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X-ray Standing Wave studies of the Structural Aspects of Ion Beam Synthesized Epitaxial $Si/CoSi_2/Si(111)$ system.

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Abstract

The atomic structure of the (111) interface between ion beam synthesized buried $CoSi_2$ epilayer (type-A) and bulk Si has been investigated by using bulk x-ray diffraction and x-ray standing wave techniques. Our results show that the $CoSi_2$ lattice is 0.7% contracted in the [111] direction with respect to the $CoSi_2$ free lattice constant. At the interface, the Co atoms (not the Si atoms) of the $CoSi_2$ epilayer are directly bonded to the surface Si atoms of the bulk Si(111) substrate conforming to the 8-fold Co coordination model. The Co–Si bonds at the interface are contracted by 0.03 ± 0.06 Å with respect to that in bulk $CoSi_2$.

I. INTRODUCTION

The heterostructures formed by growing epitaxial metallic silicides, such as $NiSi_2$ and $CoSi_2$, on silicon substrates are of considerable interest because of their fundamental importance and possible technological applications. An understanding of the basic aspects of atomic bonding geometry and the electronic properties at the interfaces of the heteroepitaxial structures contribute to their effective use in microelectronic applications. The nearly lattice matched $NiSi_2/Si(111)$ and $CoSi_2/Si(111)$ systems have been studied by various experimental [1–7] and theoretical techniques [8–10] leading to an understanding of these interfaces. Conventionally the epitaxial metallic silicide layers are grown on Si surfaces under ultrahigh vacuum (UHV) condition by Solid Phase Epitaxy (SPE), Molecular Beam Epitaxy (MBE) and Reactive Deposition Epitaxy (RPE). White *et al.* [11] used high-dose ion implantation into silicon substrates, followed by annealing, to grow buried epitaxial layers. This method is known as Ion Beam Synthesis (IBS). The epitaxial silicide layers grow in two possible orientations : type-A, where the silicide layer has the same orientation as the Si substrate, and type-B, where the silicide layer is rotated 180° about the surface normal of the Si substrate [12]. For epitaxial $CoSi_2$ layers, it is interesting to note that in the UHV procedures the B-type layers are predominantly formed whereas IBS-prepared $CoSi_2$ buried layer has the type-A dominance for thicker films. For thin layers prepared with the IBS technique, orientations of both type-A and type-B are present [13]. The IBS prepared silicides have received much attention as the electrical transport properties of epitaxial $CoSi_2$ layers formed by IBS are better than those formed by the conventional UHV procedure and the possible application of an IBS-fabricated $Si/CoSi_2/Si$ heterostructure as a metal base transistor [11,14].

A complete understanding of electronic properties of the epitaxial silicide layers requires detail knowledge of atomic bonding configuration at the interface. Possible models for both A-type and B-type have been proposed by Cherns *et al.* [2]. Either the metal atoms or the Si atoms of the silicide can be bonded to the substrate, leading to either an 5-(or 5-) or 7-fold

coordination of the interfacial metal atoms [Fig.1]. The 8-fold coordination model comprises an extra plane of Si atoms at the interface on silicide-lattice positions compared to the 5-fold coordination model. Earlier experiments by Gibson *et al.* using high resolution electron microscopy (HREM) on B-type $CoSi_2$/Si(111) samples, prepared by Co deposition on Si(111) substrates and annealing under UHV conditions, showed the evidence for 5-fold coordinated interface structure [1]. But recently Catana *et al.* used the same UHV deposition and annealing technique to obtain both B-type and A-type $CoSi_2$/Si(111) interfaces, and using the same technique (HREM) they observed sevenfold (as well as some eightfold) coordination for the B-type $CoSi_2$/Si(111) samples [15], which contradicts the observations of Gibson *et al.* For the A-type interface as well Catana *et al.* found evidence for the sevenfold coordination. Other techniques such as x-ray standing wave (XSW) [4,5] and high resolution Rutherford backscattering spectrometry (RBS) [6] found the interface of B-type $CoSi_2$/Si(111) to be 5-fold coordinated, supporting the observations of Gibson *et al.* Bulle-Lieuwma *et al.* carried out HREM studies on the IBS-prepared A-type $CoSi_2$/Si(111) interface in the Si/$CoSi_2$/Si samples and their results favor a 7-fold interface model [16]. Theoretical calculations, such as local-density-functional [8] and quantum chemical cluster [9] calculations, however, favor the 8-fold coordination model for both A- and B-type $CoSi_2$/Si(111) interfaces. Given the contradictions, it is clear that further experimental studies on the $CoSi_2$/Si(111) A-type interface are necessary. In the present work we have undertaken the study of the A-type $CoSi_2$/Si(111) interface in the IBS-prepared Si/$CoSi_2$/Si(111) system with a buried epitaxial $CoSi_2$ layer. We have used the XSW technique to determine the bonding geometry at the interface by generating standing waves with the (111) reflection from the Si substrate crystal and monitoring the Co fluorescence yield from the buried layer as a function of incident angle within the angular range of the (111) reflection from the substrate.

