PULSED ION BEAM SYNTHESIS OF β-$FeSi_2$ LAYERS ON Si IMPLANTED WITH Fe^+

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ABSTRACT

Formation of β-$FeSi_2$ layers on Si was performed by high-dose Fe^+ implantation into Si (100) at 300 K followed by pulsed ion beam treatment (PIBT) of nanosecond duration on implanted layers. It is shown that PIBT leads to the formation of a mixture of two phases (FeSi and β-$FeSi_2$) with a strained state of the silicide crystal lattice. Subsequent short-time thermal annealing at 800^0C for 20 min results in the decrease of lattice strains and in the complete transformation of the FeSi phase into the β-$FeSi_2$ phase with the production of a highly textured layer with [110] orientation. The results of the optical absorption measurements indicate the formation of a direct band gap structure with the optical gap E_g~0.83 eV.

1. INTRODUCTION

Formation of Si-based structures emitting in the visible and near infrared (IR) spectral region attracts essential interest for last 10-15 years. One of the main approaches to the fabrication of structures emitting in the wavelength λ~1.55 μm is the formation of β-$FeSi_2$ layers. β-$FeSi_2$ is the semiconducting phase of the Fe-Si system with orthorhombic structure and direct band gap E_g~0.85 eV [1-4]. This gap value corresponds to the optical wavelength λ~1.45 μm which is close to the technologically important λ~1.55 μm corresponding to the silicon transparency region and absorption minimum of the silica optical fibers. This fact allows one to create optoelectronic devices in the near IR region integrated in the silicon microelectronic technology.

In order to form β-$FeSi_2$ layers an ion-beam synthesis technique i.e. high-dose Fe^+ implantation into Si with *in-situ* heating [5] or high-temperature and long-duration annealing (T=800-900^0C, t~20 h) [6-8] is widely used. However at such thermal annealing the diffusion essential of iron atoms in the basic material takes place due to the large diffusion coefficient of Fe in Si at high temperatures (D~$5\cdot10^{-6}$ cm^2/s at T=1000^0C) and can give rise to severe device yield and reliability problems [9].

Using of nanosecond pulsed treatments by laser, electron and ion beams allows one to overcome this drawback due to local (~ 1 μm) and short-time (< 1 μs) heating of materials. At present there are many publications on pulsed laser treatment of thin metal films onto Si [10]. However they were concerned with the formation of metal silicides for interconnections, Ohmic and Schottky barrier contacts.

In order to synthesize semiconducting silicide β-$FeSi_2$ for optoelectronic applications, laser treatment of Fe films onto Si is used [11], whereas the reports on pulsed treatment of Fe^+ implanted Si are absent. In this work for the first time pulsed ion beam treatment (PIBT) of Fe^+ implanted Si is used to form a submicron β-$FeSi_2$ layers. Characteristic features of PIBT are a more uniform depth distribution of energy losses in the material compared to that under laser treatment resulting in lower surface overheating and disruption [12]. High rates of the heating, melting and recrystallization (~10^7-10^9 K/c) lead to formation of the epitaxial, defect-free and highly-doped Si layers [13-15].

2. EXPERIMENTAL

Single-crystal (100) Cz-Si wafers with an n-type resistivity of 1-4 Ω·cm were implanted by Fe^+ ions at room temperature (RT) with energy of 40 keV and dose of $1.8 \cdot 10^{17}$ cm^{-2} (ion current density of 5 μA/cm^2). After the implantation, one part of implanted samples was subjected to PIBT on a TEMP accelerator [16] (C^+-80%, H^+-20%, E=300 keV, τ=50 ns, j~50 A/cm^2, W~0.75 J/cm^2) with the total dose per pulse not exceeding of 10^{14} cm^{-2}. The other part of implanted samples was subjected to thermal annealing (TA) in a quartz furnace with ambient nitrogen at 800^0C for 20 min to compare the results. Crystal structure of formed layers was studied by glancing x-ray diffraction technique (GXRD) using FeKα radiation (λ=1.9373 Å). The azimuth dependencies of most intense diffraction peaks were measured by fixing the detector at corresponding positions and performing azimuth angle scans from 0^0 to 360^0 at a step of 3^0. IR spectroscopy in the reflection and transmission mode was employed to determine the band gap energy. The measurements were performed at RT in the spectral range λ=1100-2000 nm.

