

## SWIFT HEAVY ION INDUCED MODIFICATIONS AT Mo/Si SYSTEM

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### Abstract

Swift Heavy Ion (SHI) induced modification at Metal/Si interfaces has emerged as an interesting field of research due to its large applications. In the present study we investigate SHI induced mixed molybdenum silicide film with different ion fluences. The Molybdenum and Si thin thin films were deposited on Silicon substrates using e-beam evaporation at  $10^{-8}$  torr vacuum. Thin films were irradiated with Au ions of energy 120 MeV to form molybdenum silicide. The samples were characterized by grazing incidence X-ray diffraction (GIXRD) technique for the identification of phase formation at the interface. Rutherford backscattering spectrometry (RBS) was used to investigate the elemental distribution in the films. The mixing rate calculations were made and the diffusivity values obtained leads to a transient melt phase formation at the interface according to thermal spike model.

### INTRODUCTION

Wide applications of silicides in combination with more stringent performance requirements in very large scale integrated circuit devices, increases the need to understand the process of silicide formation. In particular the refractory metal silicides such as  $\text{MoSi}_2$ ,  $\text{WSi}_2$  and  $\text{TaSi}_2$  have increased the interest in regard to the possibility of their applications as gate and interconnect metallization materials in fabricating semiconductor devices [1-2], because of their low electrical resistance and high chemical and thermal stability. Ion Beam Mixing (IBM) has been considered as an alternative means to form metal silicide contacts in microelectronic devices using ion beam to trigger the reaction at the interface of metal and Si [3]. Two theoretical models Coulomb explosion [4] and Thermal spike [5] are invoked to explain such a mixing. According to Thermal spike model for semiconductors, SHI loose their energy predominantly by electronic excitation and ionization of target atoms, after about  $10^{-14}$  s part of the excitation energy is transferred to the lattice, by electron-phonon coupling which leads to the defects and atomic displacements at the interface.

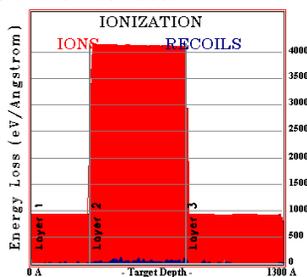


Figure 1: Energy loss distribution from 120 MeV Au ions in the Si/Mo/Si system.

A number of studies on reaction kinematics between Mo and Si have been done by solid state reaction and ion implantation techniques, for the formation of molybdenum silicide. d'Heurle et al. [6] compare the observations made with As ion implantation of energy 250 keV through Mo/W/Si, resulting the formation of two superimposed silicide layers of  $\text{MoSi}_2$  and  $\text{WSi}_2$ , with that of made on similar system by ordinary heat treatment. Same system was studied by Kwang et al. [7] using  $\text{As}^+$  ion implantation of 140-180 keV energies, which was useful to observe rapid diffusion of the implanted ions during the formation of silicide. Cheng et al. [3] have shown direct synthesis of equilibrium  $\text{MoSi}_2$  phase with a well crystalline structure on Si surface by Mo ion implantation using MEVVA ion source followed by thermal annealing. A quite similar system was studied by Liang et al. [8] also at a substrate temperature of  $100^\circ\text{C}$  during Mo ion implantation, followed by RTA and the results revealed a flat and continuous molybdenum silicide film with superior properties. Recently SHI induced mixing has been discussed by Bhattacharya et al. [9] in Mo/Si system by invoking Thermal Spike Model and they calculate the upper limit for the threshold of defect creation by electronic energy loss in Molybdenum. In the present paper, the experimental observations as well as the characterization of the observed patterns by Au ion irradiation at Mo/Si interfaces have been reported and the possible mechanism of mixing has been discussed.