With regard to the XSW method, the relevant difference between the 8-(or 5-)fold and 7- fold coordinated interfaces is the distance d_{IF} of the first Co layer from the last (111) diffraction plane of the substarte. The distance d_{IF} is same for both 8- and 5-fold coordinated interfaces [Fig.1]. Thus, while the 8-fold interface cannot be distinguished from the 5-fold

one, the structures involving 8- (or 5-) fold and 7-fold interfaces can be easily distinguis

II. XSW ANALYSIS

The XSW technique is based on the dynamical theory of x-ray diffraction and is expla in a number of publications [17–21]. Here we will give a brief account of the technique. W a monochromatic x-ray beam is Bragg-reflected from a large perfect crystal substrate, interference between the incident and the reflected waves gives rise to a standing wave in the substrate. This field also extends across the interface into the overlayer. As predi by the dynamical theory, the phase ν of the standing wave field changes by π radians as crystal is rocked through the Bragg reflection. On the low-angle side of the reflectivity c the antinodal planes of the standing wave field lie half-way between the diffraction pl and move inward with increasing angle towards a position coinciding with the diffrac planes. The position of the buried layer atoms is determined by measuring the stan wave excited fluorescence yield from those atoms along with the substrate reflectivity function of rocking angle.

Let us consider a buried epitaxial $CoSi_2$ layer to be composed of N lattice planes of fluorescing element Co with a planar spacing d_{OL} and starting at a distance d_{IF} from topmost diffraction plane of the substrate [Fig.1]. The relevant difference between the 8- (or 5-fold) and the 7-fold coordination is in the value of d_{IF}. From the models show Fig.1, the value d_{IF} for unrelaxed 7-fold and 8-(or 5-) fold coordinated interfaces is 3.5 and 2.74 Å, respectively. We introduce the parameters $\delta_{IF}=d_{IF}/d_H$ and $\gamma=d_{OL}/d_H$ -1 use the formalism given in ref.[3]. In this case, d_H is the (111) planar spacing in silicon.

The normalized fluorescence yield $Y_F(\theta)$, emitted by N overlayer planes as a functio incident angle θ is given by

$$Y_F(\theta) = 1 + R(\theta) + 2\sqrt{R(\theta)}F\cos[\nu(\theta) - 2\pi\Phi_c]$$

where the reflectivity $R(\theta)$ and the phase $\nu(\theta)$ can be calculated from the dynamical the Φ_c and F are called coherent position and coherent fraction, respectively. All poss

fluorescence yield ($Y_F(\theta)$) curves can be fitted with these two parameters. Φ_c and F are defined as follows.

$$\Phi_c = \delta_{IF} + (N-1)\gamma/2 \tag{2a}$$

$$d_{IF} = \Phi_c d_H - (N-1)\gamma d_H/2 \tag{2b}$$

$$F = f_c sin(\pi N\gamma)/N sin(\pi\gamma) \tag{3}$$

f_c contains the Debye-Waller factor and the information about the crystallinity of the epitaxial layer.

The function $sin(\pi N\gamma)/N sin(\pi\gamma)$, for a given γ, will have negative values for the value of N falling in some ranges making the coherent fraction F negative. However, to be physically meaningful F should be positive. From Eq.(1), we notice, in the last term, $Fcos[\nu(\theta) - 2\pi\Phi_c]$ and $Fcos[\nu(\theta) - 2\pi\Phi_c + \pi]$ would give rise to the same yield profile, $Y_F(\theta)$. Therefore, Eqs. (2) can be rewritten in the following form [7]

$$\Phi_c = \delta_{IF} + (N-1)\gamma/2 + \phi_0 \tag{4a}$$

$$d_{IF} = \Phi_c d_H - (N-1)\gamma d_H/2 - \phi_0 d_H \tag{4b}$$

$$F = f_c|A| \tag{5}$$

where

$$A = sin(\pi N\gamma)/N sin(\pi\gamma) \tag{6}$$

$$\phi_0 = -[sgn(A) - 1]/4 \tag{7}$$

The number of layers of the fluorescing atoms, N, is related to the epilayer thickness, T, by

$$N = T/d_{OL} = T/[d_H(1+\gamma)] \tag{8}$$

γ can be determined from the XSW experiments as was done in ref. [3] or can be determined directly from the angular separation of the x-ray diffraction peaks from the epilayer and the substrate. The value of γ or d_{OL} contain the information about the strain in the epilayer. The film thickness is determined by other methods such as RBS. Now with the known values of N and γ, d_{IF} is determined from the measured value of Φ_c from the XSW experiment. This gives the interface structure.

