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Structural and electrical properties of swift heavy ion beam irradiated Fe/Si interface

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Abstract. **The present work deals with the mixing of iron and silicon by swift heavy ions in high-energy range. The thin film was deposited on a *n*-Si (111) substrate at 10^{-6} torr and at room temperature. Irradiations were undertaken at room temperature using 120 MeV Au^{+9} ions at the Fe/Si interface to investigate ion beam mixing at various doses: 5×10^{12} and 5×10^{13} ions/cm^2. Formation of different phases of iron silicide has been investigated by X-ray diffraction (XRD) technique, which shows enhancement of intermixing and silicide formation as a result of irradiation. *I–V* measurements for both pristine and irradiated samples have been carried out at room temperature, series resistance and barrier heights for both as deposited and irradiated samples were extracted. The barrier height was found to vary from 0·73–0·54 eV. The series resistance varied from 102·04–38·61 kΩ.**

Keywords. **Ion beam mixing; XRD; Schottky barrier height; series resistance.**

1. Introduction

When a metal comes into contact with a semiconductor, a charge transfer takes place between them as the Fermi levels for the two are normally different, resulting in the formation of a potential barrier at the interface. Schottky barrier rectifies the flow of carriers under applied bias voltages. To evaluate the Schottky barrier height, an alloyed interface without rectification effect, i.e. an ohmic electrode, is normally prepared on the other side of the semiconductor substrate. The barrier height can be estimated by the current–voltage (*I–V*) method in which the electron current variation through the interface is measured with bias voltages applied to the Schottky diode (Sze 1981).

The phenomena of Schottky barrier formation at metal–semiconductor interface has been studied intensively for over four decades, yet it remains one of the most active areas of solid-state physics (Brillson and Brucker 1983). When the doping level in the silicon is low, the Schottky barrier acts as a diode that has a lower turn-on voltage than a *p–n* junction diode. With this advantage, the Schottky diode has been frequently used in high-speed devices (Stefan Sassen *et al* 2000). When a bias is applied to the junction, it can make the barrier either lower or higher from the semiconductor side (Brillson 1982). The iron silicide phases at Fe/Si interfaces are formed by interdiffusion and intermixing at room temperature or by annealing samples at elevated temperatures (Crescenzi *et al* 1990; Sirotti *et al* 1994; Telling *et al* 2001). In a reactive interface such as silicide–Si interface, there is an interfacial layer, which tends to dominate the Schottky barrier height. The layer should control not only barrier height, but other interfacial properties as well. The most important characteristic of the metal–semiconductor interface is the nature of the potential barrier between the Fermi level of metal and the majority carrier's band edge of the semiconductor. This potential barrier has central importance in determining the performance of semiconductors, necessary in forming metal–semiconductor interface, and depends upon the barrier height (Ottavani *et al* 1980). The Schottky barrier height of metal/Si varies from 0·93 eV (IrSi) to 0·55 eV ($ZrSi_2$) (Mathias and Vidvuds 1998). Irradiation with GeV energy ions has been found to produce intermixing in Fe/Si multilayer (Bauer *et al* 1993). It was shown by Dunlop *et al* (1994) and Tombrello (1995) that the trails of damage can be made in metals by high levels of electronic energy loss, S_e. Threshold S_e for such columnar damage varies from metal to metal. For example, S_e for Fe is ~5 keV/Å (Dunlop *et al* 1994). Recently, researchers have shown interest in atomic mixing, materials modification and phase changes using ion beam mixing of high energy where inelastic collisions or electronic stopping are responsible for the energy loss (Assmann *et al* 1998; Kraft *et al* 2002; Chaudhary *et al* 2004; Diva *et al* 2004). Veenu Sisodia and Jain (2004) studied mixing induced by swift heavy ion irradiation at Fe/Si interfaces. Swift heavy ion induced intermixing in the metallic systems and underlying mechanism responsible for the interdiffusion process

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is not yet clear. More detailed studies done on the system suggests that for low (dE/dX) values, in addition to damage creation, intermixing occurs mainly via thermal diffusion process.

In the present work, we chose ion beam sputtering (IBS) method as the alternate method for the fabrication of iron thin films on Si substrate. Fe/Si bilayer system is studied under the swift heavy ion irradiation and effects on the system were observed as a result of 120 MeV Au^{+9} ion irradiation. X-ray diffraction (XRD) technique was employed to study the irradiation effects at the interface. I–V curves at room temperature, Schottky barrier height and series resistances have been investigated.

