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Study of the ion implanted Fe depth distribution in Si after pulsed ion beam treatment

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The behaviour of Fe implanted into Si(100) during subsequent pulsed ion - beam treatment (PIBT) has been studied. A two-step $^{56}Fe^{+}$ ion implantation at energies of 60 and 20 keV and total doses of 10^{16} – $2x10^{17}$ cm^{-2} was used. As crystallization due to PIBT took place, Fe segregated towards the surface of the samples for the lower dose used (10^{16} cm^{-2}) and diffusion into the bulk of the Si samples occured for higher doses ($1x10^{17}$ cm^{-2} and $2x10^{17}$ cm^{-2}). The Fe concentration profile was shifted rigidly, without Fe losses. Both the movement of the Fe layer and the maximum concentration of Fe in the Si crystallized region were characterized by Rutherford backscattering spectroscopy (RBS) in combination with channelling (RBS/C).

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1. Introduction

The conventional ion beam synthesis (IBS) technique for the formation of semiconducting silicides consists of two steps: ion implantation of metal ions into Si and annealing. Several methods of annealing have been used for the preparation of silicides: conventional furnace annealing, rapid thermal annealing (RTA), laser annealing and pulsed ion-beam treatment (PIBT) [1-4]. Among these PIBT is very suitable because it affects only a local surface layer of the material (~1 μm) during a short time (< 1 μs), which eliminates the unwanted impurity diffusion into the base material [4].

Ion implantation is a non - equilibrium process. An excess of implanted atoms over the solid solubility in the system results in segregation or precipitate formation after annealing. This effect is considered to be important for the formation of a stoichiometric silicide phase in Si by IBS. Semiconducting β-$FeSi_2$ is one of the most extensively studied materials due to its potential applications for optical sources and silicon-based optoelectronic components.

In the present work the depth profiles of Fe ions of as-implanted and PIBT-annealed Si wafers were studied by Rutherford backscattering spectroscopy (RBS).

2. Experimental

Ion implantation was carried out in a type ILU-4 ion accelerator. In order to form an unburied surface layer a two-step $^{56}Fe^{+}$ ion implantation in n-type (100) Si wafers at energies of 60 and 20 keV was performed, using three different doses: $D_1=5\times10^{15}$, $D_2=5\times10^{16}$ and $D_3=1\times10^{17}$ cm^{-2}, resulting in total doses of 1×10^{16} cm^{-2}, 1×10^{17} cm^{-2} and 2×10^{17} cm^{-2} , respectively.

The samples were subjected to PIBT from a TEMP accelerator [4] using a high-power nanosecond ion beam (80% of C^{+}, 20% of H^{+}, E = 300 keV, τ = 50 ns, and W = 1.2 J cm^{-2}; five pulses were used). The total dose of C^{+} and H^{+} ions in the course of PIBT did not exceed 1×10^{14} cm $^{-2}$ per pulse. The C and H ranges in Si are well beyond the thicknesses of the initially formed amorphous layers. The C range is about 703 nm with a straggle of 118 nm and the more penetrating H component has a range of 3.08 μm with a straggle of 157 nm in Si [5]. Computer simulation of Si heating shows that during PIBT the melt thickness amounts to 1 μm and the melt duration amounts to 400 ns [4].

The depth distribution of ion-beam implanted Fe atoms in Si wafers was studied by backscattering spectrometry. RBS measurements were performed using a 3 MeV He^{+} beam from a Van de Graaff accelerator in glancing angle geometry at 97°, under random and channeling conditions.

3. Results and discussion

The initial $^{56}Fe^{+}$ implantation profiles, shown in Fig. 1 were simulated by the SRIM computer code [5]. The implanation conditions are given in Table 1. Fe peak volume concentrations calculated by SRIM and experimentally obtained from the RBS spectra of as-implanted samples are in good agreement.