In order to obtain the values of Φ_c and F from the XSW experiment, the measured fluorescence yield is fitted to Eq.1. The best fit gives Φ_c and F. The normalized fluorescenc yield $Y_F(\theta)$ is related to the experimental fluorescence yield, Y_F (expt), by

$$Y_F(expt) = CY_F(\theta) \tag{9}$$

The normalization factor C is proportional to the number of Co atoms within the range of the interference field and thus to the number of metal layers (N).

III. EXPERIMENTAL

An Si wafer (p-doped) with (111) orientation was implanted with 200 keV Co^+ ions to a dose of 2×10^{17} /cm^2 while the substrate was kept at 350°C. This was followed by an anneal treatment of one hour at 600°C and 30 minutes at 1000°C to form 680 ± 50Å thick A-type epitaxial $CoSi_2$ buried layer under 880 Å of crystalline Si. This sample will be denoted by Si/$CoSi_2$/Si(111) and is schematically shown in the inset of Fig. 3. The method of this preparation of an epilayer is known as ion beam synthesis (IBS). A review of the method of preparation and characterization of buried epitaxial layers by ion implantation is given in Ref.[22]. In the IBS-prepared $CoSi_2$ epilayer there appears to be a critical size between 200 and 300 Å; below and above this thickness B-type and A-type epilayers, respectively are formed [16].

The x-ray diffraction (XRD) and the XSW measurements were carried out at the Hamburg Synchrtron Radiation Laboratory (HASYLAB), DESY. The experimental arrangement

has been described in details elsewhere [23,24]. With the use of an asymmetrically cut double-crystal monochromotor the synchrotron x-radiation from DORIS was collimated and monochromatized to obtain 9.2 keV photons incident on the sample [Fig.2]. The asymmetric Si(111) crystal was used to reduce the angular divergence of the exit beam from the monochromator to $\sim$ 1/5 of the Si(111) natural reflection width. In addition, the slightly dispersive Ge(111) $-$ Si(111) combination suppresses the harmonics. The Co K_α fluorescence yield was measured with a Si(Li) detector and the Bragg reflected x-ray intensity (reflectivity) was measured with an ionization chamber [Fig.2]. High resolution topographs were taken to select a perfect crystalline region on the sample for the XSW measurement.

IV. RESULTS AND DISCUSSIONS

The thickness (T) of the $CoSi_2$ layer has been determined to be 680 $\pm$ 50 Å with the RBS technique. It is well known that the lattice structure of $CoSi_2$ is of the CaF_2 type cubic and the lattice constant is 1.2 % smaller than that of Si. That is, the (111) planar spacing in $CoSi_2$ is 3.097 Å. However, for the buried epitaxial $CoSi_2$ layer the (111) planar spacing (i.e., the value of d_{OL}) has been determined to be 3.075 $\pm$ 0.0005 Å. This value was determined from the angular positions of the (111) diffraction peaks from the substrate Si and the $CoSi_2$ epilayer (Fig.3). The measured value of d_{OL} corresponds to a perpendicular strain in the buried $CoSi_2$ layer of $-$ 0.7% with respect to the $CoSi_2$ free lattice constant. This corresponds to γ = -19.26 $\times$ 10^{-3}, whereas a pseudomorphic growth would correspond to γ = -23.0 $\times$ 10^{-3}. For a complete absence of strain, that is with the $CoSi_2$ free lattice parameter, γ = -12.0 $\times$ 10^{-3}. Our measured value of γ = -1.926% is in good agreement with those measured by Vantomme *et al.* [25] for IBS-prepared $CoSi_2$ films of thicknesses in the range 100 $-$ 600 Å. With the known film thickness T and the measured value of d_{OL} (or γ), the number of $CoSi_2$ layers N can be determined from Eq.(8). The value of N and γ have been determined to be 221 $\pm$ 16 and -0.0193 $\pm$ 0.0002, respectively. The results of the XSW experiment, namely, the Si(111) reflectivity [$R(\theta)$], and the Co K_α fluorescence yield

[$Y_F(\theta)$] with the corresponding fit are shown in Fig.4. The parameters Φ_c and F have b obtained by fitting the experimental Co fluorescence yield with the theoretical one [Eq.(The values are Φ_c = 0.756 $\pm$ 0.006 and F = 0.15 $\pm$ 0.05. From Eqs. 4(b),(6) and (d_{IF}(expt) = 2.67 $\pm$ 0.06 Å.