2. Experimental

2.1 *Sample preparation*

Fe film of thickness, 30 nm, has been deposited on n-type Si (111) wafer of resistivity 1–10 Ωcm, by ion beam sputtering deposition method using argon (Ar) ions. Fe plates of purity, 99·999%, have been used as target. These plates were located at an angle of 45° to incident ions. To remove native oxide layer from the surface, Si wafers were cleaned by HF. The cleaned substrates were loaded in the deposition chamber. The base pressure of the chamber was kept below $1\cdot2 \times 10^{-6}$ torr using turbo molecular pump. The diameter of the beam used was 30 mm. During the deposition, vacuum was maintained at $1\cdot6 \times 10^{-5}$ torr. The deposition was carried out at a rate of 32 Å/min at room temperature.

2.2 *Irradiation*

Fe/Si samples were irradiated using 120 MeV Au^{+9} ions using 15 UD pelletron accelerator at IUAC Delhi, at two fluence values, 5×10^{12} and 5×10^{13} ions/cm^2, at room temperature. The samples were irradiated uniformly over an area of 1×1 cm^2 by scanning the ion beam of 1 pna current using an electromagnetic scanner at 10^{-6} torr vacuum. Room temperature I–V measurements for both the pristine and irradiated samples have been carried out using the Keithley Electrometer – 6517A. Schottky barrier heights and series resistances of these samples have been calculated using I–V characteristics.

2.3 *XRD technique*

As deposited and irradiated samples were studied using XRD to find out the presence of any phase or crystal structure at the interface. The difference between X-ray spectra of as deposited and irradiated samples allow to separate the irradiation effects created due to heavy ion irradiation.

3. Results and discussion

3.1 *Structural study by XRD*

Figure 1(a) shows the diffraction pattern of the bilayer system. X-ray diffraction pattern of the as deposited sample give separate crystalline Bragg peaks corresponding to Fe(110), Fe (200) and Si (111), which do not show formation of any silicide. This system after irradiation at higher fluences shows crystalline peaks of Fe as well as Bragg peaks corresponding to different planes of Fe_2Si, FeSi and $FeSi_2$. XRD measurement revealed that irradiation promotes the transformation of Fe_2Si to FeSi and FeSi to $FeSi_2$. At 5×10^{12} ions/cm^2, fluence shows the formation of crystalline Fe_2Si (100), FeSi (211) and $FeSi_2$ (002) (figure 1(b)). Figure 1(c) shows the XRD pattern of the same system irradiated at a fluence of 5×10^{13} ions/cm^2, leading to the formation of two dominant peaks of two phases, $FeSi_2$ (002) and FeSi (111), where $FeSi_2$ (002) is the most stable phase.

XRD pattern shows the Bragg peak of Si (111) and Fe (110) at same intensity. These diffractograms and X-ray analysis clearly indicate the formation of different silicide phases at the interface.

3.2 *Electrical measurements*

For electrical measurements, silver paste was applied on the top and bottom to make contact on the sample. Cur-

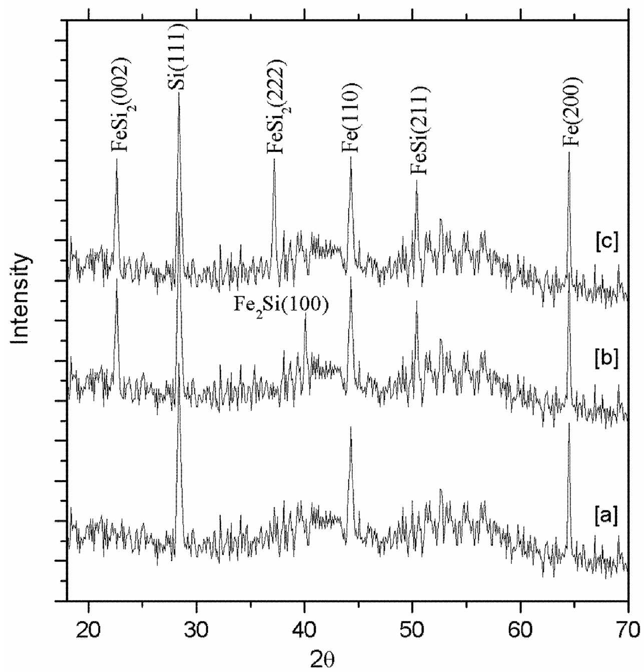

Figure 1. XRD of (a) as deposited sample, (b) irradiated sample with 120 MeV Au^{+9} ions at a dose of 5×10^{12} ions/cm^2 and (c) irradiated sample with 120 MeV Au^{+9} ions at a dose of 5×10^{13} ions/cm^2.

