



Luminescence of silicon nanoparticles from oxygen implanted silicon

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ARTICLE INFO

Keywords:

Oxygen implantation
Silicon nanoparticles
Photoluminescence

ABSTRACT

Oxygen with a kinetic energy of 20 keV is implanted in a silicon wafer (100) at different fluences, followed by post-implantation thermal annealing (PIA) performed at temperatures ranging from 1000 to 1200 °C, in order to form luminescent silicon nanoparticles (SiNPs) and also to reduce the damage induced by the implantation. As a result of this procedure, a surface SiO_x layer (with 0 < x < 2) with embedded crystalline Si nanoparticles has been created. The samples yield similar luminescence in terms of peak wavelength, lifetime, and absorption as recorded from SiNPs obtained by the more conventional method of implanting silicon into silicon dioxide. The oxygen implantation profile is characterized by elastic recoil detection (ERD) technique to obtain the excess concentration of Si in a presumed SiO₂ environment. The physical structure of the implanted Si wafer is examined by grazing incidence X-ray diffraction (GIXRD). Photoluminescence (PL) techniques, including PL spectroscopy, time-resolved PL (TRPL), and photoluminescence excitation (PLE) spectroscopy are carried out in order to identify the PL origin. The results show that luminescent SiNPs are formed in a Si sample implanted by oxygen with a fluence of 2 × 10¹⁷ atoms cm⁻² and PIA at 1000 °C. These SiNPs have a broad size range of 6–24 nm, as evaluated from the GIXRD result. Samples implanted at a lower fluence and/or annealed at higher temperature show only weak defect-related PL. With further optimization of the SiNP luminescence, the method may offer a simple route for integration of luminescent Si in mainstream semiconductor fabrication.

1. Introduction

Strong luminescence from silicon nanoparticles attracted a substantial interest in the nineties, mainly due to the potential use in semiconductor technology for electro-optical applications [1,2]. An early method to embed Si nanoparticles (SiNPs) in a dielectric material is Si implantation with an energy range of 50–200 keV in amorphous silicon oxide, followed by thermal annealing [3–5]. After implantation, the oxide layer created in the implanted region becomes sub-stoichiometric SiO_x (with 0 < x < 2). Post-implantation annealing (PIA) can then be employed to stimulate a phase separation in the silicon oxide layer forming Si nanostructures in the SiO₂ matrix [6]. For lower fluences (i.e. < 10¹⁶ atoms cm⁻²), well-separated SiNPs are formed by nucleation and growth processes [7]. On the other hand, for higher fluences (i.e. > 10¹⁷ atoms cm⁻²), closely adjacent SiNPs, or network-like Si-nanostructures can be formed via spinodal decomposition [8]. However, despite extensive research, the optical efficiency of the nanoparticles formed in these processes is limited mainly due to low yield

of nanoparticle formation and non-radiative defects, quenching the luminescence [9].

Separation by implantation of oxygen (SIMOX) is a very known and well-established ion-beam-based technique to form a buried SiO₂ layer in Si wafers, which has been employed for over three decades [10–12]. The SIMOX process includes oxygen implantation in a Si-wafer at a very high fluence of O ions (> 10¹⁷ atoms cm⁻²), followed by a subsequent thermal annealing. The thickness of the SiO₂ layer depends on ion energy and fluence, annealing temperature, etc. Under proper conditions, a uniform high quality SiO₂ layer with well-defined interfaces to the Si matrix above and below can be successfully achieved [13]. These silicon on insulator (SOI) wafers have been used in many technological applications such as high quality microelectronic integrated circuits (e.g. MOSFET), photonics, and RF-devices, and, when compared to conventional bulk Si wafers, offer advantages such as low parasitic capacitance and supreme radiation hardness [14–16].

In this work, the basic principle of the SIMOX process is employed to create a SiO₂ layer embedded in a Si matrix, although the concentration

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of implanted oxygen corresponds to a sub-stoichiometric SiO_x instead of a stoichiometric SiO_2 . In addition, a mixed phase system is formed after the PIA, containing SiO_2 as well as embedded SiNPs. The formation of small Si clusters in the SiO_x layer has been noticed also for the SIMOX process [17,18], although considered as an undesired artefact. Here, we make use of this effect to demonstrate the possibility of an alternative way to manufacture luminescent SiNPs for easy integration in standard Si processing.

2. Methods

A relatively low-energy O-implantation has been chosen to make the detection of SiNP luminescence easier, since a thick Si surface layer will absorb the photons. According to simulations based on Monte Carlo simulations [19,20], sputtering is expected at these high fluences, removing up to ~ 10 nm of the Si from the surface. Two (100) p-type Si wafers were implanted at room temperature by 20 keV O^+ at two ion fluences: 5×10^{16} and 2×10^{17} atoms cm^{-2} , corresponding to compositions at the mean projected range of $\text{SiO}_{0.15}$ and $\text{SiO}_{0.4}$ (O concentration of 15 and 40 at%), respectively. The wafers were mounted on a polished and thick metal plate in order to conduct beam induced heat away from the sample. Samples were also tilted at 7° with respect to the incident beam to decrease any possible channeling during the beginning of the implantation. The ion flux during the implantation was kept constant around 10^{13} atoms $\text{cm}^{-2} \text{s}^{-1}$. Simulated depth profiles of oxygen implanted in the Si matrix were obtained from the Monte Carlo codes, i.e., TRIM [19] and TRIDYN [20], where the latter accounts for sputtering and swelling, which is unavoidable for high fluence implantation. After the implantation, the wafers were cut into smaller pieces of $0.5 \times 0.5 \text{ cm}^2$. Post-implantation thermal annealing (PIA) was performed at temperatures of 1000, 1100, or 1200 °C for 90 min in an argon ambient.

