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Effect of Ion Implantation Temperature on Formation of Nanometric β-FeSi2 Layer

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Abstract: A nanometric buried layer of iron disilicide was synthesized by ion implantation in Si(1 1 1) p-type at different temperatures using 195 keV Fe ions with a dose of 2.10^{17} Fe^+/cm^2. The investigation of the phase composition is carried out by Rutherford backscattering spectrometry (RBS), whereas the structural characterization is obtained by X-ray diffraction (XRD) pole figure. The process of the silicidation has been investigated at a function of the ion implantation temperatures ranging from 200 to 440 °C. The precipitates favor epitaxial growth with respect to Si(1 1 1) planes with epitaxial relationships β-$FeSi_2$(2 2 0) //Si(1 1 1) and/or β-$FeSi_2$ (2 0 2) // Si(1 1 1).

Keywords: Ion beam synthesis, β-$FeSi_2$, RBS, XRD pole figure.

1 Introduction

The study of transition metal silicides has attracted a great deal of interest for their applications as contact materials, gate electrodes, or interconnect materials in microelectronic devices [1-3]. The iron silicides have many phases and have been much studied for their unusual properties that cannot be explained by traditional means, and for their applications in microelectronics devices [4]. Iron disilicide (β-$FeSi_2$), is one of the promising candidates for thermoelectric materials [5-7], also was first applied as a bioactive material for the application of tissue engineering and could be used as a novel antitumor agent [8]. Among the iron phases, β-$FeSi_2$ is semiconducting with a band gap of about 0.80 eV [9-12]. It crystallizes in orthorhombic structure (space group: Cmca), with lattice constants a=0.9865 nm, b=0.7791 nm and c=0.7833 nm at room temperature [13-15]. Since the first successful fabrication of buried epitaxial silicides by ion beam synthesis (IBS) had been reported by White et al. [16], the IBS technique has considerably improved. In comparison with other methods, the significant interest in IBS has been directed to the formation of semiconducting iron disilicide (β-$FeSi_2$), the band gap, free of dislocation loops for appropriate implantation temperature and annealing conditions [17-19]. In this work, we report the results of the formation of buried iron disilicide layers by IBS and the characterization using Rutherford backscattering spectrometry (RBS) and X-ray diffraction (XRD) pole figure.

2 Experimental details

An iron silicide layer was produced by 195 keV Fe^+ ion implantation with a dose of 2.10^{17} Fe^+/cm^2 into a chemically cleaned p-type Si (1 1 1) wafer with a high current implanter from the DANPHYSIK A/S. During the implantation, the substrates were heated at different temperature in the range of 200 – 440 °C. The implantation conditions led to the formation of β-phase and the recrystallization of ion beam damaged Si substrates. Rutherford backscattering spectrometry (RBS) was performed with 1.7 MeV He^+ ions at a scattering angle of 170° between the incoming and outgoing beam lines using a Si-surface barrier detector with a resolution of 15 keV full width at half maximum (FWHM) and the experimental spectra were analyzed with the SIMNRA program. XRD pole figure measurements were performed in a $\theta - 2\theta$ geometry using CuK_α radiation to characterize the phases and their orientation relationship with the Si substrates.

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3 Results and Discussion

In Figure 1 shows the RBS spectrum of a Si(111) sample implanted at T_i=200 °C with an iron dose of 2.10^{17} Fe^{+}/cm^2, obtained in the random direction. The arrows (labeled Fe and Si) indicate the energy for backscattering from these elements at the surface. The SIMNRA simulation of RBS spectrum allowed to obtain the depth profiles of Si and Fe elements (see inset, Figure 1) and to confirm the formation of an Fe–Si intermixed layer during the ion implantation.

