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Iron distribution in the implanted silicon under the action of high-power pulsed ion and laser beams

R. Bayazitov [a,*], R. Batalov [a], R. Nurutdinov [a], V. Shustov [a], P. Gaiduk [b], I. Dézsi [c], E. Kótai [c]

[a] *Kazan Physical-Technical Institute of RAS, Sibirsky Trakt 10/7, 420029 Kazan, Russia*
[b] *Belarussian State University, F. Scarina Avenue 4, 220050, Minsk, Belarus*
[c] *KFKI Research Institute for Particle and Nuclear Physics, H-1525 Budapest 114, Hungary*

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Abstract

The results of the investigation of the phase composition, microstructure and dopant depth distribution in silicon layers implanted with iron ions and annealed with pulsed ion and laser beams are given. X-ray diffraction data indicate the phase transition FeSi → β-$FeSi_2$ with increasing of the pulse energy density. After ion implantation and pulsed treatments, silicon layers have a cellular structure related with the low solubility of iron in silicon. Depending on the iron atomic concentration, either segregation of the dopant to the surface or diffusion into silicon takes place. This dependence is explained by rapid diffusion of iron in liquid silicon and increase of the dopant distribution coefficient when increasing dopant concentration. The results of the computer simulation agree well with experimental data on the iron depth distribution and give the segregation co-efficient close to 1 at the highest dopant concentration.

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1. Introduction

Pulsed treatment of implanted semiconductors with laser, electron and ion beams is the efficient method to form highly doped layers and thin film compounds. Earlier was shown [1] that during pulsed ion beam treatment (PIBT) deeper diffusion than that at pulsed laser annealing (PLA) is observed resulting in the formation of deep highly doped layers. In the case of low-soluble impurities, such as iron in silicon ($N \sim 10^{16}$ cm^{-3}), in addition to diffusion, motion of the impurity to the surface

* Corresponding author. Tel.: +7 8432 72 12 41; fax: +7 8432 72 50 75.
E-mail address: bayaz@kfti.knc.ru (R. Bayazitov).

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(segregation) and synthesis of metal silicides takes place.

Among different phases in the Fe–Si system, semiconducting iron disilicide (β-$FeSi_2$) is of special interest for industrial applications. Due to its direct bandgap ($E_g \sim 0.85$ eV) and high absorption co-efficient ($\alpha \sim 10^5$ cm^{-1}) this material could be used in Si-based optoelectronics as a light emitter in the 1.5 μm range, solar cell and photodetector [2]. Continuous layers and precipitates of β-$FeSi_2$ on Si substrate are formed by two main approaches, namely by iron ion (Fe^+) implantation into Si and vacuum deposition of Fe film onto Si. At the second stage of synthesis, Si crystals are subjected to prolonged thermal treatment (up to 20 h) at elevated temperatures (up to 950 °C) in order to crystallize films and to eliminate defects [3,4]. However, such thermal treatments are undesirable in microelectronics due to uncontrolled diffusion of Fe atoms and electrically active dopants (boron, phosphorous) in device structures.

An alternative to prolonged thermal annealing could be pulsed treatments of implanted (Si:Fe^+) and vacuum deposited (Fe/Si) structures with nanosecond laser, ion and electron beams. Such treatments are accompanied by melting and crystallization of near-surface Si layers (up to 1 μm) during a short time interval (up to 1 μs) and allow one to anneal separate parts of the wafer or device [5]. The main feature of ion beams compared to laser ones is the more uniform depth distribution of absorbed energy and its independency on optical parameters of the materials. This results in deep melting without overheating and disruption of the surface. In this work the behavior of Fe atoms implanted in Si at pulsed treatments is studied on the basis of the investigation of the phase composition and microstructure of near-surface Si layers and also the depth distribution of Fe atoms in Si and its concentration dependence.

2. Experiment

Single-crystal Si wafers grown by the Czochralski method with the n-type conductivity, resistivity of 4–5 Ω cm and (1 0 0) orientation were implanted by 40 keV Fe^+ ions with respective fluences of $\Phi_1 = 7 \times 10^{15}$ and $\Phi_2 = 1.8 \times 10^{17}$ cm^{-2}. Implantation was carried out at room temperature with the ion current density of $j < 5$ μA/cm^2 in order to avoid in-situ annealing. According to the SRIM calculation [6], the projected range of Fe^+ ions at this energy is equal to $R_p = 37$ nm, straggling is equal to $\Delta R_p = 13$ nm.

PIBT of amorphized Si layers was carried out in the chamber of an ion accelerator which generated a wide-aperture beam (3 cm in diameter) mainly consisting of carbon and hydrogen ions (C^+ ~80%, H^+ ~20%). The beam ion energy amounts to 300 keV, pulse duration amounts to 50 ns. Irradiation of samples was carried out with various energy densities ($W_1 = 0.7$ and $W_2 = 1.2$ J/cm^2) by three pulses. The total fluence of C^+ and H^+ ions implanted into Si during pulsed treatment does not exceed 5×10^{14} cm^{-2}. For comparison, PLA of the implanted Si layers was carried out by the radiation of a ruby laser. PLA details and its results can be found elsewhere [7]. The phase composition of Si layers after ion implantation and pulsed treatments was studied using glancing incidence X-ray diffraction (GXRD) and electron microdiffraction. The microstructure of near-surface Si layers was investigated using transmission electron microscopy (TEM) in plan-view and cross-section. The depth distribution of Fe atoms was studied using Rutherford backscattering spectrometry (RBS) of helium ions (He^+) with the energy of 1 and 3 MeV. Detectors of scattered particles were fixed at the 97° and 165° with respect to the normal of the surface. Such geometries gave the depth resolution in the 10–25 nm range [8].

The computer simulation of the iron distribution in Si during pulsed treatments was performed for two stages with the numerical calculations of the temperature fields produced by nanosecond pulsed beams and the dopant diffusion in the melt created [1]. The re-distribution of the implanted iron atoms was determined by the diffusion co-efficient in the molten silicon and the segregation co-efficient $k = C_s/C_l$, where C_s and C_l are the atomic concentrations in the solid and liquid phase at the crystallization front.