From the models shown in Fig.1, ignoring the small difference in bond length betw Si$-$Si and Co$-$Si, the value of d_{IF} expected for the 7-fold coordination is 3.52 Å and th for 8- (or 5-) fold coordination is 2.74 Å. Fig.5 shows the computed coherent position a coherent fraction for the 8-(or 5-) fold and the 7-fold coordination of Co at the interf and the experimental values of Φ_c and F. It is clear that our experimentally determi Φ_c, and consequently d_{IF}, is in good agreement with the 8- (or 5-) fold model and we rule out the 7-fold model. In other words, the Co atoms of the $CoSi_2$ layer are direc bonded to the surface Si atoms of the substrate. It should be noted that this analysis ref to the $CoSi_2$/bulk Si interface (see the inset of Fig.3). The difference Δd_{IF} = d_{IF}(ex - d_{IF}(8-fold) = - 0.07 Å shows that the Co atoms of the Co-Si bond at the interface relaxed inward by 0.07 $\pm$ 0.06 Å. In other words, if the substrate surface Si atoms are their ideal position the Si-Co bond length at the interface would be 2.28 $\pm$ 0.06 Å (Si- bond length in bulk $CoSi_2$ is 2.31 Å). Our result is in agreement with the surface extenc x-ray absorption fine structure (SEXAFS) results of Rossi *et al.* [26] who measured a va of 2.26$-$2.35 Å for one and two $CoSi_2$ layers. Rossi *et al.* also ruled out the 5- and 7-f coordination of Co. In previous XSW measurements on epitaxially grown B-type $CoSi_2$ Si(111) surface it was concluded that the Co atoms at the interface are five-fold coordinat In the XSW measurement fivefold coordination cannot be distinguished from the eightf one as both the models would give the same d_{IF}. Recent local-density-functional (LDF) and quantum chemical cluster [9] calculations showed that the eightfold coordination, both B and A type, is much more favorable than the fivefold coordination. So, the 8-f coordination for the B-type interface appears to be established. In the two sets of previ XSW measurements on B-type $CoSi_2$/Si(111) samples it was observed that the Co ato at the interface are relaxed outward by 0.05$\pm$0.03 Å and 0.14$\pm$0.05 Å for films in

ranges 3–9 [4] and 20-51 Co layers [5], respectively. Here we observe for the A type $CoSi_2$ film containing 221 Co layers an inward relaxation of the interface Co atoms by 0.07±0.06Å. Whether this difference in the relaxation is due to the additional epitaxial Si layer [27] on top of the buried $CoSi_2$ layer or beacuse the film is A-type is not clear. The sample used in the SEXAFS study [26] had a Si bylayer on top of the $CoSi_2$ layer; however, the type of the interface was not known. The diffrence in the relaxation for the 8-fold A and the 8-fold B type interfaces may lie in the fact that the A-type interface has an overcoordinated Si atom whereas the B-type interface has an undercoordinated Si atom. Indeed, a persual of the contour plots of the constant valence charge density obtained from the LDF theory [28] for the 8-fold A, 8-fold B and bulk $CoSi_2$ shows that the Si–Co bond at the A type interface is stronger compared to both the B-type interface and bulk $CoSi_2$. This may be attributed to the Si-Co bond length contraction at the A-type interface. A difference in the relaxation for the A and B type interfaces was also observed for the $NiSi_2$/Si(111) system [3,7].

The measured coherent fraction in the present experiment is higher than the theoretical value. One notices this trend for large film thicknesses. Jegenhagen *et al.* [7] studied $NiSi_2$ epilayer on Si(111) with film thickness in the range 63–976 Å (20–314 Ni layers). There one notices that the measured coherent fraction falls below the theoretical value for thin layers and above for thick layers. For larger thicknesses the assumption of a constant planar spacing (d_{OL}) may need to be modified. In fact, the measured full width at half maximum (FWHM) of the (111) diffraction peak from the $CoSi_2$ layer is more than what is expected from a perfect 680 Å $CoSi_2$ layer with uniform (111) planar spacing [29]. However, this minor modification is not expected to change the conclusion regarding d_{IF} and the interface coordination.

