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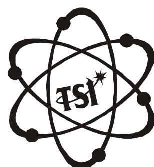

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Structural and optical characterization of β-$FeSi_2$ layers formed by ion beam synthesis

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ABSTRACT

Buried layer of semiconducting iron disilicide has been synthesized by implantation of Fe ions with an energy of 195 keV and a dose of $2x10^{17}$ Fe^+/cm^2 into Si(111) wafers, maintained at 500°C, followed by annealing in a N_2 atmosphere at 750°C for 90 min. Rutherford Backscattering Spectrometry (RBS) and X-ray diffraction (XRD) pole figure have been used to investigate the growth and the structure of the formed iron disilicide, and the depth profile of atomic composition of Fe and Si elements. The precipitates favor epitaxial growth with respect to Si(111) planes with the epitaxial relationships of β-$FeSi_2$(220)//Si(111) and /or β-$FeSi_2$(202)//Si(111). The optical characteristics of the obtained samples have been measured at room temperature (RT) by means of Infra-Red (IR) and Raman spectroscopies, and have been correlated with the structural properties.
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INTRODUCTION

Semiconducting iron disilicide (β-$FeSi_2$) is considered as a promising material for silicon based optoelectronics due to its band gap of about 0.8 eV[1,2]. This energy corresponds to a wavelength of 1.55 µm, which is of great interest for applications in optical fiber based telecommunications, infrared detectors, and thermoelectronics devices[3-5]. The iron disilicide ($FeSi_2$) exists in two phases. The tetragonal α-$FeSi_2$ (lattice parameters a=b=0.266 nm and c=0.514 nm) is a metallic phase[6] and the orthorhombic β-$FeSi_2$ is a semiconducting phase with lattice parameters a=0.9863 nm, b=0.7791 nm, and c=0.7833 nm at room temperature[7]. The ion beam synthesis (IBS) is widely used for the formation of epitaxial silicides[8,9].

The aim of this work is to investigate the formation by the IBS technique of iron silicide layer in Si(111) substrate by means of Rutherford backscattering spectrometry (RBS), X-ray diffraction (XRD) pole figure, and the IR and Raman characteristics of the studied samples.

EXPERIMENTAL

A buried iron silicide layer was produced by implanting iron ions at T_i=500°C with a dose of $2x10^{17}$ Fe^+/cm^2 and an energy of 195 KeV into a P-type single crystal Si(111) wafer. The ion source is a DANPHYSIK high current operated at 20-200 KeV, with magnetic scan, current limit< 10 mA, and target station with a possibilities to move large and heavy

samples. The as-implanted samples were then annealed in N_2 atmosphere at 750°C for 90 min.

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. The experimental energetic spectra were analyzed with RUMP computer program[10]. XRD pole figure measurements were performed in a θ-2θ geometry using CuK_α radiation. The IR transmittance and Raman spectra were taken at room temperature (RT) in the range of 150-550 cm^{-1} and 150-550 cm^{-1} respectively.

RESULTS AND DISCUSSION

Figure 1 shows the random RBS spectrum of the Fe as-implanted Si(111) substrate at T_i=500°C. The arrows (labeled Fe and Si) indicate the energy for backscattering He^+ ions from these elements at the surface. The RUMP simulation of RBS spectrum allows to establish the depth profile of Fe and Si elements (see inset, Figure 1) and to confirm the formation of thin $FeSi_2$ buried layer (62 nm).

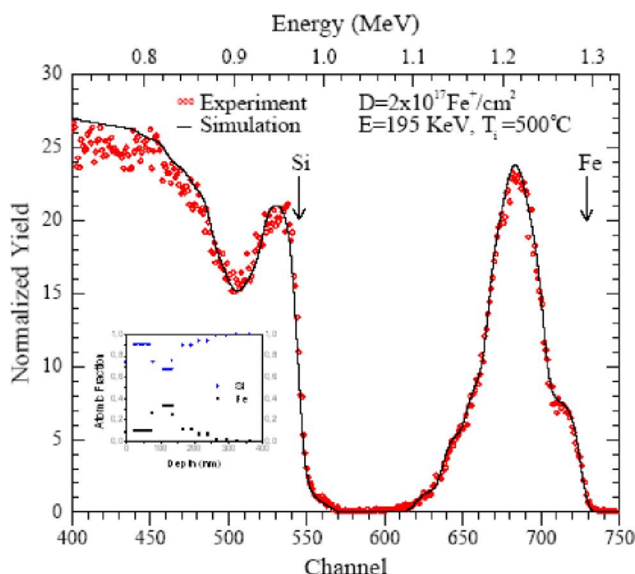

Figure 1 : Random RBS spectrum for the as-implanted samples. Inset shows the depth profiles of Si and Fe elements deduced from the RUMP analysis.