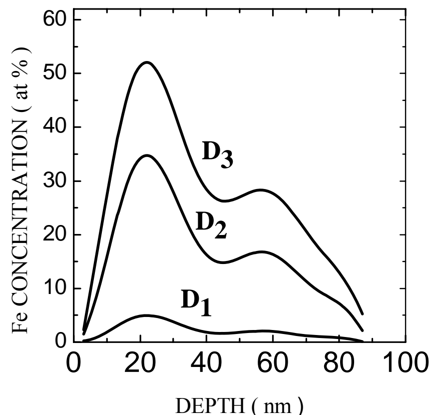

Fig. 1. Fe $^+$ Implantation profiles simulated by SRIM.

Table 1. Summary of the implantation conditions, theoretical calculations and experimental results for the peak Fe concentration of the as-implanted depth profiles.

Sample	Ion impl. $^{56}Fe^+$ Energy, Doses	SRIM N_{Fe} (%)	Exp. N_{Fe} (%)
D_{11} (as-impl.) D_{12} (PIBT)	60 кeV, 5×10^{15} cm^{-2} plus 20 кeV, 5×10^{15} cm^{-2}	5	4.6
D_{21} (as-impl.) D_{22} (PIBT)	60 кeV, 5×10^{16} cm^{-2} plus 20 кeV, 5×10^{16} cm^{-2}	32	23
D_{31} (as-impl.) D_{32} (PIBT)	60 кeV, 1×10^{17} cm^{-2} plus 20 кeV, 1×10^{17} cm^{-2}	52	49

RBS random and aligned (channeling (RBS/C)) spectra of a Fe implanted Si substrate with a D_1 dose, before and after annealing, are shown in Fig. 2 a,b,c. An apparent difference was observed between the RBS random and aligned spectra of Fe (Fig. 2(b) and Fig. 2(c), respectively). The depth of the initially formed amorphous layer (Fig. 2(b)) was estimated to be 108 nm. The peak positions from a SRIM simulation, indicated in the inset of Fig. 2(a) coincides with the measured spectrum. During PIBT, the amorphous layer completely recrystallizes. All implanted Fe atoms after PIBT are in substitutional sites (Fig. 2(c)). Fig. 2(a) shows random spectra of as-implanted and annealed samples. After annealing, the Fe peak shifts to the surface. The redistribution of Fe atoms to the Si surface (segregation), characteristic of low-solubility impurities in Si ($N_{Fe} \sim 10^{15}$ cm^{-3} at 1000 ^{o}C [6]), is observed.