For the study of the B-type $CoSi_2$/Si(111) system high resolution electron microscopy (HREM) was used by Gibson *et al.* [1]. As a definite structure assignment may be hampered by the uncertainities in the HREM image simulation parameters, they identified the 5-fold coordination of the interface Co atoms as the most likely model. This was later on supported by XSW [4,5] and ion scattering [6] studies. However, using the HREM technique Catana

et al. [15] obtained evidence for 7-fold (in some cases eightfold) coordination for the B-type interface, which contradicts even the previous HREM studies. For the A-type interface as well they showed evidence for sevenfold coordination. In both the HREM studies [1,15] the sample preparation procedures were essentially the same – by room temperature Co deposition on Si and annealing under UHV condition. On the IBS-prepared Si/$CoSi_2$/Si(111) systems, there were HREM studies by Bulle-Lieuwma *et al.* [16] on both A and B type $CoSi_2$/Si(111) interfaces. Through the computer simulations of the HREM images they obtained evidence for eightfold coordination of the B-type and sevenfold coordination of the A-type interface. It should be noted that theoretical calculations show the lowest interface energy for the eightfold B-type interface. For the A-type interface the sevenfold configuration has 26% (~ 0.2 eV) higher interface energy compared to the eightfold configuration [8,28], making the latter more likely. This agrees with our observations.

V. CONCLUSIONS

We have made x-ray diffraction and x-ray standing wave measurements on a buried $CoSi_2$ layer in the Si(880 Å)/$CoSi_2$(680 Å)/Si(111) system prepared by Ion Beam Synthesis, namely, Co ion implantation into Si(111) and subsequent annealing. The $CoSi_2$ layer was A-type. The (111) planar spacing and the strain in the $CoSi_2$ were determined with high resolution x-ray difrraction measuremnts. These values were used in further XSW analyses leading to the atomic structure of the $CoSi_2$/Si(111) substrate interface. We have found evidence for the eightfold coordination of the Co atoms at the interface, which means that the Co atoms of the silicide layer are directly bonded to the surface Si atoms of the substrate. The positions of the interface Co atoms are slightly relaxed towards the substrate. Assuming the substrate Si atoms to be at their ideal positions the inward relaxation corresponds to a Co–Si bond length of 2.28±0.06 Å i.e., 0.03 Å shorter than that in bulk $CoSi_2$. It was not possible to determine the structure of the upper Si/$CoSi_2$ interface in the present study. However, knowledge of this interface structure would provide an insight into the growth

process of the ion beam synthesized epilayer and the critical thickness for the B → A-type growth.

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FIGURES

FIG. 1. Possible models of the $CoSi_2$/Si(111) interface for both type-A and type-B systems. Open and filled circles represent Co and Si atoms, respectively. The Co atoms are 5-fold coordinated [(a) and (c)] when the extra plane of Si atoms are absent at interface. For details, see the text.

FIG. 2. Schematic experimental setup at the ROEMO station, HASYLAB at DESY. The white synchrotron x-ray beam is monochromatized and collimated in angle by using a symmetrically cut Ge(111) crystal (C1) and an asymmetrically cut Si(111) crystal (C2). The reflectivity [$R(\theta)$] was measured with the Ionization chamber (I3) and the fluorescence yield [$Y(\theta)$] was measured with the Si(Li) detector.

FIG. 3. Bulk x-ray diffraction pattern obtained from the sample when scanned by varying the angle of incident θ in steps of 0.002°. From the values of the angular positions of the (111) diffraction peaks, we obtained the (111) planar spacing in the $CoSi_2$ layer. The sample is schematically shown in the inset.

FIG. 4. $R(\theta)$ and $Y(\theta)$ are the reflectivity and the fluorescence yield, respectively. Circles : experiment; Lines : best fit to the XSW theory. The fit gives Φ_c=0.756±0.006 and F=0.15±0.05. The error bars are included in the size of the circles.

FIG. 5. Coherent position (Φ_c) and coherent fraction (F) computed from the experimentally determined number of Co layers (N) and strain (γ) for different interface models. (a) (i) and (ii) represent the computed coherent position for the 8-(or 5-) fold and the 7-fold model, respectively. The open square (with error bars) is the experimentally determined coherent position. (b) Solid line represent the computed coherent fraction and the open square (with error bars) represent the experimental value.