### EXPERIMENTAL DETAILS

A trilayer system, Si (50nm) /Mo (50nm) /Si (30nm) has been deposited onto Si (100) substrate using electron beam evaporation at vacuum of  $4 \times 10^{-8}$  torr. The deposition rate was  $0.2 \text{ \AA}/\text{sec}$  for Si and  $1.0 \text{ \AA}/\text{sec}$  for Mo. This system was then irradiated with 120 MeV Au ions using 15 UD Pelletron Accelerator at Inter University Accelerator Centre (IUAC) New Delhi, India, at different fluences from  $10^{12}$  to  $10^{14}$  ions/ $\text{cm}^2$  at room temperature under  $10^{-6}$  torr vacuum. The electronic and nuclear energy losses were 36.64 keV/nm and 0.69 keV/nm for Mo and 12.94 keV/nm and 0.21 keV/nm for Si have been calculated using SRIM 2003 program [10]. Grazing incidence X-Ray diffraction (GIXRD) measurements were performed using  $\text{CuK}\alpha$  radiation. The elemental distribution in all samples was determined by Rutherford Backscattering Spectroscopy (RBS) using 3 MeV  $\text{He}^+$  ion beam at backscattering angle  $170^\circ$  of the Dynamitron Accelerator, at University of Stuttgart, Germany. Fits to the spectra were obtained with the help of the RUMP computer code [11]. Irradiation effect on the surface morphology of the Mo/Si thin film system has been studied using AFM in tapping mode.

**RESULTS AND DISCUSSION**

*Structural Information by GIXRD*

X-Ray Diffraction patterns of the as-deposited as well as irradiated thin films at different fluences are shown in Fig. 2.

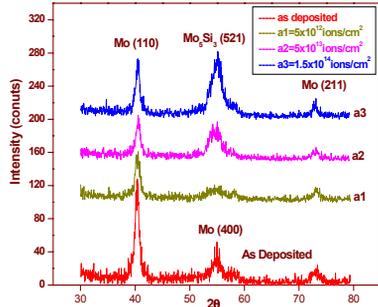


Figure 2: GIXRD curves of as-deposited and irradiated Mo/Si system.

The as deposited XRD pattern giving the separate crystalline Bragg peaks of Mo corresponding to planes (110, 400 and 211). The sample irradiated at lowest dose  $5 \times 10^{12}$  ions/cm<sup>2</sup> shows a broad peak of Mo<sub>5</sub>Si<sub>3</sub> with minimum intensity and it increases with increasing the fluence. At highest dose of  $1.5 \times 10^{14}$  ions/cm<sup>2</sup> a sharp peak of tetragonal-Mo<sub>5</sub>Si<sub>3</sub> was formed, while the other two crystalline peaks of Mo with planes (110) and (211) remains at the same position. The diffraction peak at  $2\theta=55.13^\circ$  corresponding to (521) plane allows the positive identification of Mo<sub>5</sub>Si<sub>3</sub> phase (JCPDS X-Ray Powder file data file 34-0371). Hence XRD measurements revealed that irradiation promotes the movement of atoms at the interface leading to the formation of a mixed compound in the form of metal silicide.

*RBS Analysis*

The RBS spectra of as-deposited and irradiated Mo/Si thin film system at various fluences are given in Fig. 3. Sample irradiated at lowest dose  $5 \times 10^{12}$  ions/cm<sup>2</sup> shows a very little shift in the peaks of Mo and Si, which are not clearly observable but with the help of RBS data and its calculation using RUMP code determines a little mixing of the order of 1.5nm. In case of irradiation at fluences  $5 \times 10^{13}$  and  $1.5 \times 10^{14}$  ions/cm<sup>2</sup> a little decrease in the slope and shift towards the lower edge of Mo peak and in front edge of Si peak indicates, that the mixing occurred at these interfaces. These profiles for Mo/Si system were extracted from the RBS spectra with the help of RUMP simulation code. They were fitted with a Gaussian error function and the values for mixing length, interface variance, mixing rate and mixing efficiency corresponding to each irradiation dose are tabulated in Table 1. The observed increase in the variance was calculated by

$$\Delta\sigma^2 = \sigma^2(\phi) - \sigma^2(0)$$

where  $\sigma^2(\Phi)$  and  $\sigma^2(0)$  are the variances of irradiated sample at fluence  $\Phi$  and unirradiated sample respectively.

**Applications of Accelerators**

**U02 - Materials Analysis and Modification**

The maximum mixing length corresponds to the formation of t- Mo<sub>5</sub>Si<sub>3</sub> at Mo/Si interface.

