Depth-Resolved X-ray Absorption Fine Structure Study of Fe/Si Interfaces Using X-ray Standing Waves

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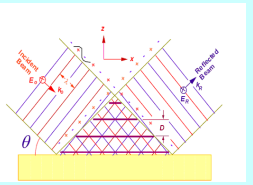
Introduction

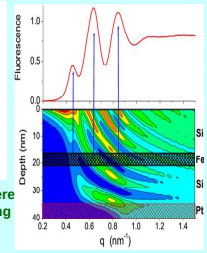
- Magnetic multilayer like Fe/Si have great importance, because they exhibit antiferromagnetic coupling between Fe layers for certain thickness of intervening Si spacer layers.
- Coupling between Fe layers is known to depend upon the structure of the spacer layer (amorphous or crystalline; Si, FeSi or $FeSi_2$)
- Typically the width of the interfacial region is of the order of a few nanometers (nm), therefore we need such experimental technique which characterize the interfacial structure should have a depth resolution of similar order.
- The conventional depth profiling techniques like Rutherford back-scattering spectrometry (RBS) , Secondary ion mass spectrometer (SIMS) have a typical depth resolution of a few nm.
- In the present work, we demonstrate that XAFS measurement can be made depth selective by making use of X-ray standing waves generated by total external reflection of X-rays incident on the sample at grazing angle.

X-ray Standing Waves



Incident and Reflected waves interfere with each other generates a standing wave

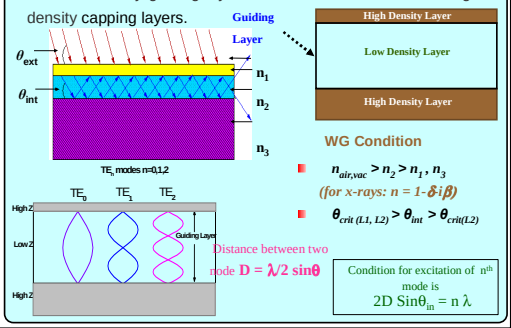
Standing Wave period: $D = \frac{\lambda}{2\sin\theta}$



Field intensity inside the multilayer structure : Substrate/ Pt/Si/Fe/Si

X-ray Wave-Guide (WG) structure :

- One low density guiding layer is sandwiched between two higher density capping layers.



WG Condition

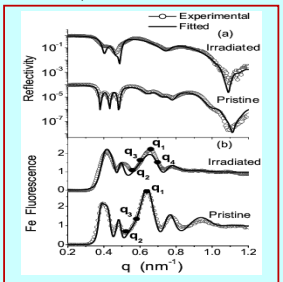
- $n_{air,vac} > n_2 > n_1, n_3$ *(for x-rays: $n = 1-\delta-i\beta$)*
- $\theta_{crit\,(L1,\,L2)} > \theta_{int} > \theta_{crit(L2)}$

Distance between two mode $D = \lambda/2\sin\theta$

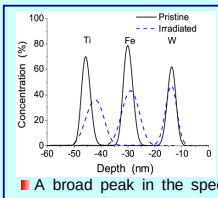
Condition for excitation of n^{th} mode is $2D\,\mathrm{Sin}\theta_{in} = n\lambda$

Results

- The multilayer structure: substrate/Cr(20nm)/Au(60nm)/Si(12.5nm)/W(3nm)/Si(12.5nm)/Fe(3nm)/Si(12.5nm)/Ti(3nm)/Si(12.5nm), prepared by electron beam evaporation with a base pressure of the order of 2×10^{-9} mbar.
- ⇨ Samples were irradiated with 100 MeV Au^{7+} ions at Inter-University Accelerator Center, New Delhi in order to induce intermixing of metal layers with Si.
- ⇨X-ray reflectivity, XRF and XAFS measurements (in fluorescence mode) were done at ID32 beam line of ESRF, Grenoble, France.



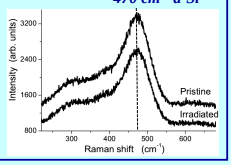
X-ray reflectivity and Fe Fluorescence of the multilayer before and after irradiation with 100 MeV Au ions at a fluence of 1×10^{13} ions/cm².

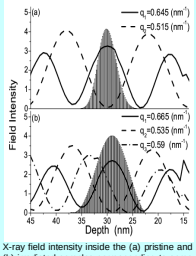


- Ti exhibits strong mixing with Si, leading to a large broadening of its depth profile.
- W depth profile exhibits only a slight broadening.
- Fe layer exhibits an intermixing with Si, which is intermediate between that of Ti and W.

470 cm⁻¹ a-Si

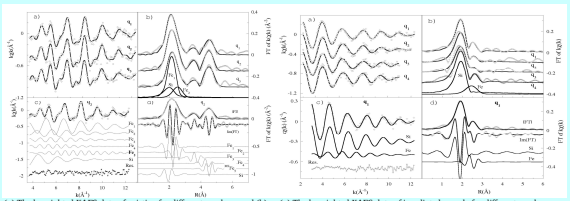
- A broad peak in the spectrum at 470 cm^{-1} is characteristic of amorphous Si (a-Si).
- This shows that Si layers in the as-deposited film are amorphous in nature, and even after irradiation these layers remain amorphous.