Figure 2 shows the RBS spectra of the as-implanted and annealed samples at 750°C for 90 min. As can be seen, the height of Fe signal slightly decreases whereas the energetic width increases. In the same time, the Si signal around channel 500, corresponding to the buried $FeSi_2$ layer, is slightly extended to the surface with a thickness about 88 nm.

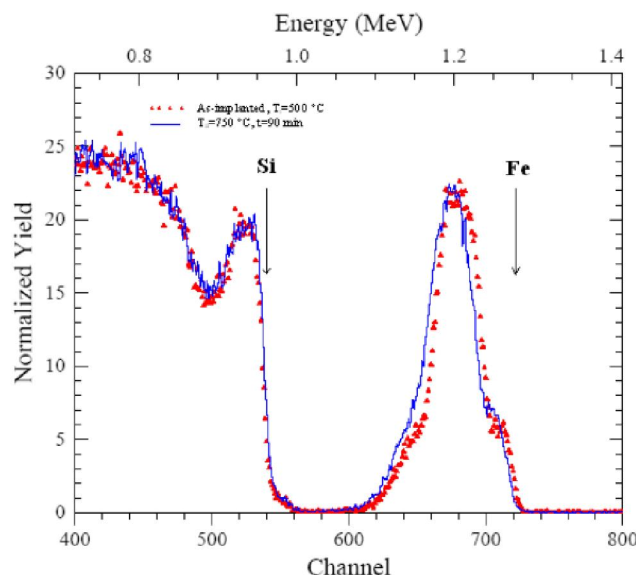

Figure 2 : RBS spectra for the as-implanted and annealed samples at 750°C for 90 min.

The figure 3(a) shows the partial pole figure of the annealed samples in N_2 atmosphere at 750°C for 90 min. The poles are measured with steps of 5° of φ and χ angles (φ is the rotation angle around the surface normal and χ is the tilt angle of the sample) in the whole range of φ and in the range χ=35-40°. The poles with the heights of 39.17, 38.11 and 34.92 at the scattering angle 2θ=29.112° are β-$FeSi_2$(220) /(202) reflections. These results indicate the formation of epitaxial β-$FeSi_2$(220) and /or β-$FeSi_2$(220) on the Si(111) substrate. The figure 3(b) presents the partial pole figures of α-$FeSi_2$ reflections in the whole range of φ and χ=35-45° at the scattering angle 2θ=37.668° of the annealed sample. The six poles near the centre with heights of 33.05, 37.97, 8.92, 26.63, 9.18 and 26.04 are α-$FeSi_2$(101) reflections. It is interesting to note that the intensities of the three poles of β-$FeSi_2$ and α-$FeSi_2$ increase in the case of the annealed sample in comparison with those obtained in the as-implanted sample which have been reported elsewhere[11]. This fact attests of the increase in the amount of β and α phases. The infrared (IR) transmittance spectra measured at RT in the range of 150–500 cm^{-1} for as-implanted and annealed samples are shown in figure 4. The five main peaks can be assigned to the five active IR internal modes of the

iron sites characteristic for β-$FeSi_2$. The values of frequencies are 262.4, 295.1, 310, 345.3 and 422.2 cm^{-1}, and are in a good agreement with those previously published by Daraktchieva et al.[12]. The IR spectra of the as-implanted and annealed samples at 750°C for 90 min are comparable and they reveal the formation of β-$FeSi_2$ phase. The absorption at 310 cm^{-1} can be explained by an initial nucleation of β-$FeSi_2$ precipitates during the implantation of iron into silicon substrate.

