STRUCTURAL AND OPTICAL PROPERTIES OF Si/β-$FeSi_2$/Si HETEROSTRUCTURES FORMED BY ION IMPLANTATION AND MBE

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The method of ultrahigh vacuum and low-temperature cleaning of Si(100) and Si(111) samples implanted by Fe^+ ions with different fluencies (Φ = 10^{15} -1.8×10^{17} cm^{-2}) and subsequent epitaxial growth of a Si layer has been applied for the first time. The possibility of the formation of atomically smooth and reconstructed Si surfaces after Fe^+ implantation and nanosecond pulsed ion-beam treatment has been shown. It was found that smooth Si films with thickness up to 1.7 μm and with reconstructed surface grow up to fluence $\Phi = 10^{16}$ cm^{-2}. The formation of β-$FeSi_2$ precipitates inside Si matrix after the growth of epitaxial Si layer by MBE has been confirmed by optical spectroscopy. Low temperature photoluminescence measurements in the range of 1300-1700 nm showed that light emission of the formed Si/β-$FeSi_2$/Si heterostructures is due to contributions from β-$FeSi_2$ precipitates and dislocations.

Introduction

In recent years the considerable attention has been paid to the formation of isolated precipitates and continuous layers of semiconducting iron disilicide (β-$FeSi_2$) in Si due to the possibility of application of β-$FeSi_2$ in optoelectronics as a light emitter in the 1.5-1.6 μm range. The main methods for the formation of β-$FeSi_2$ are Fe^+ implantation of Si [1] and reactive deposition epitaxy of Fe layers followed by molecular beam epitaxy (MBE) of Si layer [2]. Both methods include the high-temperature (up to 900 °C) and long-time (up to 20 hours) furnace annealing undesirable for device structures because their parameters essentially degrade at elevated temperatures. Pulsed treatments of the implanted layers by nanosecond laser, ion and electron beams can be alternative to thermal annealing. Such treatments allow one to localize heating of Si crystal for its area and depth. Moreover, high rates of heating, melting and subsequent crystallization taking place during pulsed treatments lead to the formation of defect-free epitaxial Si layers. We have demonstrated earlier the formation of β-$FeSi_2$/Si heterostructures by low-energy Fe^+ implantation and pulsed treatments by ion and laser beams [3,4]. For subsequent fabrication of light-emitting diodes the formation of Si/β-$FeSi_2$/Si heterostructures is highly preferably.

In this paper a new low temperature growth technology including Fe ion implantation and Si MBE is applied for the first time. The structural and optical properties of the grown Si/β-$FeSi_2$/Si heterostructures are studied.

Experiment

The implantation of Fe^+ ions into monocrystalline Si wafers with (100) and (111) orientations was carried out at room temperature with ion energy E = 40 keV (R_p = 37 nm, ΔR_p = 13 nm) and fluencies in the range $\Phi = 10^{15} - 1.8\times10^{17}$ cm^{-2}. The details of sample preparations are given in Table 1. Pulsed ion-beam treatment (PIBT) of the implanted Si layers was carried out using pulsed ion accelerator which generated high-energy (E = 300 keV) nanosecond (τ = 50 ns) carbon ion beams (C^+). Pulse energy density varied between W = 1.2-1.5 J/cm^2 and the fluence of C^+ ions does not exceed $\Phi \sim 10^{13}$ cm^{-2}.

Si overgrowth was performed in two UHV chambers with base pressures $p = 10^{-10}$ and 10^{-9} Torr. Both chambers were eouipped with sublimation p-type Si sources (N_p = $10^{[illegible]}$ cm^{-3}) for MBE growth. The first chamber was equipped with Auger electron spectrometer (AES) used for measuring of impurity concentrations on Si surface before and after cleaning procedure, the last one had the low energy electron diffraction (LEED) facility for *in-situ* studying of the structure of the grown Si layers. Si deposition rate was controlled by quartz sensor of thickness. Si samples were annealed by applying of direct current.

Table 1. Parameters of samples

Sample	Substrate	Implanted fluence, (cm^2)	Type of conductivity	Resistivity, (Ωcm)
A	Si(111)	10^{16}	*p*	20
B	Si(111)	1.8×10^{17}	*p*	20
C	Si(100)	10^{15}	*n*	4.5
D	Si(100)	10^{16}	*n*	4.5
E	Si(100)	1.8×10^{17}	*n*	4.5

Atomic force microscopy (AFM) investigations of samples morphology were performed using multimode SPM Solver P47. Optical spectra of the samples before and after Si overgrowth were investigated using automatic spectrophotometer Hitachi H-3010 at 300 K.

Photoluminescence (PL) measurements were carried out at T = 5 K in the range of 1300-1700 nm using He-Ne laser (λ = 632.8 nm, 40 W/cm^2). PL spectra were analyzed in spectrometer on the basis of double monochromator and detected by Ge photodiode from «Edinburgh Instruments».