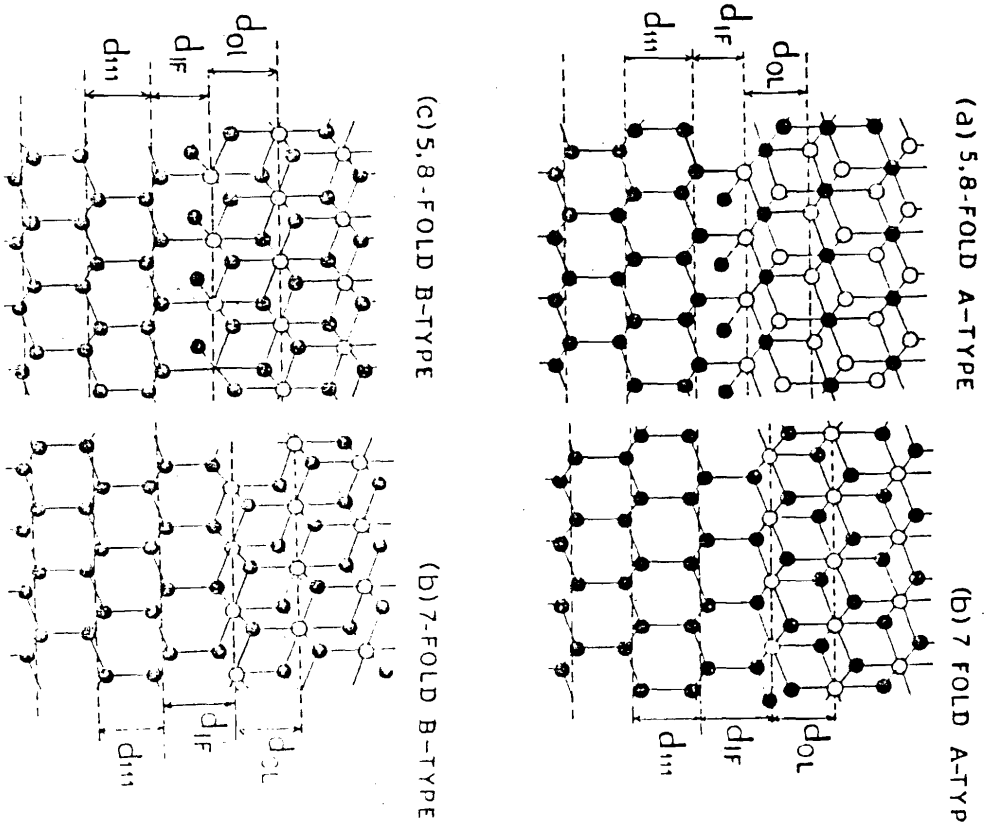
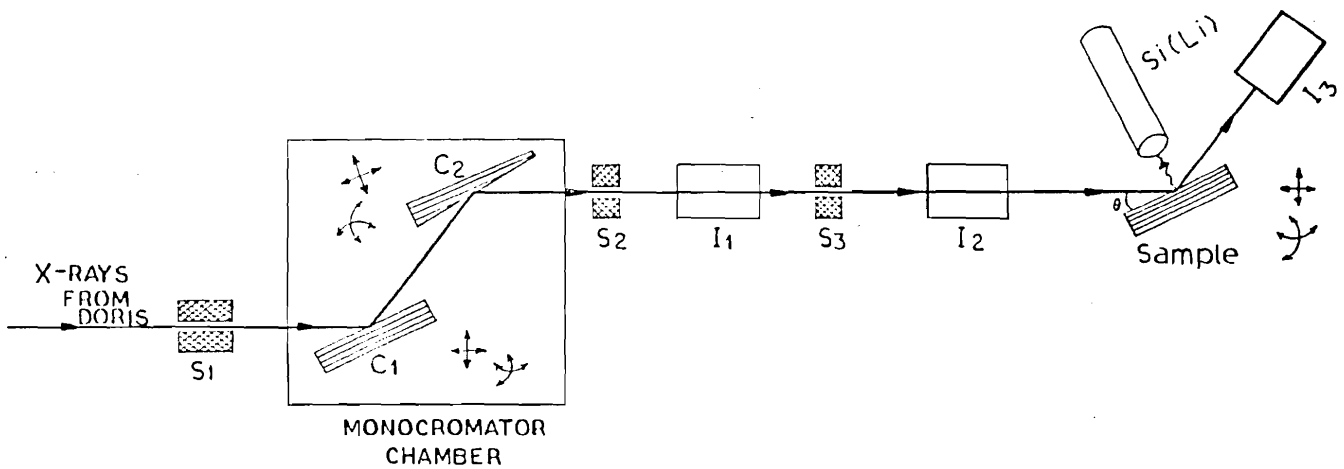


Fig. 1.