RESULTS AND DISCUSSION

After ion implantation no reflections are present in the GXRD pattern (not shown) indicating that complete amorphization of the implanted layer takes place. Fig.1 shows GXRD patterns of the samples subjected to various treatment regimes after ion implantation. From fig.1 (a) one can see that after PIBT two phases takes are mixed: the metallic FeSi and semiconducting β-$FeSi_2$. The most intensive peak in the spectrum belongs to the Bragg reflections from (220)/(202) planes of the β-$FeSi_2$ phase. The position of this peak ($2\theta=36.1^0$) differs from the table value ($2\theta=36.9^0$). Disilicide crystal lattice deformation estimated from the difference of interplane distances in the strained and unstrained states is ε~2 %. Similar behavior for other diffraction peaks present in the spectrum is observed. The difference observed in the positions of Bragg reflections can be explained by a strained state of silicide crystal lattice which is caused by the rapid liquid-phase crystallization after PIBT.

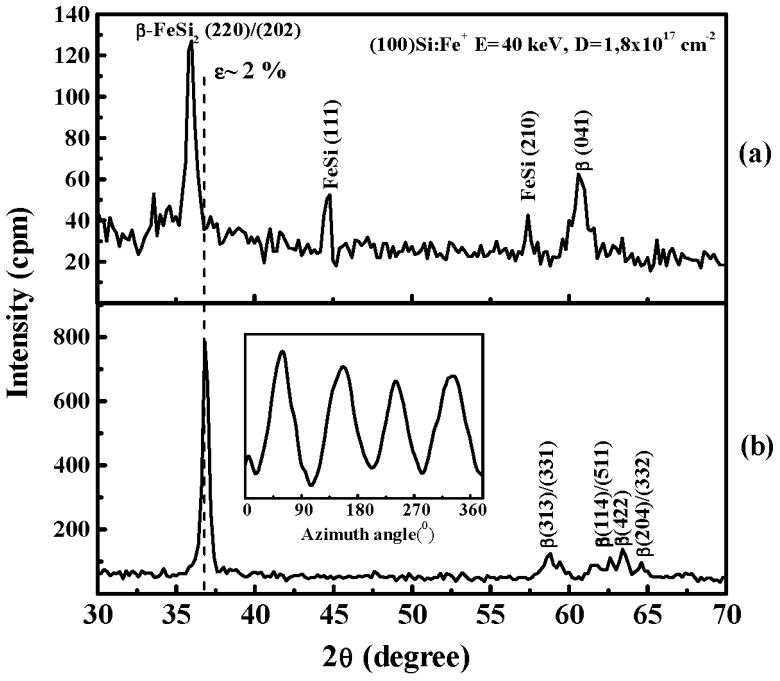

Figure 1. GXRD patterns of the implanted Si (40 keV/1.8·10^{17} Fe^{+}/cm^{2}). (a) after PIBT (0.75 J/cm^{2}) and (b) after PIBT and additional TA (800^{0}C, 20 min). In the inset an azimuth dependence of β-FeSi$_2$ (220)/(202) diffraction peak is shown.

In order to remove the lattice strains and to transform the residual amount of the FeSi phase into the β-FeSi$_2$ one a short-time TA (800^{0} C, 20 min) was performed. GXRD pattern after additional TA is shown in fig. 1 (b). One can see the essential increase of (220)/(202) β-FeSi$_2$ peak intensity and its shift to the value of 2θ=36.9^{0}, indicating that the strains in the silicide lattice are removed. Moreover, Bragg reflections of the FeSi phase disappear as well. The ratio of the integrated intensities I_{220}:I_{422} is about 8.7 whereas in randomly oriented β-FeSi$_2$ powders this ratio is about 1.25. This fact indicates that the preferable grain orientation (texture) is present. In the inset of fig. 1 (b) an azimuth dependence of the (220)/(202) peak is shown, indicating the presence of the high-degree texture with [110] orientation on Si (100).