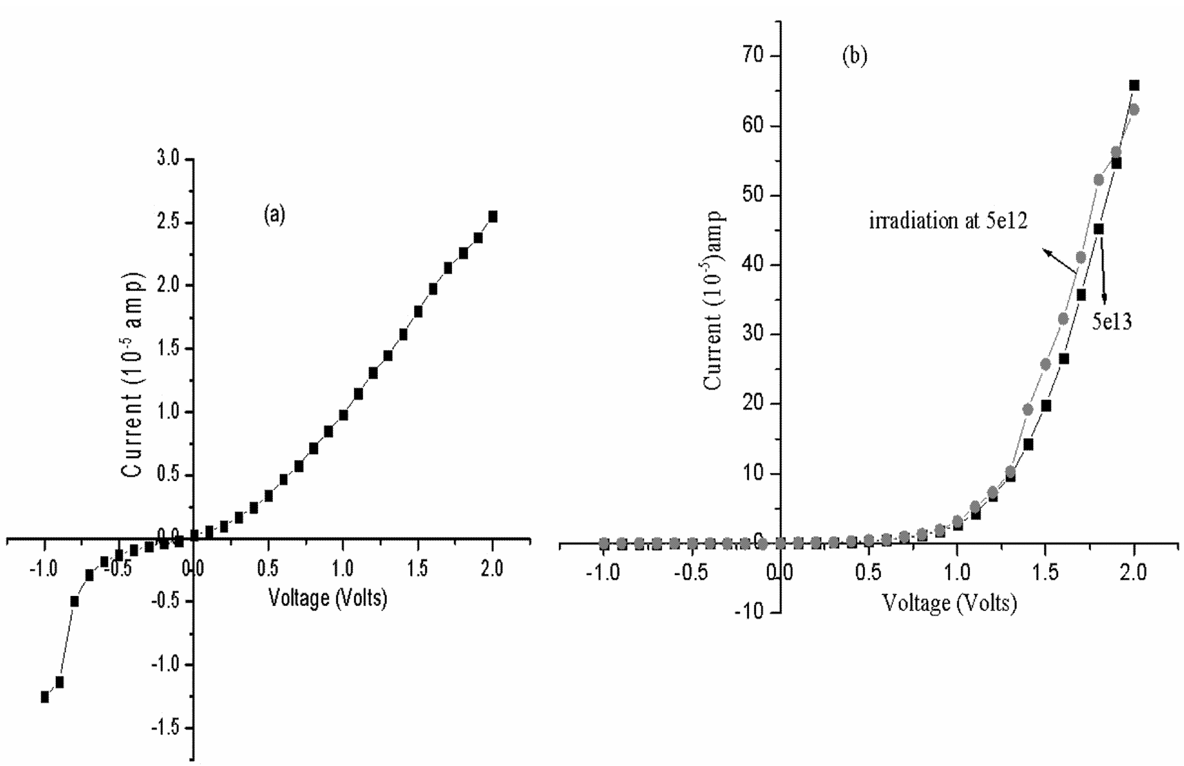

Figure 2. *I–V* curve for (a) pristine sample and (b) irradiated sample.

Table 1. The values of barrier heights and series resistances.

Samples	SBH (eV)	Series resistance (kΩ)
Pristine	0·73	102·04
Irradiated at 5×10^{12} ions/cm^2	0·62	43·8
Irradiated at 5×10^{13} ions/cm^2	0·54	38·61

rent–voltage (*I–V*) measurements have been made for as-deposited and irradiated samples. The current across a metal–semiconductor junction is mainly due to majority carriers. Figures 2(a) and (b) are typical curves of I vs V for both the pristine and irradiated samples at two fluence values, 5×10^{12} and 5×10^{13} ions/cm^2.

3.3 *Schottky barrier heights*

Schottky barrier is an intrinsic energy barrier formed at the interface of most metal–semiconductor junctions. In the present work, the effect of swift heavy ion irradiation on the barrier height formed at the Fe/Si interface has been reported. For a Schottky barrier diode the relation between the applied forward bias and current of the device is due to the thermionic emission and can be written as

$$I = AA^{**}T^2 \exp(-q\Phi_B/KT)\{\exp(qV_{\text{eff}}/nkT) - 1\},$$

where A, A^{**}, T, q, K, n, V_{eff} and Φ_B are the cross-sectional area of the metal/semiconductor interface, the modified Richardson constant for the metal/semiconductor, temperature (300 K), the electronic charge, the Boltzmann's constant, the ideality factor, the effective bias across the interface and the barrier height, respectively.

Modified Richardson constant,

$$A^{**} = \left(\frac{4\pi m^* K^2 e}{h^3}\right) = 31{\cdot}2\ \text{A/cm}^2\text{K}^2.$$

The effective mass of the electron in Si is taken as $m^* = 0{\cdot}26\ m_0$. The value of I_s has been calculated from extrapolating the linear region of I vs V. The values of barrier heights and series resistances are shown in table 1.

4. Conclusions

XRD measurements clearly indicate that the mixing increases with increasing fluence and gives a stable structure at the highest fluences. A significant increase in current (I) has been observed after irradiation. It has also been observed that all the irradiated samples have less resistance than as deposited. Series resistance also decreases after irradiation. In brief, from the present study, it can be concluded that ion beam mixing is a useful tool to modify the phase structure and the barrier height quite significantly.

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