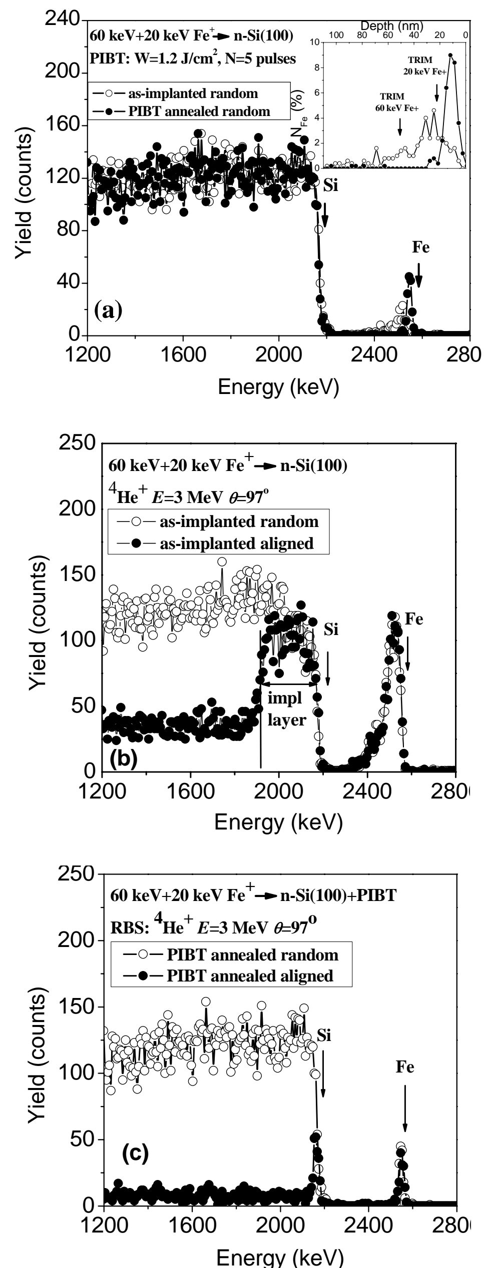

Fig. 2. RBS random and aligned spectra of implanted Si with an ion dose D_1.

In the case of the higher D_2 dose, the Fe impurity profile has a different behavior (Fig. 3(a)). Due to the high sputtering yield for Fe in Si (2.39 at.ion^{-1} for 20 keV and 2.64 at.ion^{-2} for 60 keV [5]) the initial implantation profile shifts to the surface. The maximum Fe concentration in the initial depth profile is ~ 23 %. The higher Fe concentration within the a-Si affects the redistribution during the crystallization process. A large fraction of the implanted Fe atoms diffuses toward the Si substrate. At the same time, some of the Fe atoms diffused to the Si surface are sputtered during the implantation process. Figs. 3(b) and 3(c) show RBS/C for the same samples. The depth of the amorphous layer created after the implantation – 130 nm (Fig. 3(b)) is close to that theoretically predicted by SRIM – 132 nm. All of the deeper-diffused Fe atoms occupy substitutional sites, while for the diffused atoms close to

the surface, some of the Fe atoms (~21 %) are on interstitial sites (Fig. 3(c)).

A similar behavior of the crystallization process after PIBT of Fe implanted Si with the highest total dose of $D_2 = 2\times10^{17}$ cm^{-2} (Fig. 4(a)) is observed. The accumulation of defects in the tail of the initial implantation profile leads to a slight increase in the depth of the amorphous layer - 133 nm (Fig. 4(b)). The Fe concentration at the maximum of the profile is close to the theoretical calculated value (Table 1). Fig. 4(a) shows significant diffusion during PIBT, toward the substrate. The RBS/C spectrum (Fig. 4(c)) reveals complete recrystallization of the Si matrix. Similarly to the case of the D_2 dose, the deeper diffused Fe atoms occupy substitutional sites while the atoms close to the surface are on interstitial sites. An indication of this is the difference (~ 27%) between the aligned and random spectra (Fig. 4(c)) estimated by Rutherford Universal Manipulation Program (RUMP) [7]. A similar behavior of Fe implanted atoms in Si after laser annealing was observed by Bayasitov et al. [3].