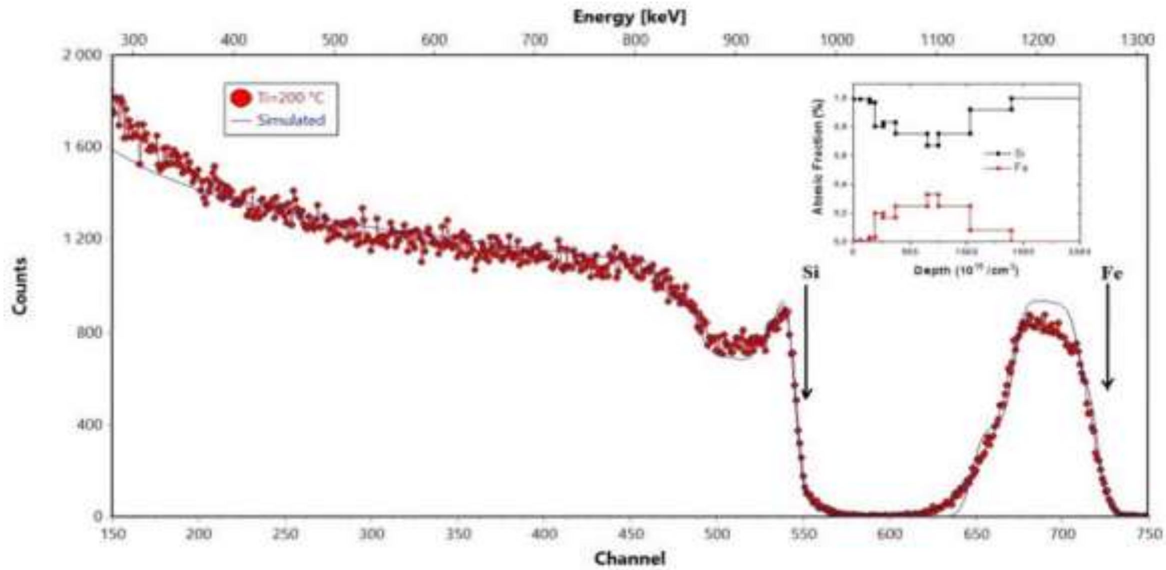

Fig. 1: Random RBS spectrum for the implanted sample at 200 °C. Inset shows the depth profiles of Si and Fe elements deduced from the SIMNRA analysis.

Figure 2 shows the RBS spectra of the samples implanted at different temperatures. As it can be seen, the height of Fe signal around channel 708 slightly decreases whereas the temperature of implantation increases. In the same time, the Si signal, around channel 500, corresponding to the intermixed buried layer is extended to the surface whereas the temperature of implantation decreases.

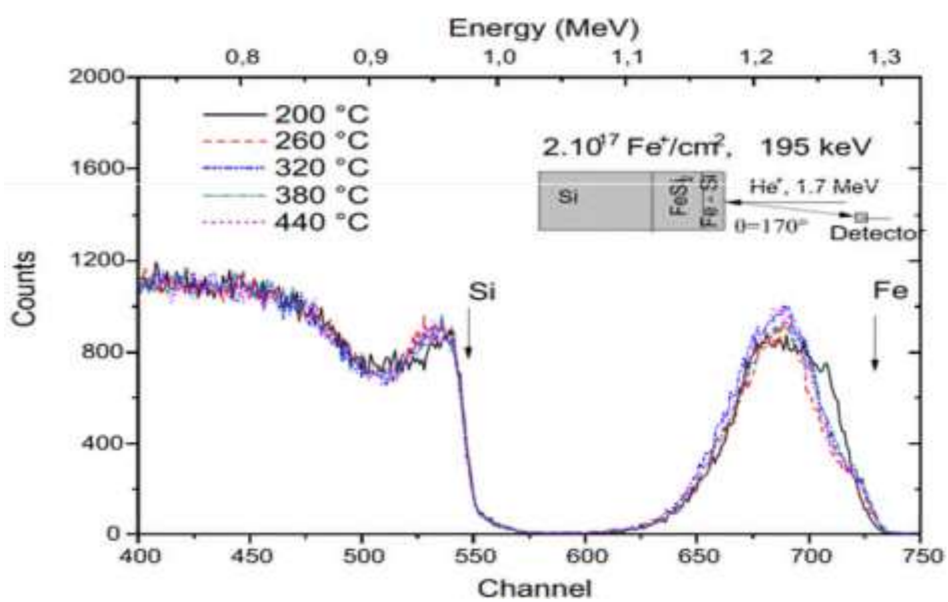

Fig. 2: RBS spectra for the samples implanted at different temperatures.

The effects of ion implantation temperatures on the amorphization of Si during low temperature implantation will be even more significant. It is noticed that $FeSi_2$ phase was observed for all the ion implantation temperatures.

Figure 3 shows the thickness of $FeSi_2$ buried layers as a function of ion implantation temperatures deduced from SIMNRA simulation of RBS spectra. As it can be seen, the thickness of $FeSi_2$ increases whereas the implantation temperature increases.

This result reveals in the evidence the interactions between iron and silicon atoms during the ion implantation at different temperatures, and it is in a good agreement with XRD analysis.

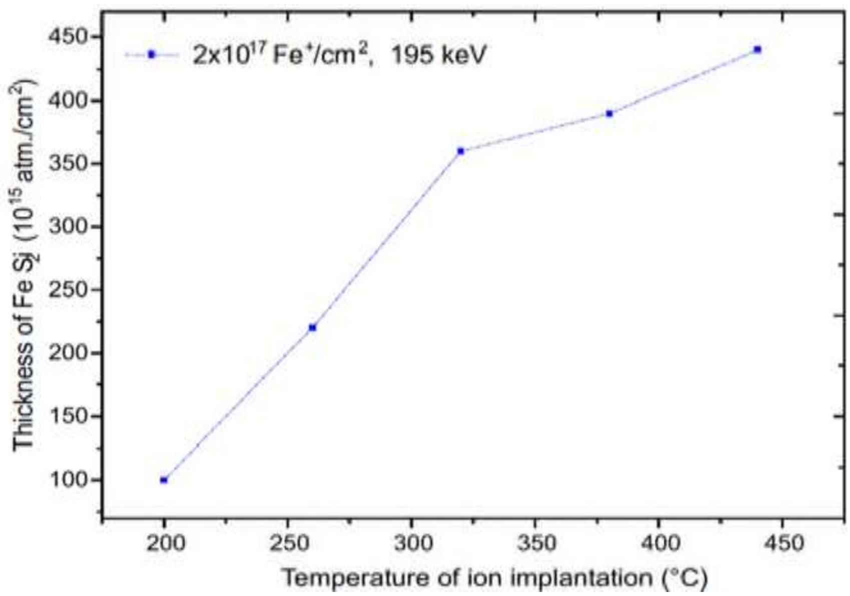

Fig. 3: The $FeSi_2$ thickness as a function of ion implantation temperature.