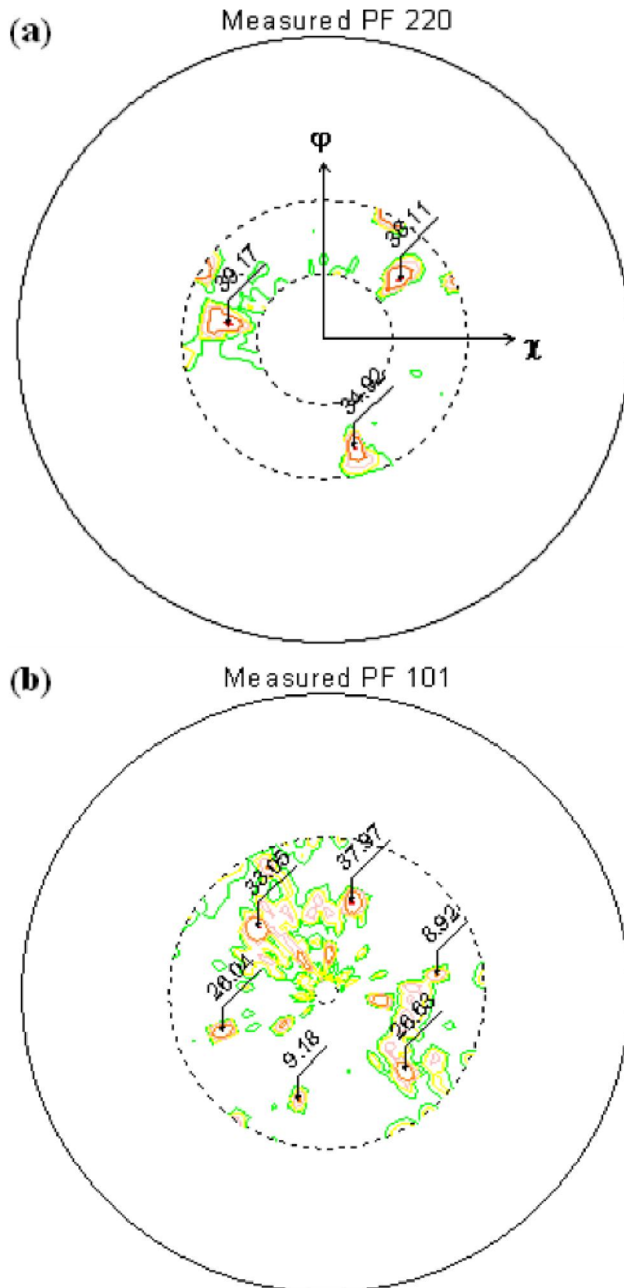

Figure 3 : XRD Pole figures of β-$FeSi_2$(220) at 2θ=29.112° (a), and α-$FeSi_2$(101) at 2θ=37.668° for the annealed sample (b).

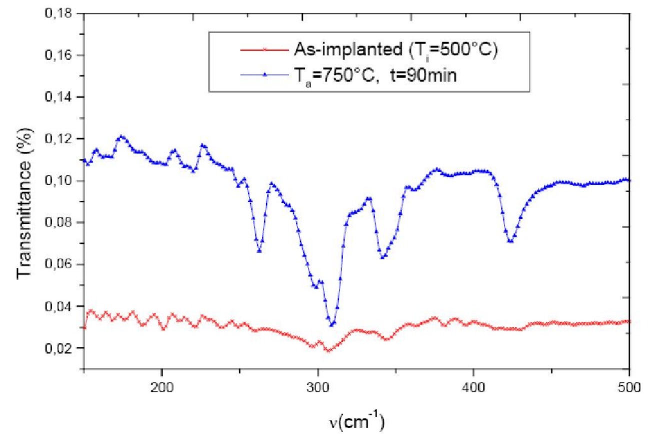

Figure 4 : IR spectra for the as-implanted and annealed samples.