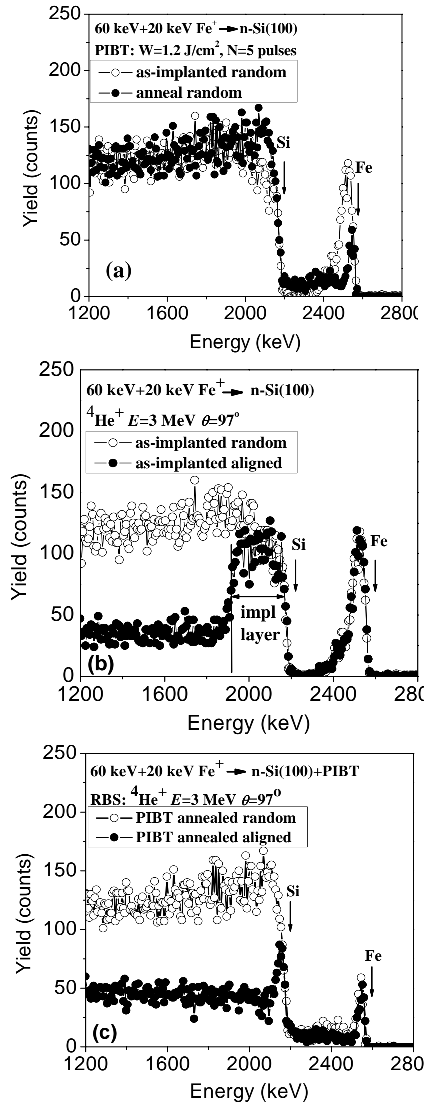

Fig. 3. RBS spectra of the Fe-implanted samples with a total dose of 1x10^{17} cm^{-2}, before and after PIBT annealing.

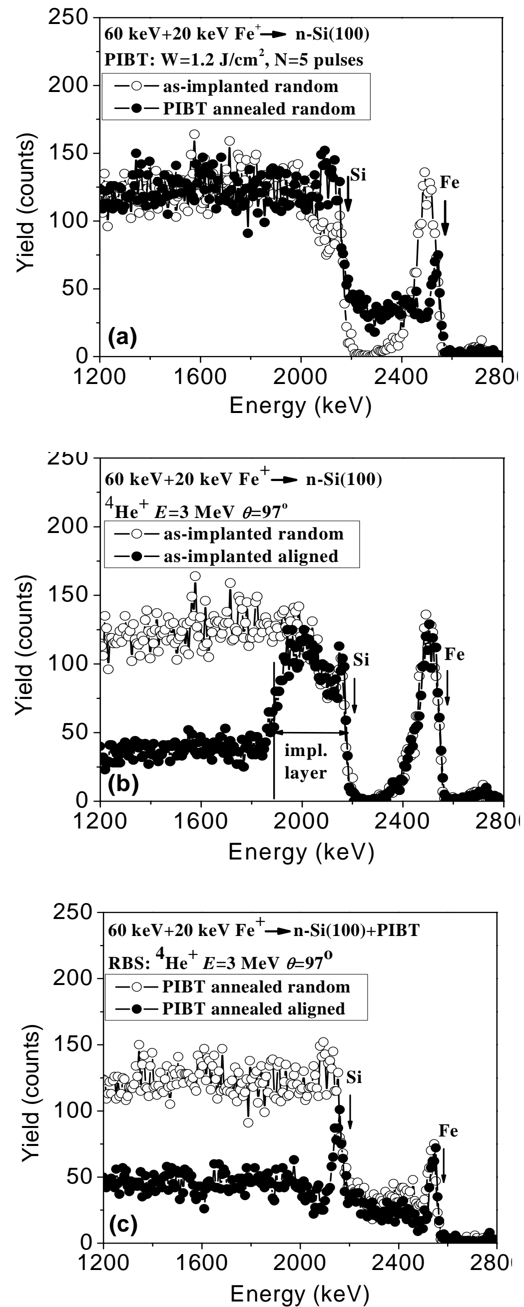

Fig. 4. RBS spectra of the Fe-implanted samples with a total dose of 2×10^{17}cm^{-2} before and after PIBT annealing.

4. Conclusions

During PIBT, significant redistribution of ion implanted Fe atoms in Si takes place. Depending on the initial Fe concentration, either segregation of the dopant to the surface or diffusion into the Si substrate occurs.

For the lowest implanted dose (1×10^{16} cm^{-2}) all implanted Fe atoms are incorporated in substitutional sites near the surface. For the intermediate dose (1×10^{17} cm^{-2}) implanted atoms diffuse into the Si and some of them remain in interstitial sites (~ 23 %). For the highest implanted dose (2×10^{17} cm^{-2}), the fraction of Fe atoms in the interstitial sites increases to 27 % after PIBT.

The results of a computer simulation agree well with the experimental data on the iron depth distribution of the as implanted samples.

The results of this investigation show the possibility of forming structures with a high concentration of Fe dopants by a non-equilibrium method – IBS.

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