S_1, S_2, S_3 — SLITS

I_1, I_2, I_3 — IONIZATION CHAMBERS

C_1 — SYMMETRIC Ge(111) CRYSTAL

C_2 — ASYMMETRIC Si(111) CRYSTAL

SCHEMATIC EXPERIMENTAL SETUP

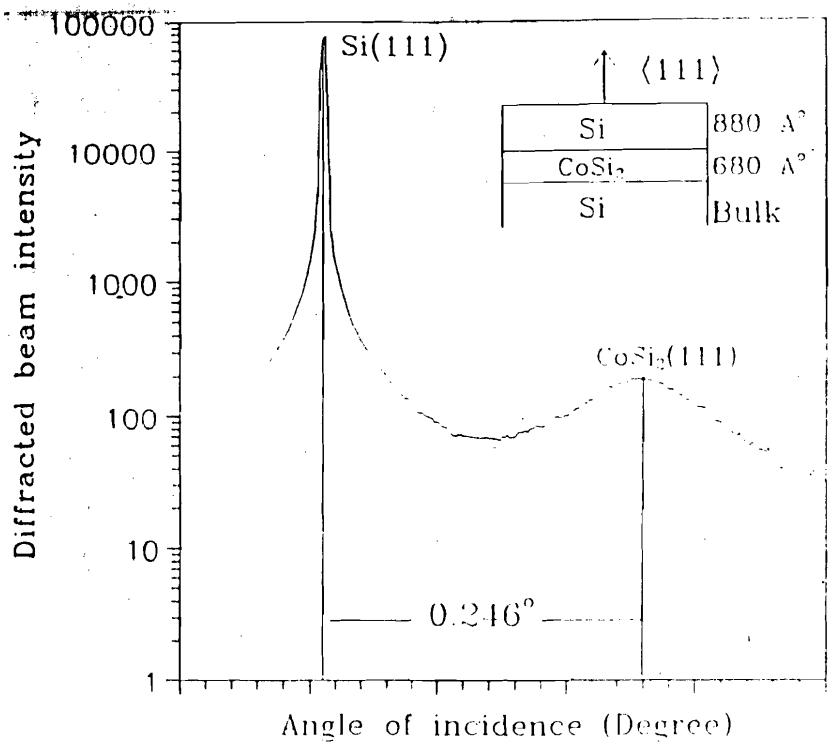

Diffracted beam intensity
100000
10000
1000
100
10
1
Si(111)
⟨111⟩
Si
880 Å
CoSi2
680 Å
Si
Bulk
CoSi2(111)
0.246°
Angle of incidence (Degree)

Fig-3

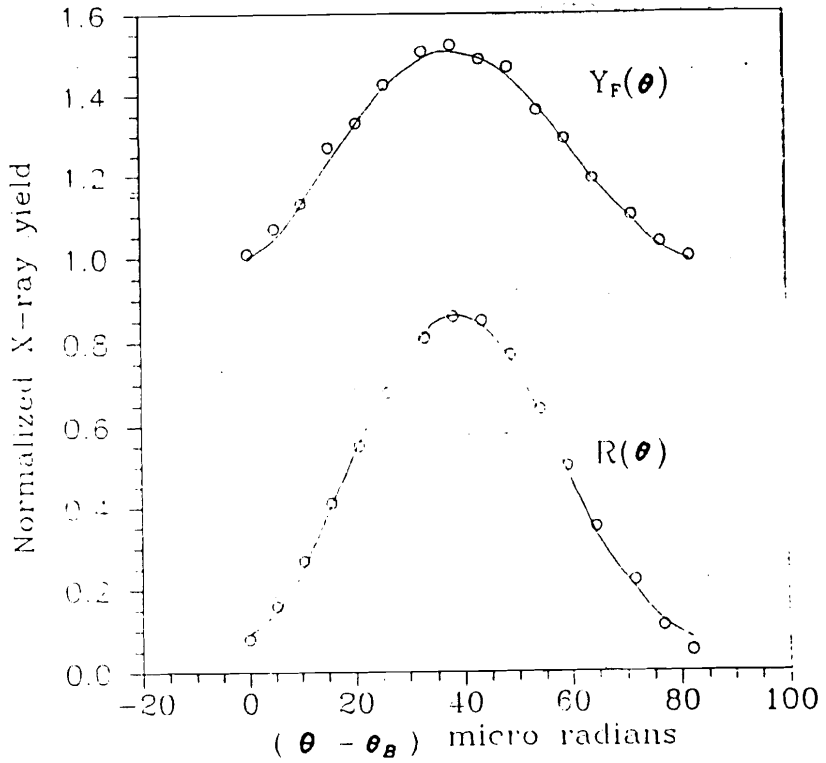

Normalized X-ray yield
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-20
0
20
40
60
80
100
$Y_F(\theta)$
$R(\theta)$
$(\theta - \theta_B)$ micro radians

