sufficient to identify the composition of the buried interface at sub-nanometer scale. We have shown possibility of determining phase composition at buried interfaces using soft x-ray resonant reflectivity (SXRRR) tuning photon energy at the absorption edges of constituent element *[for details please see M. Nayak, G. S. Lodha, A.K. Sinha, R.V. Nandedkar, S.A. Shivashankar Applied Physics Letter, 89 (2006)181920]*. We demonstrate this for a Mo-Si multilayer (ML) system, measuring soft x-ray reflectivity by tuning photon energy at Si L-absorption edge (L_{II} =12.34 and L_{III}=12.41nm) using Indus-1 SR. The $[Mo(30Å)/Si(60Å)]_5$ MLs were fabricated on float glass substrate using e-beam evaporation system. Before the SXRRR measurements, the micro-structural parameters were determined with XRR measurements with a Cu target (0.nm). Figure A.5.1 shows the measured and fitted XRR spectra of ML sample. The fitted data for three possible (different) interlayer phase compositions show clearly that conventional XRR is not sensitive to the composition of phases formed at buried interface. This is due to the small difference in optical constants among these compositions.

Figure A.5.2 shows the soft x-ray resonant reflectivity measured spectra using Indus-1 SR. The experimental data are fitted for three different compositions i.e. $MoSi_2$, Mo_5Si_3 and Mo_3Si. For two different photon wavelengths, good agreement between measured and best-fit curve is obtained for the $MoSi_2$ composition, not only near the Bragg peak but also in the Kiessig oscillation region and at grazing angles of incidence around the critical angle of total reflection. The fitted result reveals the formation of $MoSi_2$ composition at the interfaces.

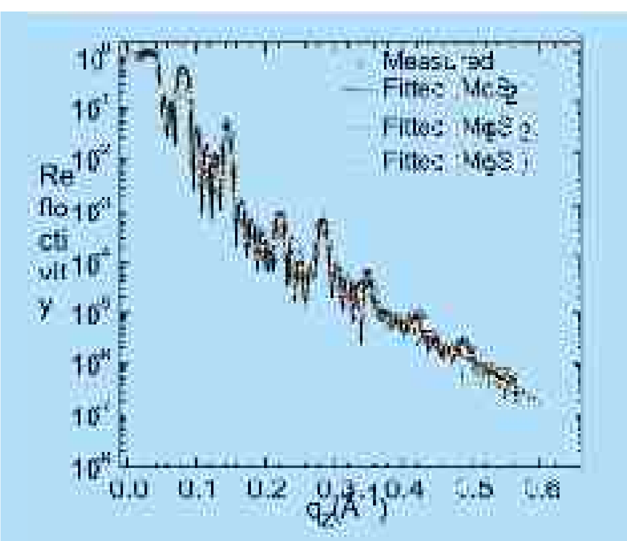

Fig. A.5.1 *XRR spectrum at Cu K wavelength of [Mo (30Å)/Si(60Å)]$_5$ ML.*

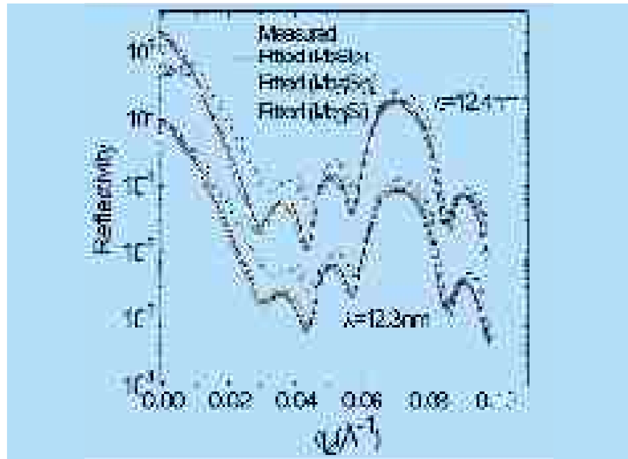

Fig. A.5.2 *Measured and fitted soft x-ray reflectivity of using Indus-1 SR near Si L-edge.*

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A.6 Z-contrast imaging in NbC/Si soft x-ray multilayer

Chemical roughness or the formations of nanocrystallites at the interface of multilayer structure used in soft x-ray mirrors deteriorate the performance of these mirrors. Conventional electron microscopy (CTEM) bright field (BF) imaging is usually not helpful as the strong diffraction contrast arising from the matrix obscures its presence. Since the precipitates differ most often from matrix by elemental content, atomic number (or z) contrast imaging seems to be well suited.

Z-contrast imaging is a common option in a scanning electron microscope (STEM). Here Z-contrast is realized by using an annular dark field (ADF) detector, which collects the electron scattered to high angles. Nano precipitates can be revealed routinely with this technique. Atomic resolution STEM work requires a microscope equipped with a field emission gun, and an exceptionally quite room environment. However, such options are not cheap or commonplace. Although Z-contrast imaging can also be realized in a conventional microscope (CTEM) by hollow cone illumination as well, the illumination cone convergence is limited to about 10 mrad, which is rather small compared to a 50/200mrad collection angle for high angle annular dark field (HAADF) STEM detectors. Hashimoto *(Hashimoto H, Kumao A, Himo K, Endoh H.E., Yotsumoto H& Ono A (1973) Journal of electron Microscopy 22,123)* first demonstrated the possibility to image heavy atoms and clusters by conventional dark field operation.