X-ray field intensity inside the (a) pristine and (b) irradiated samples corresponding to some of the q values at which XAFS measurements were taken.

- ❖ At $q=q_1$, the position of an antinode coincides with the center of the Fe layer, while at $q=q_2$, a node coincides with the center of the Fe layer.
- ❖Thus at $q=q_1$, larger contributions from the Fe ions located in the center of the layer, while at $q=q_2$, one should get the preferential information about the interfacial regions.

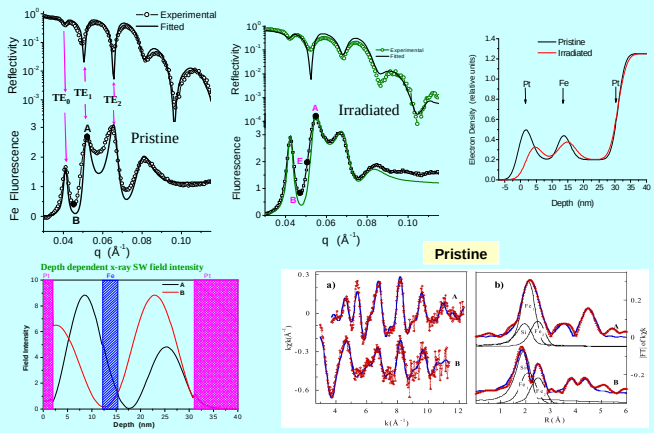


(a) The k-weighted XAFS data of pristine for different q values, and (b) their Fourier transforms

(a) The k-weighted XAFS data of irradiated sample for different q values, and (b) their Fourier transforms

- XAFS signals of the pristine film present features typical of -Fe and high frequency oscillations suggesting some degree of medium-range atomic order. On the contrary, XAFS signals of the irradiated sample have broad oscillations rapidly decreasing with k typical of weak scatters Si and suggesting higher structural disorder as for an amorphous phase. **[Ajay Gupta et al., Phys. Rev. B 76, 195401 (2007)]**.
- For $q=q_1$ the value of N_{Si}/N_{Fe} is less than 2.1, which is similar to FeSi phase. At $q=q_3$ & q_4 is agreement with $FeSi_2$ phase.
- Thus, the depth-selective XAFS analysis for all four q values together suggest a depth-dependence of Fe atomic environment for the irradiated sample: in the center of the layer, the Fe ions present a short-range order similar to that found in the stoichiometric FeSi phase, and in the interfacial region, the structure become richer in Si and the local structure around Fe becomes similar to that of the $FeSi_2$ phase.

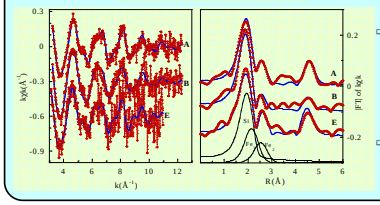
- The Waveguide structure: substrate/Cr(20nm)/Au(60nm)/Si(16nm)/Fe(4nm)/Si(11nm)/Au(2nm)



✓At q = A, the position of an antinode coincides with the center of the Fe layer , while at q= B, an antinode coincides with the interface of the Fe layer.

- ❖ From the depth selective XAFS one is able to resolve the structure of interfacial region from that of the center of the Fe layer.
- ❖ At q=A, the structure consists of mainly bcc–Fe with only 20% contribution of Fe-Si bonds
- ❖ while at q=B, the XAFS data matches with that of crystalline FeSi.
- ❖ After irradiation total thickness of multilayer structure Si/Fe/Si is decreases , this may be due to densification of amorphous Si layers.
- ❖From the electron density profile Fe layers get completely mixed with Si.

Irradiated with 120 MeV ions to a fluence of $1x10^{13}$ ions/cm²



⇨ The XAFS data of the irradiated samples does not show any sharp features characteristic of α-Fe phase, suggesting that Fe layer is completely mixed with Si.

⇨ However, different phases (FeSi and $FeSi_2$) are formed at different depths

Conclusions

⇨ **Swift heavy ion induced intermixing of Ti, Fe, and W marker layers with Si in a single film has been studied using x-ray fluorescence and XAFS measurement.**

⇨ **From XAFS measurements, in the pristine film the Fe layer consists of crystalline bcc-Fe with small amount of Si dissolved in it, and with FeSi phase in the interfacial regions.**

⇨ **After an irradiation with 100MeV Au ions, Fe layer gets completely mixed with Si and forms a highly disordered or amorphous structure. It is observed that in the center of the intermixed layer the short-range order around Fe ions is similar to FeSi phase, while in the interfacial region $FeSi_2$ type of short-range order is observed with number of Fe-Fe near neighbours decreasing with the distance from the center.**

Acknowledgement

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