Figure 4 shows the XRD pole figure of the sample implanted with a dose of 2.10^{17} Fe^+/cm^2 at T_i =340 °C. As can be seen, the poles with the heights of 11.36, 11.36 and 12.86 near the center and at scattering angle 2θ = 29.112° in the periphery are β-$FeSi_2$(2 2 0) /β-$FeSi_2$(2 0 2) reflections, are measured with steps of 5° of ϕ and χ angles (ϕ and χ are the azimuth and rotation axes perpendicular to the substrate, respectively) in the whole range of ϕ and a limited range of χ of three β-$FeSi_2$ poles.

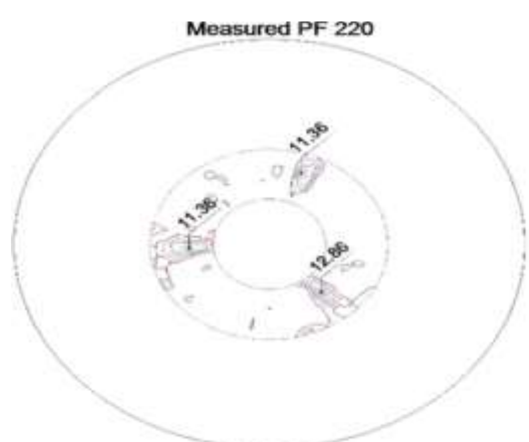

Fig. 4: X-ray pole figure plot of (2 2 0) diffraction peak of β-$FeSi_2$ and Si(1 1 1) for the sample implanted at 380 °C.

As a result, the epitaxial relationship is described as follows:β-$FeSi_2$(2 2 0) and/or β-$FeSi_2$(2 0 2)

//Si(1 1 1). In order to estimate the formation of β-$FeSi_2$ at different implantation temperatures a part of a pole figure of the most intense reflections β-$FeSi_2$ (220), β-$FeSi_2$ (202) near the pole figure center (for χ in the limits of 25° and 50°) at the scattering angle 2θ=29.112 ° are measured. The intensity values proportional to the amount of β-$FeSi_2$ is shows in Figure 5. The value is the sum of the peak intensities of the three β-$FeSi_2$ poles shown in the pole figure.

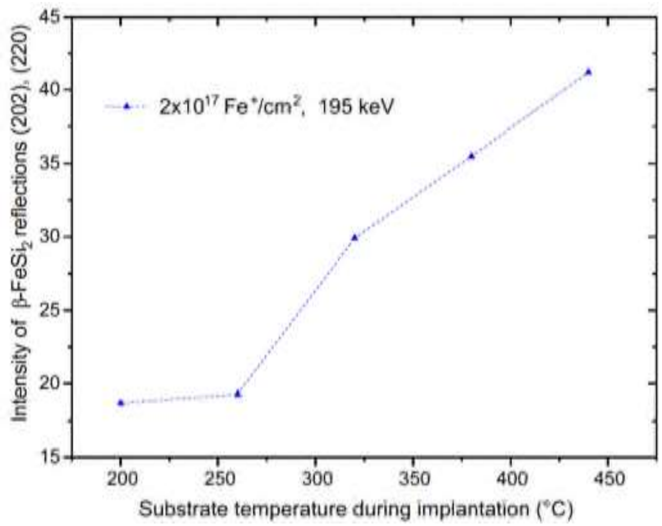

Fig. 5: The intensity values of β-$FeSi_2$(2 2 0) and/or β-$FeSi_2$(2 0 2) //Si(1 1 1) as a function of ion implantation temperature.

The formation of iron disilicide and well crystallized β-$FeSi_2$ layer can be synthesized when the implantation temperature increases. It is obvious that with the rise of the implantation temperarture, the (2 2 0)/(2 0 2) peak of β-$FeSi_2$ became stronger and larger amount of β-$FeSi_2$ was formed.

4 Conclusions

In this study, the formation of iron disilicide was investigated under different conditions. The implantation of 195 keV Fe^+ with a dose of 2.10^{17} at./cm^2 in Si(1 1 1) substrates at different temperatures allows the formation of a continuous buried β-$FeSi_2$ layer. The buried layer is grown epitaxially on Si(1 1 1) substrate with the relation of β-$FeSi_2$(2 2 0) and/or β-$FeSi_2$(2 0 2) // Si(1 1 1). The thickness of $FeSi_2$ increases whereas the implantation temperature increases. The formation of nanometric iron disilicide and well crystallized β-$FeSi_2$ layer can be synthesized when the implantation temperature increases.

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