Fig. 4

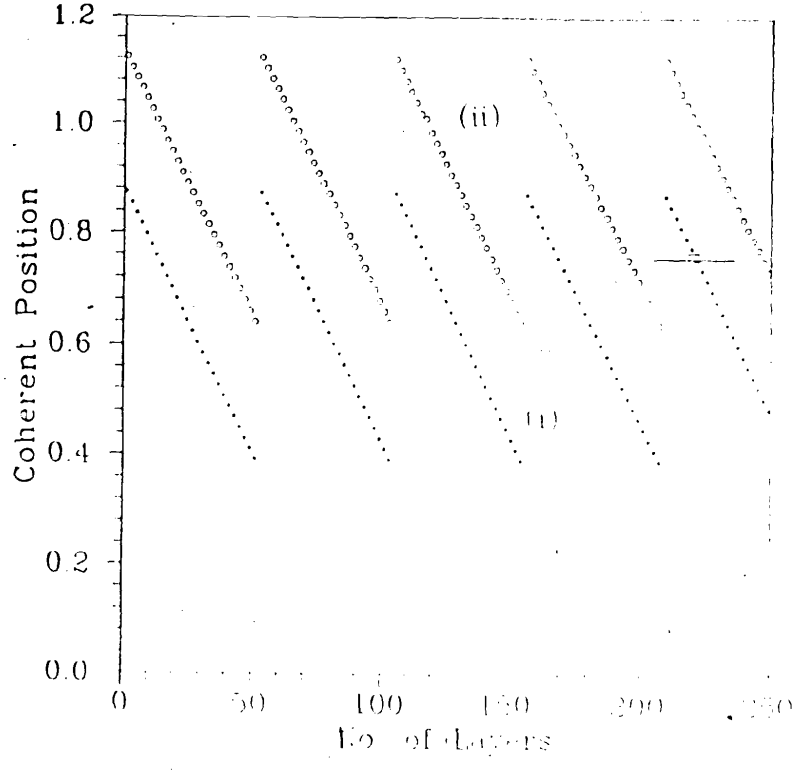

1.2
1.0
0.8
0.6
0.4
0.2
0.0
Coherent Position
(ii)
(i)
0
50
100
150
200
250
No. of Layers

Fig.5(a)

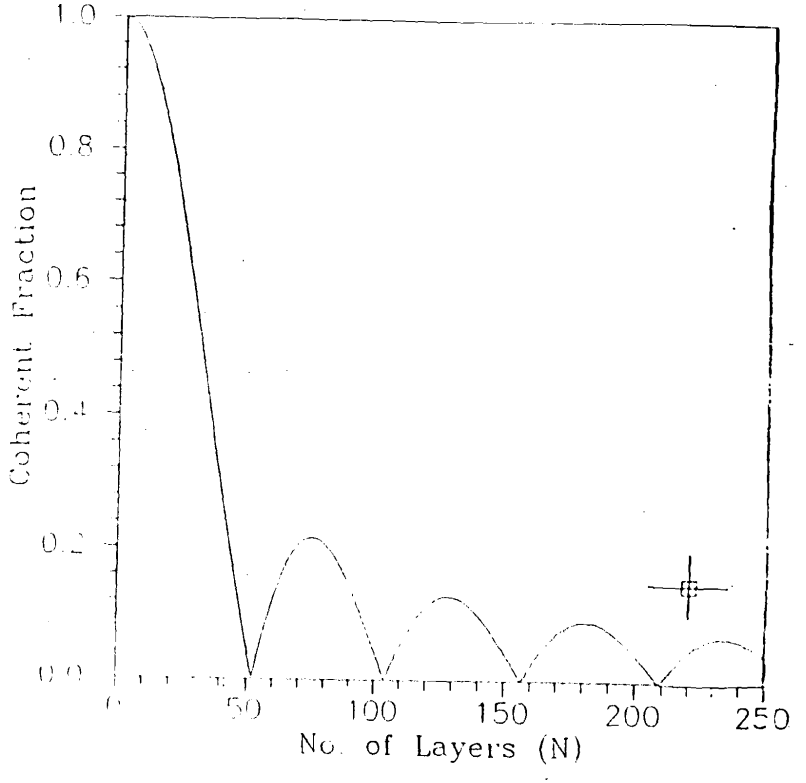

1.0
0.8
0.6
0.4
0.2
0.0
Coherent Fraction
0
50
100
150
200
250
No. of Layers (N)

Fig.5(b)