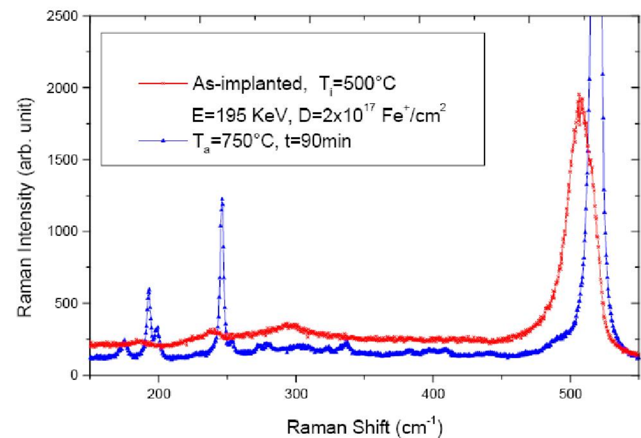

Figure 5 : Raman scattering spectra at RT for the as-implanted and annealed samples.

Figure 5 illustrates the Raman scattering spectra obtained at RT for as-implanted and annealed samples. The crystalline silicon has a typical line at 520 cm^{-1}. As can be seen, no important lines are detected in the as-implanted sample, because the amount of β-$FeSi_2$ is too small. However, in the case of the annealed samples, the Raman peaks have different intensities and are associated to Fe–Si vibrational modes[13], indicating the formation of β-$FeSi_2$ phase. We notice that all experimental peaks are red shifted compared to those obtained theoretically[13]. This shift may be explained by the stress caused during the implantation and the heat treatment.

CONCLUSION

β-$FeSi_2$ phase was fabricated by IBS technique with a dose of $2x10^{17}$ Fe^+/cm^2 and an energy of 195 KeV in Si(111) substrates at T_i=500°C followed by an anneal-

ing in N_2 atmosphere at 750°C for 90 min. The buried layer is grown epitaxially on Si(111) substrate with the epitaxial relationships of β-$FeSi_2$(220) and/or β-$FeSi_2$ (202) //Si(111). A mixture of β-$FeSi_2$ and α-$FeSi_2$ is observed. The IR transmittance spectra show the five main peaks of β-$FeSi_2$, and the absorption at 310 cm^{-1} indicates the initial nucleation of β-$FeSi_2$ precipitates during the implantation. The Raman signals for β-$FeSi_2$ are slightly shifted toward lower energies.

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REFERENCES

[1] M.C.Bost, J.E.Mahan; J.Appl.Phys., **74**, 1138 (**1993**).

[2] B.Schuller, R.Carius, S.Mantl; J.Appl.Phys., **94**, 207 (**2003**).

[3] D.Leong, M.Harry, J.K.Reeson, K.P.Homewood; Nature, **387**, 686 (**1997**).

[4] Y.Ozawa, T.Ohtsuka, Cheng Li, T.Suemasu, F.Hasegawa; J.Appl.Phys., **95**, 5483 (**2004**).

[5] A.Heinrich, H.Griessmann, G.Behr, K.Ivanko, J.Schumann, Vinzelberg; Thin Solid Films, **381**, 287 (**2001**).

[6] N.Kbayashi, H.Katsumata, H.L.Shen, M.Hasegawa, Y.Makita, H.Shibata, S.Kimura, A.Obara, S.Uekusa, T.Hatano; Thin Solid Films, **270**, 406 (**1995**).

[7] Y.Dusaussoy, J.Protas, R.Wandji, B.Roques; Acta.Cryst.B, **27**, 1209 (**1971**).

[8] D.Gerthsen, K.Radermacher, Ch.Deiker, S.Mantl; J.Appl.Phys., **71**, 3788 (**1992**).

[9] D.J.Oostra, C.W.T.Bulle-Lieuwma, D.E.W.Vandenhoudt, F.Felten, J.C.Jans; J.Appl. Phys., **74**, 4347 (**1993**).

[10] L.R.Doolittle; Nucl.Instr.and Meth.B, **9**, 344 (**1985**).

[11] R.Ayache, E.Richter, A.Bouabellou; Nucl.Instr.and Meth.B, **216**, 137 (**2004**).

[12] V.Daraktchieva, M.Beleva, E.Garonova, Ch.Angelov; Vacuum, **58**, 415 (**2000**).

[13] H.Kakemoto, Y.Makita, S.Sakuragi, T.Tsukamoto; Jpn.J.Appl.Phys., **38**, 5192 (**1999**).