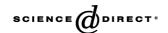
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## Structural properties of swift heavy ion beam irradiated Fe/Si bilayers

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#### Abstract

The Fe/Si multilayers were prepared by electron beam evaporation in a cryo-pumped vacuum deposition system. Ag<sup>+</sup> and Au<sup>+</sup> ions of 100 MeV at two different fluencies such as  $1 \times 10^{12}$  ions/cm<sup>2</sup> and  $1 \times 10^{13}$  ions/cm<sup>2</sup> at a pressure of  $10^{-7}$  torr were used to irradiate the Fe/Si samples. The irradiated samples were analyzed by High-Resolution XRD and it reveals that the irradiated films are having polycrystalline nature and it confirms the formation of the  $\beta$ -FeSi<sub>2</sub>. The structural parameters such as crystallite size (*D*), strain ( $\epsilon$ ) and dislocation density ( $\delta$ ) have been evaluated from the XRD spectrum. The role of the substrates and the influence of swift heavy ions on the formation of  $\beta$ -FeSi<sub>2</sub> have been discussed in this paper.

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Keywords: Fe/Si bilayer; Ion irradiation; β-FeSi<sub>2</sub>; Structural; Thin films

### 1. Introduction

Ion irradiation is one of the powerful techniques to synthesize metastable phases in thin film from multilayered elemental structures for a variety of applications [1]. This process involves ion irradiation induced mass-transport popularly known as ion beam mixing (IBM) and phase transformations. IBM is a local rearrangement of atoms across the interfaces induced by energetic ions [2,3]. In lowenergy regime, the mechanism of mixing at interface is well understood as the energy transfer to the material by elastic collision that causes target atoms to move from their lattice positions and generate defects and subsequent atomic mobility across the interface [4,5]. On the other hand, IBM induced by electronic excitations in the high-energy regime is being intensively investigated to understand the mechanism and to exploit it for novel applications. Recently, swift ion beam induced mixing has been investigated in Cu/W, Tb/Fe, Co/Si and many other combinations [1,6-8].

Semiconducting  $\beta$ -FeSi<sub>2</sub> with a direct band gap of 0.85 eV is attractive for Si-based opto-electronic applications

[9,10]. Various methods for growth of  $\beta$ -FeSi<sub>2</sub> have been employed, such as reactive epitaxy deposition [11–13], pulsed laser deposition [14], and ion beam synthesis [15–18]. On the other hand, it is expected that irradiation with focused ion beams to Fe/Si structures will induce atomic mixing and enhance silicidation locally, which can be utilized for nano-fabrication of  $\beta$ -FeSi<sub>2</sub> [19]. For this purpose, effects of ion beam irradiation on silicidation in Fe/Si structures were investigated.

Various experimental techniques have been utilized to understand the phases and properties induced by IBM [5–8]. If the change induced by IBM at the interface is small (within a few nanometers), X-ray absorption measurement is a useful tool to probe the local electronic structure of materials including identification of different phases. It provides significant information about unoccupied molecular orbitals [20]. Apart from this, based on the analysis of the chemical bonding of multilayers before and after ion beam irradiation, one can attempt to understand the mechanism responsible for IBM.

In the literature, no data is available on the formation of semiconducting silicides by swift heavy ion beam irradiation. This investigation is the first of its kind and an attempt has been made to form a  $\beta$ -FeSi<sub>2</sub> semiconducting silicide by swift heavy ion beam irradiation. The  $\beta$ -FeSi<sub>2</sub> synthesis was

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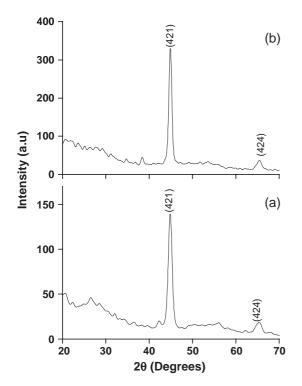


Fig. 1. X-ray diffraction spectrum of  $\beta$ -FeSi<sub>2</sub> thin films on Si (100) irradiated with 100 MeV of Ag ions: (a) fluence at  $1 \times 10^{12}$  ions/cm<sup>2</sup>; (b) fluence at  $1 \times 10^{13}$  ions/cm<sup>2</sup>.

carried out using swift heavy ion beam irradiation on Si (100) and Si (111) substrates. The influences of the heavy ion beam irradiation on the structural properties of Fe/Si layers and the formation of  $\beta$ -FeSi<sub>2</sub> on different substrates have been discussed in this paper.