Fig. 2 shows the AFM morphology of the implanted Si surface after above treatments. One can see the formation of silicide grains with sizes up to 400 nm in plan whereas the surface roughness is about 4-5 nm.

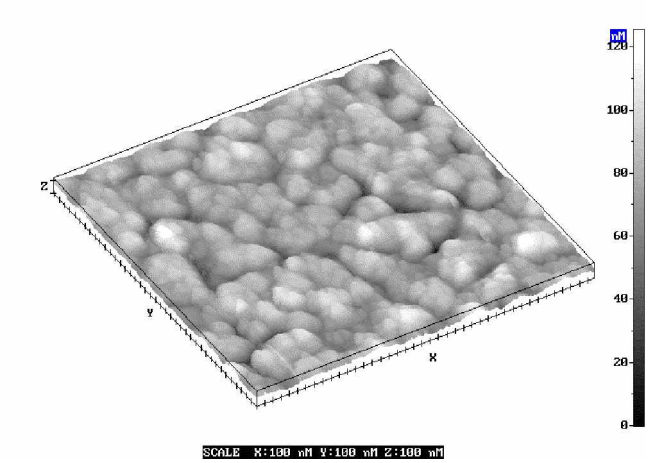

Figure 2. AFM morphology of the implanted Si (40 keV/1.8·10^{17} Fe^{+}/cm^{2}) after PIBT (0.75 J/cm^{3}) and additional TA (800^{0} C, 20 min).

The dependence of the absorption coefficient α on the photon energy E for the direct interband transitions is given by [17]

$$\alpha = A\left(E - E_g\right)^{1/2}, \qquad (1)$$

where A is a constant that is associated with specific features of the band structure and E_g is the magnitude of the direct band gap. The absorption exponent αd (d is the layer thickness) is found according to the equation

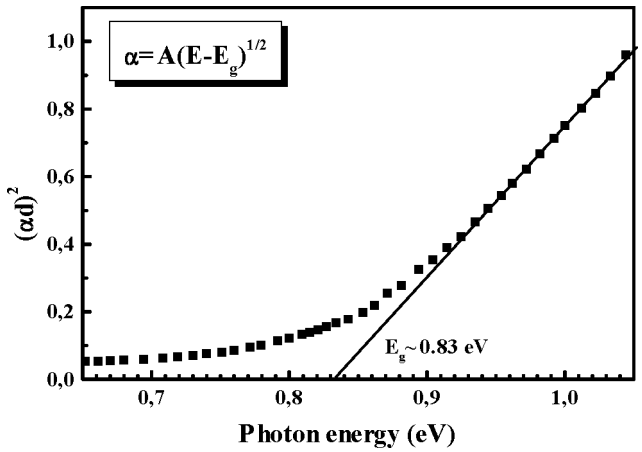

Figure 3. Square of the absorption exponent vs photon energy for the implanted Si after PIBT (0.75 J/cm^{2}) with additional TA (800^{0}C, 20 min). The solid line shows an extrapolation of the absorption data to determine E_g value.

$$\alpha d = \ln\left(\frac{1-R}{T}\right), \qquad (2)$$

where R and T are the reflectance and transmittance, respectively. From the dependence of $(\alpha d)^2$ on E one can determine the E_g value by extrapolating the straight line down to the intersection with the E axis (fig. 3). The obtained E_g value (~0.83 eV) is close to those of ion-beam synthesized β-$FeSi_2$ given in the literature [2-4].

Work is in progress to investigate the photoluminescence properties of the formed β-$FeSi_2$ layers in the near IR region.

3. CONCLUSIONS

We have shown that PIBT of Fe^+ implanted Si leads to the formation of the mixture of two phases (FeSi and β-$FeSi_2$) with a strained state of the silicide crystal lattice. Subsequent short-time TA (800^0C, 20 min) results in the decrease of lattice strains and the complete transformation of FeSi phase into β-$FeSi_2$ one with the production of a highly textured layer with [110] orientation on Si (100). The results of the optical absorption measurements indicate the formation of a direct band gap structure with the optical gap E_g~0.83 eV.

Acknowledgments

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