PL lines have been found, whose appearance correlates with the Ge content [2,3]. The conclusion has been drawn that Ge atoms, when present in a sufficiently high concentration, may become, at least at certain annealing stages, major sinks for mobile defect components, thus inhibiting the formation of other defects commonly observed in Ge-free Si. In this work we extend these studies to molecular beam epitaxy (MBE) grown silicon doped with higher concentrations of Ge.

2. Experiment

A Ge-free MBE Si layer (sample A) and two Ge-doped MBE Si layers (Si:Ge layers) (sample B, $x_{Ge} = 0.69$ at.% and sample C, $x_{Ge} = 1.25$ at.%) with a thickness of 3 μm

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doi:10.1016/j.nimb.2006.04.068

were grown at 800 °C on top of (0 0 1) Si substrates. The Ge content in the used Si:Ge layers was determined by Rutherford backscattering spectroscopy (RBS) using 1.5 MeV He^+ ions. Samples B and C were intentionally doped with Sb to be n-type. The concentration of conduction electrons measured by the capacitance–voltage technique amounted to $9\times10^{15}\,cm^{-3}$ in sample B and to $3\times10^{15}\,cm^{-3}$ in sample C. These values should correspond roughly to the concentration of Sb donor atoms in the samples, since we expect the contamination resulting from unwanted compensating acceptor atoms in our MBE system to be lower than $10^{14}\,cm^{-3}$. Sample A was not intentionally doped during growth; however, an n-type doping of about $3\times10^{14}\,cm^{-3}$ resulted from the contamination of the growth chamber with Sb.

All samples were irradiated with 875 keV protons with a fluence of $10^{16}\,H^+/cm^2$ through a 10 μm thick Al foil. The energy of the protons and the thickness of the Al foil were chosen based on a TRIM calculation [4] in order to place the profile of the damage (vacancies/interstitials) inside the 3 μm thick Si:Ge layers. The proton energy necessary to achieve this localization of the damage inside the Si:Ge layers without the use of an Al foil would be too low for the accelerator used in our experiments. Furthermore, at a lower implantation energy the hydrogen profile would be much narrower than the Si:Ge layers. The maximums of the concentration profiles of vacancies/interstitials and of hydrogen atoms, which are estimated using a TRIM calculation for the used irradiation fluence ($10^{16}\,H^+/cm^2$), are 2×10^{21} and $1.25\times10^{20}\,cm^{-3}$, respectively. Both profiles are located at 2.2 μm below the surface of the layers and have a full-width-at-half-maximum of about ~1 μm. We should note that the TRIM calculations are performed at a temperature of 0 K and at room temperature most of the vacancies and interstitials formed by the irradiation recombine. In moderately doped silicon, this recombination of interstitials with vacancies is quite intense at room temperature and only about 1% of the vacancies/interstitials formed upon the irradiation should remain in the sample [5]. Therefore, we estimate a maximum of the concentration profile of vacancies/interstitials after the irradiation at room temperature of about $2\times10^{19}\,cm^{-3}$, which is considerably lower than the maximum of the concentration profile of hydrogen atoms ($1.25\times10^{20}\,cm^{-3}$). One should also note that the maxima of the concentrations of vacancies/interstitials and of hydrogen atoms produced by the irradiations are several orders of magnitude higher than the concentration of Sb donors.

After irradiation the samples were annealed for 15 min in a nitrogen atmosphere at temperatures between 100 and 650 °C in steps of 50 °C. The PL measurements were performed with a Bruker IFS 66v FTIR spectrometer equipped with a liquid nitrogen cooled Ge detector with the samples placed in a helium gas flow cryostat. For the PL measurements, in a wide range of power densities, we used the 488 nm line of an Ar^+ laser. The temperature of the samples varied from 4 up to 300 K.

3. Results

The evolution of the PL spectra with annealing temperature, T_a, is illustrated in Fig. 1 for all samples under study. In the PL spectrum of sample A, after irradiation and prior to any annealing, only the W centre of intrinsic origin [6,7] is observed. With increasing annealing temperature T_a the W centre transforms into the X centre, as discussed in [6,7]. The W centre is believed to be an aggregate of two or three Si interstitials, I_2 or I_3, while the X centre is ascribed to an aggregate of four Si interstitials, I_4, as described in [8]. Simultaneously, several lines (AA1–AA5 and AA18) that have not been previously reported appear in the PL spectra. All the lines observed in this work and the respective T_a intervals are listed in Table 1.

The addition of 0.69 at.% of Ge to the layers (sample B) strongly affects the PL spectra, particularly in the near band edge (NBE) region (Fig. 1). Whereas the W and X centres are again observed at their typical annealing temperatures, new NBE spectra start to appear at $T_a\approx500$ °C and reach their maximum intensity at $T_a\approx550$ °C. The NBE lines studied in detail in this work have been labelled AA6–AA16, see Fig. 1. Despite forming a group, these lines appear separately and they do not stem from transitions between different sublevels belonging to one and the

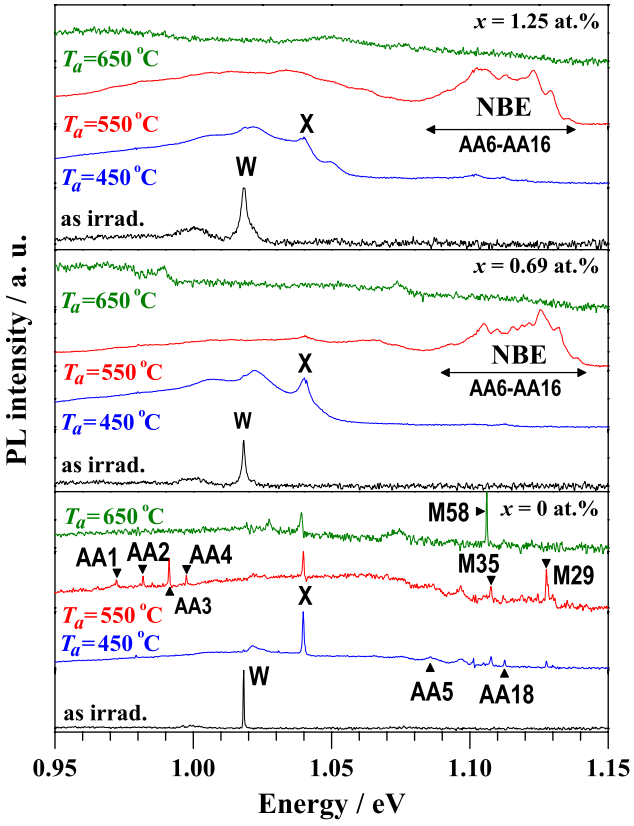

Fig. 1. PL spectra measured at 5 K after irradiation and annealing in MBE grown Si samples with Ge content x_{Ge} ranging from 0% to 1.25%. The x_{Ge} values and the annealing temperatures T_a are indicated in the figure. The parameters of the observed lines are indicated in Table 1.