## 2. Experimental procedure

Fe/Si bilayer was prepared by electron beam evaporation on (100) and (111) oriented single crystal silicon substrates. The substrates were first degreased in organic solvents (TCE, acetone and methanol one after another). The substrates were dipped into 10% HF solution for 1–2 min before loading into e-beam chamber. The iron coating was done under a vacuum of  $\sim 10^{-8}$  torr using cryo pump and Turbo based UHV evaporator.

The ion irradiation was carried out using a 15UD Pelletron accelerator with a beam current of 4 nA at Nuclear Science Centre, New Delhi. Au and Ag ions of 100 MeV with varying fluencies of  $1 \times 10^{12}$  ions/cm<sup>2</sup> and  $1 \times 10^{13}$ 

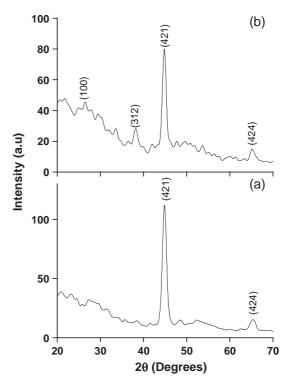


Fig. 2. X-ray diffraction spectrum of  $\beta$ -FeSi<sub>2</sub> thin films on Si (111) irradiated with 100 MeV of Ag ions: (a) fluence at  $1 \times 10^{12}$  ions/cm<sup>2</sup>; (b) fluence at  $1 \times 10^{13}$  ions/cm<sup>2</sup>.

ions/cm² irradiated the multilayer at room temperature. The vacuum inside the irradiation chamber was of the order of  $1\times 10^{-6}$  torr. The projected range of 100 MeV ions in the multilayer as calculated using TRIM95 code is about 8.93  $\mu m$ , which is greater than the total thickness of the multilayer. Thus, the bombarding ions pass through the entire film and deposit in the Si substrates. The electronic energy loss (Se) is of  $\sim 3.91~keV/nm$  against the elastic nuclear energy loss (Sn) of 0.022 keV/nm. The as deposited and irradiated multilayers were characterized by High-Resolution X-ray diffraction (HRXRD) using  $CuK_{\alpha}$  radiation.

#### 3. Results and discussion

## 3.1. $Ag^+$ ion irradiation

Detailed information on the nature and relative quantity of different iron silicide phases was obtained from the XRD analysis. Fig. 1 shows the X-ray diffraction patterns of 100

Table 1 The calculated structural parameters of the  $\beta$ -FeSi $_2$  thin films on Si (100) irradiated with 100 MeV of Ag ions at two different fluencies

Fluence at $1 \times 10^{12}$ ions/cm <sup>2</sup>						Fluence at $1 \times 10^{13}$ ions/cm <sup>2</sup>					
2θ (°)	d (Å)	hkl	D (Å)	$\frac{\varepsilon \times 10^{-3}}{(\ln^2/\text{m}^{-4})}$	$\frac{\delta \times 10^{15}}{(\text{lin/m}^2)}$	2θ (°)	d (Å)	hkl	D (Å)	$\varepsilon \times 10^{-3}$ (lin <sup>2</sup> /m <sup>-4</sup> )	$\frac{\delta \times 10^{15}}{(\text{lin/m}^2)}$
44.83	2.022	421	223	1.62	1.98	44.87	2.019	421	257	1.42	1.52
65.28	1.429	424	219	1.65	2.08	65.38	1.427	424	219	1.65	2.08

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