However in the case of a highly defective matrix, mostly its defect rather than the precipitates will be revealed with this method.

Here we show that nanometer-sized precipitates (shown in circle) of atomic number higher than those of surrounding crystalline/amorphous matrix can be clearly revealed in a conventional microscope by high angle centered dark field (HACDF) imaging after minimizing the diffraction contrast. The effect is similar to that of z-contrast STEM, albeit with a spatial resolution limited to 3-4 nm. In our studies cross sectional samples for TEM examination were prepared from multilayed sample of NbC/Si (10 layer pairs) on silicon substrate. Mechanical polishing, dimpling and low angle Ar-ion milling were used. Microscopy was carried out using Philips CM200 equipped with W cathode operated at 200kV. Figure A.6.1 shows the bright field image of the NbC/Si multilayer. High angle dark field image was obtained by using one of the diffraction spot. For z-contrast imaging, sample was tilted to such an extended that sample does not remain in the Bragg condition thus eliminating the diffraction contrast. Adjacent figure shows the z-contrast imaging of the same region from where bright field image was obtained. Dark band is due to the NbC and light bands are from Si. Dark bands contain some dark patches, which shows the presence of precipitate of NbC and Si in nanometer scale. These precipitates are shown in the circle. The chemical sensitivity to atomic number differences between precipitate and matrix is about 14.

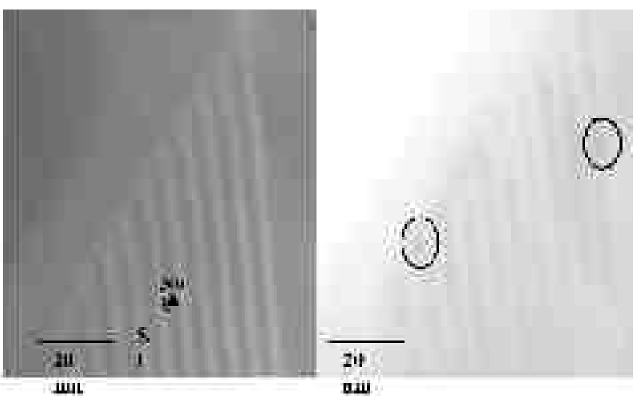

Fig. A.6.1 *Cross sectional TEM bright filed image of NbC/Si soft x-ray multilayer. Adjacent micrograph shows the Z contrast image of the same region.*

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Infrastructure

Computer Centre

Commissioning of high throughput cluster - Nalanda

32 node cluster 'Nalanda'was reconfigured with CONDOR clustering software to optimize parallel and sequential jobs. Currently each node has Pentium IV 2.8 GHz processor with 2 GB RAM. Intel Fortran, lf95, Absoft Fortran 90/95 compilers and parallel library MPICH for each of these compilers, are configured on the cluster. Math kernel library, SCALPACK, BLAS, CBLAS libraries are also configured on this cluster.

Many application programs like ADF (Amsterdam Density Functional - a Fortran program for calculations on atoms and molecules), WIEN97 & WIEN2K (computation of electronic structure of solids within density functional using Linearized Augmented Plane Wave (LAPW) method) and CPMD: Car-Parrinello Molecular Dynamics - Electronic Structure and Molecular Dynamics Program are successfully ported and running on the 32 node cluster. Transport software package (a computer program used to design charged particle beam transport systems) of version 1_5a for linux was also configured on the cluster with check-pointing facility.

Upgradation of computing infrastructure

A high end computing server (Chi) based on Quad Alpha 21264 RISC processors (1.25 GHz and 16 MB L2 cache, 8 GB RAM) , two Xeon based servers (Beta, Gama) with (2x3.6 GHz processors, 2 MB L2 cache, 4 GB RAM) and one Itanium2 based server (Epsilon) with (1.6 GHz processor, 9 MB L3 cache and 8 GB RAM) were commissioned and released to the scientific computing users.

Quad Alpha Server is a HP ES45 series server with Fort (Fortran90) compiler, Ladebug debugger, Compaq 'C' compiler, Compaq math libraries (cpml, cxml) and Parallel library MPICH version 1.2.7. Beta server is configured with Red Hat Linux 9, lf95, Absoft fortran 90, Intel fortran & 'C' compilers, Intel debugger, Math Kernel Library, Nag Fortran library and transport package. Gama server is configured with 64-bit Red Hat Enterprise Linux version 4.0, 64 bit compilers-GNU Fortran 95, Intel fortran & 'C', Intel debugger and Math Kernel Library.

Epsilon server is configured with 64-bit Red Hat Enterprise Linux version 3.0 , 64 bit compilers - Intel fortran & 'C', Intel debugger and Math Kernel Library.