The concentrations of the implanted oxygen, as well as the oxygen profile in the Si wafers, were investigated by a time-of-flight elastic recoil detection (ToF-ERD) technique [21] at Uppsala University using 36 MeV $^{127}\text{I}^{8+}$ as primary projectiles. In addition to the quantitative composition analysis, grazing incidence X-ray diffraction (GIXRD) was performed to further characterize the structure of SiNPs embedded in the SiO_x layer. The optical properties were studied by photoluminescence (PL) techniques.

A 405-nm emission laser diode with a power range of 10–40 mW cm^{-2} was used to excite electronic states in samples, and their PL spectra were detected by a spectrometer connected to a CCD array, operating at -100°C . Time-resolved PL (TRPL) and photoluminescence excitation (PLE) measurements were used to complement the information and enable an identification of the PL origin. A single photon energy in the range of 1.9–3.4 eV, generated from a white light source connected to a monochromator, was used to excite the electronic states in the samples for the PLE measurements.

3. Results and discussion

3.1. Physical structure

The oxygen concentrations and depth profiles in the implanted Si wafers, for low-fluence ($\text{SiO}_{0.15}$) and high-fluence ($\text{SiO}_{0.4}$), deduced from ToF-ERD spectra are presented in Fig. 1. The implantations simulated with TRIM and TRIDYN are also shown for comparison, where the high fluence effects are found different. The oxygen profiles measured by ERD for both samples are distributed in the same region as the simulations, although the projected range of experimental data are slightly shorter than the simulations. It is important to point out that the tails of the experimental profiles reach slightly beyond the simulated profiles, which is related to straggling effects of the heavy-projectile bombardments for the ToF-ERD measurements. According to the TRIDYN output, the change in the density induced by the high-fluence

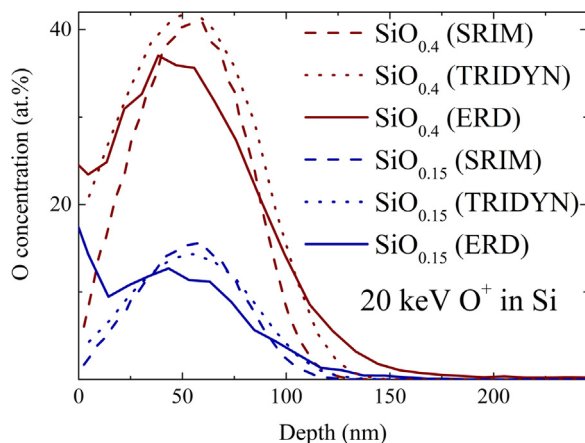


Fig. 1. The concentration profiles for oxygen implanted in Si obtained from two different simulation codes (dashed and dotted lines): SRIM and TRIDYN, together with experimental ToF-ERD profiles (solid lines). The ERD profiles show oxygen concentrations close to the surface higher than the simulations.

implantation leads to a difference in the oxygen concentration between these simulations.

The oxygen implantation will amorphize the implanted Si layers from the surface to a depth beyond the mean projected range [22]. After the PIA, the oxygen atoms will bond to the native Si atoms, forming a relatively low quality SiO_2 , and leave an excess Si concentration around the mean projected range of the oxygen. Generally, the excess Si is a crucial parameter for the formation of SiNPs, affecting their size and density. In Fig. 2, the oxygen profiles obtained experimentally from ERD, used to calculate excess Si in the presumed SiO_2 matrix, are shown as a function of depth in the implanted Si matrix. The profiles of excess Si feature a minimum value at the projected range of implanted oxygen, and then asymptotically increases to 100% (i.e. no presence of oxygen) at larger depths (> 150 nm). The minimum values of excess Si, beyond the surface region, for the $\text{SiO}_{0.15}$ sample and $\text{SiO}_{0.4}$ sample are 80 and 45 at%, respectively. In addition, there is a slight enhancement of oxygen concentration nearby the surface (< 10 nm), mainly due to preferential sputtering of Si and/or surface contamination.

Fig. 3 shows the GIXRD spectra for $\text{SiO}_{0.4}$ sample annealed at 1000 °C, measured at an incidence angle of 0.2° and 0.5° . It can be seen that there are no pronounced peaks for the lower incidence angle, while three distinct peaks centered at the detection angles of 28.54° , 47.49° , and 56.13° , are observed, corresponding to the diffraction at crystalline

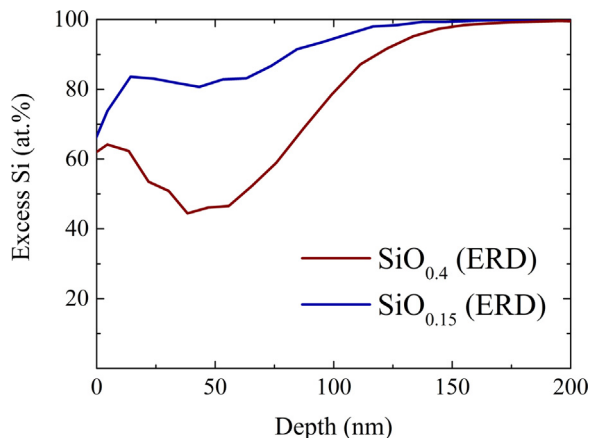


Fig. 2. Excess Si compared to a presumed SiO_2 matrix, obtained from ERD. Apart from the surface, Minimum values of excess concentration of Si for the low- and the high-fluence implantation are 45 and 80 at%, respectively.

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