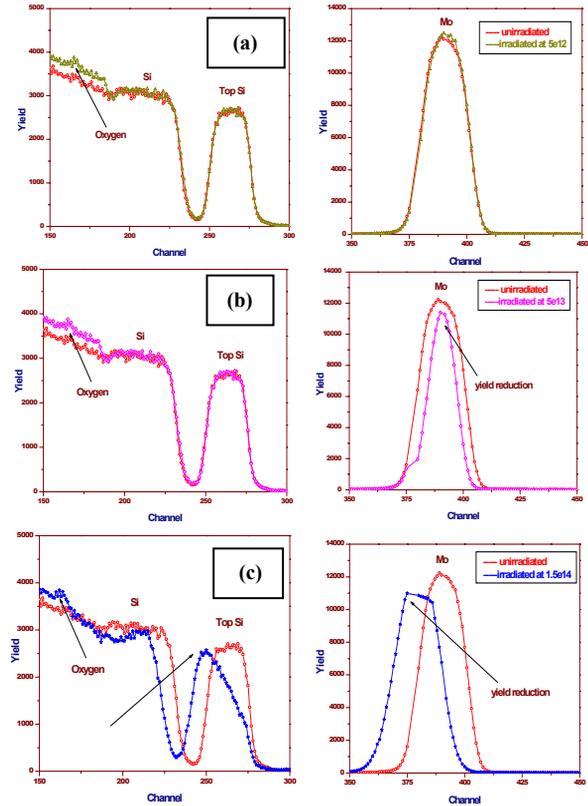


Figure 3: RBS Spectra of as deposited and irradiated Mo/Si system at fluences (a)  $5 \times 10^{12}$  (b)  $5 \times 10^{13}$  and (c)  $1.5 \times 10^{14}$  ions/cm<sup>2</sup>.

Table 1: Mixing width, Interface variance, and Mixing Rate with Ion fluence

Fluence $\Phi$ (ions/cm <sup>2</sup> )	Mixing width $\sigma$ (nm)	Interface variance $\Delta\sigma^2(\Phi)=\sigma^2(\Phi)-\sigma^2(0)$ (nm <sup>4</sup> )	Mixing rate $k=\Delta\sigma^2(\Phi)/\Phi$ (nm <sup>4</sup> /ion)
Unirradiated	0	-	~21.3
$5 \times 10^{12}$	1.5	2.25	
$5 \times 10^{13}$	3.4	11.56	
$1.5 \times 10^{14}$	5.7	32.49	

It is clear from Table 1 that the value of  $\Delta\sigma^2$  increases linearly with increase in ion fluence hence supporting the results of GIXRD. The mixing rate is defined as  $k = \frac{\sigma^2(\phi)}{\phi}$  was calculated from the data given in Table 1.

In assumption of Thermal Spike Model for semiconductor system [12] each incident ion loses its energy during its transit across the material mainly by electronic excitation. Temperature of electronic system rises for a typical time span of  $10^{-15}$  s which is followed by transfer of energy from electrons to the target via the electron – phonon

coupling, inducing the local temperature rise ( $\geq 1000\text{K}$ ) in a very narrow zone. The rise and decay of the lattice is governed by two coupled differential equations [5]. For the temperatures above the melting point the lattice melts followed by fast quenching. The melting of lattice facilitates atomic motion through this zone and an enhanced diffusion takes place dominantly in each cylindrical melt zone, as the diffusivity in molten state is several orders of magnitude higher than in the corresponding solid. Thermal Spike Model has also been used previously to explain ion beam mixing in various Metal/Si systems [13, 14]. The Diffusion during transient thermal spike follows the equation to calculate the Diffusion coefficient as

$$D = \frac{\Delta\sigma^2(\phi)_{MI}}{2t_s}$$

where  $t_s$  is the duration of the transient melt phase and  $\Delta\sigma^2(\phi)_{MI}$  is mono ion mixing effect [15] which is defined as

$$\Delta\sigma^2(\phi)_{MI} = \frac{k}{(\pi r^2)}$$

where  $k$  is mixing rate,  $r$  is the radius of molten ion track. Taking the typical track radius as 1.5nm and  $t_s$  as  $\sim 1\text{ps}$  for another metal Ni, the data for which is available [16], the diffusivity  $D$  at the interface turns out to be of the order of  $\sim 10^{-6} \text{m}^2 \text{s}^{-1}$ . The value is a characteristic and clearly in the range of the interdiffusion constants known from liquids and hence supports the thermal spike model of mixing.

## CONCLUSION

The present work describes the mixing behaviour of Mo and Si under SHI irradiation using 120MeV Au ions. XRD Results indicates that SHI induced mixing has taken place at the interface of Mo/Si system, which results in the formation of  $t\text{-Mo}_5\text{Si}_3$ , that is not a stable phase in the series of Mo/Si interface reacted phases but it is suitable for microelectronics. From RBS analysis, diffusivity value suggests a transient molten phase at the interface following the Thermal spike Model. Therefore the IBM is a successful tool to modify the metal/Si interfaces.

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