Results and discussion

After Fe^+ implantation and PIBT the surface of samples *A* and *B* (Table 1) represents the cellular structure which also was observed earlier in [4] by TEM. The formation of cellular structure is related to low solubility of Fe in Si (~ 10^{16} cm^{-3}) and to Fe segregation on Si cell walls due to instability of the solid/liquid interface. The surface of samples *C* and D after PIBT was quite smooth (σ_{rms} = 0.23 and 0.4

nm). Increase of the fluence up to 1.8×10^{17} cm^{-2} (sample *E*) results in the increase of local surface non-uniformity as well as occurrence of areas with large relief (σ_{rms} = 2.62 nm) and with $FeSi_2$ crystallites occurred on the surface in the form of granular film. The formation of β-$FeSi_2$ phase is confirmed by optical reflectance spectroscopy data, type of absorption spectra and the presence of interband transitions (2.7 eV) corresponding to β-$FeSi_2$ [5].

A new low-temperature (LT) cleaning procedure suitable for Si overgrowth upon Si layers implanted by Fe^+ ions has been studied. The sample kept at *T* = 850 ^{0}C was exposed to the Si atomic flow with small rate of about 0.1 nm/min for 15-20 minutes which provides decomposition of thin SiO_2 film. AES data revealed that all oxide and carbon contaminations were completely removed and clean Si surface was obtained as a result of this procedure. This procedure was successfully applied for the first time for Fe^+ implanted samples.

After LT cleaning the samples *C* and *D* demonstrated Si(100)2×1 LEED pattern that corresponds to the formation of smooth and atomically clean surface. For fluence higher than 10^{16} cm^{-2} (sample *E*) no LEED pattern was observed that can be related to high residual density of defects. Thus, the increasing of ion fluence results in the increase of defect concentration on Si surface after PIBT in nanometer scale and these defects persisted after LT cleaning procedure.

Si overgrowth on the surface of all samples was performed after LT cleaning. After Si overgrowth (T_{Si} = 700 ^{0}C) on the samples *C* and *D* a smooth (σ_{rms} = 0.08 нм) epitaxial film with thickness of 1700 nm was obtained and LEED Si(100)2×1 pattern was observed without any additional annealing. The annealing of defects on the surface takes place during Si deposition and then the growth goes on epitaxially and surface ordering takes place. The increasing of the fluence up to 1.8×10^{17} cm^{-2} (sample *E*) results in polycrystalline growth of silicon and the sample surface becomes rougher (σ_{rms} = 86.2 nm). The pinholes observed in AFM images indicate a 3D growth mechanism and agglomeration of Si crystallites. The similar tendency was observed during Si overgrowth on the samples *A* and *B* after LT cleaning; however, the surface roughness was 7.0 nm and 11.8 nm, respectively.

The reflection spectroscopy data obtained from all samples after Si overgrowth reveal that in the energy range below 2 eV the behavior of the reflection coefficient is in line with that for Si. Hence, β-$FeSi_2$ crystallites do not occur on the surface after Si overgrowth. The observed optical interference from Si/β-$FeSi_2$/Si heterostructures in the transparency wavelength range (higher 1200 nm) proves the formation of abrupt interfaces.

The study of PL properties of Si/β-$FeSi_2$/Si heterostructures obtained by ion implantation, PIBT and MBE has been carried out at *T* = 5 K. It was shown that the intensity of PL depends on a fluence of the implanted ions, crystalline quality of grown epitaxial silicon layer and substrate orientation The maximum PL intensity was observed for sample *D*. Figure 1 shows experimental PL spectrum of this sample and its deconvolution into three Gaussian components peaked at 0.784, 0.811 and 0.855 eV. The position of first sub band is well agreed with the energy of PL band related to β-$FeSi_2$ precipitates [3]. Other two sub bands are close to *D*1 and *D*2 lines [6] and relates to dislocation structures formed during Si growth. More detailed structural studies are needed to confirm the formafion of dislocations during MBE growth.

Thus, in this work for the first time the formation of Si/β-$FeSi_2$/Si heterostructures was performed using ion implantation, PIBT and MBE. The obtained heterostructures have abrupt interfaces, emit light in the 1.5-1.6 μm region and suitable for the fabrication of electroluminescent devices.

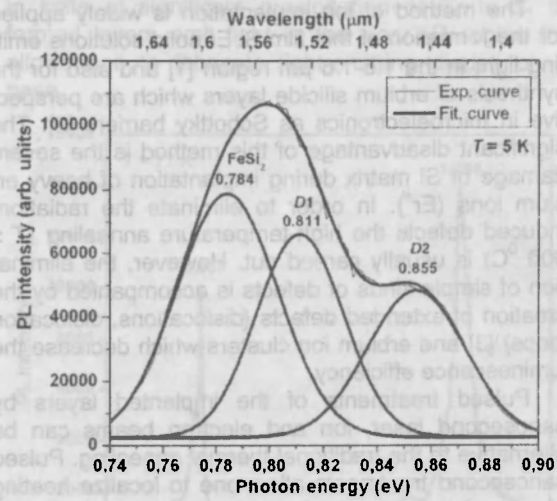

Fig.1. PL spectrum of sample *D* and its fitting using three Gaussian components corresponding to β-$FeSi_2$ phase and dislocation lines

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