PS12.02.08 FOCUSING COLLIMATORS FOR A MICROFOCUS X-RAY SOURCE. U.W. Arndt[1], A. Inneman[2] and L. Pina[3], [1]MRC LMB Cambridge CB2 2QH, UK, [2]Koma, K Lesu 965/4 14200 Prague 4, Czech Republic, [3]Czech Technical University, Bréhová 7, 11519 Prague 1, Czech Republic

We have constructed two types of specularly-reflecting focusing mirrors for 8keV X-rays: ellipsoidal mirrors made by an electroforming replication of appropriately shaped mandrels, and double Kirkpatrick-Baez-Franks mirror-blocks containing two pairs of orthogonal elastically-bent planar-elliptical mirrors. They are used with a magnetically focused X-ray tube, produced in collaboration with JVP Long and P Duncumb, which allows the mirrors to be mounted within 10 mm of the electron focus of which an image is formed on the specimen 600 mm from the source. This arrangement permits a large collecting angle at the source and a small crossfire at the sample: our best collimators produce a flux per unit tube power more than 100 times that obtained with a pinhole-collimated beam with the same cross-fire of about 0.001 radians. We have tested our system at low tube-power; we expect to be able to dissipate more than 25 watts in our X-ray tube, at which point we should exceed the X-ray intensity at the sample obtained with conventional collimation of a 2.5 kW rotating-anode X-ray generator beam.

PS12.02.09 DETERMINATION OF STRUCTURE DEFECTS IN MERCURY CADMIUM TELLURIDE MULTILAYER MATERIALS. Fuju Yu, Shanghai Institute of Technical Physics, Chinese Academy of Sciences, Shanghai 200083, China.

Some structure defects at heterojunction regions, such as microtwins, stacking faults, mismatch dislocations, and orientation differences between multilayer structures: mercury cadmium telluride/cadmium telluride and cadmium telluride/gallium arsenide as well, were studied by TEM (transmission electron microscopy). For the heterojunctions of mercury cadmium telluride/ cadmium telluride/gallium arsenide multilayers gown by MBE (molecular beam epitaxy) method, it is clearly shown that the buffer layer cadmium telluride acts as an effective barrier for mercury cadmium telluride epilayer for most of structure defects, and orientation differences between multilayer structures mercury cadmium telluride/cadmium telluride and cadmium telluride/gallium arsenide were found to be the more orientation difference accompanies the more lattice mismatch degree. There is a transient layer with intensive strain and a thickness at about 30 Angstrom, between buffer layer cadmium telluride and substrate. The transient layer distributed near homogeneously over a large area was just happened at the beginning of epitaxial growth of buffer layer due to large lattice mismatch as well as inappropriate growth rate (perhaps too fast) or other insufficient condition. It seems likely that the transient layer relaxes the lattice mismatch strain at heterojunction cadmium telluride/gallium arsenide, therefore no mismatch dislocation was created during the following growth of buffer layer and the epilayer could be smoothly grown afterwards. It is surprising to find that the epilayer can still be formed in an epitaxial orientation upon this transient layer, and this suggests either that the substrate can influence the overgrowing epilayer through the intervening layer, or that this layer forms interactively later, just similar to the case in the (cadmium, zinc)sulfide/gallium arsenide compounds.

PS12.02.10 INTERFACE EVOLUTION AFTER THERMAL TREATMENT OF TUNGSTEN/SILICON MULTILAYERS. M.Jergela, V.Holyb, Z. Bochnicekb, E.Majkovaa, S.Lubya, R.Senderaka a Institute of Physics of the Slovak Academy of Sciences, Dubravska cesta 9, 842 28 Bratislava, Slovakia b Faculty of Science, Masaryk University, Kotlarska 2, 611 37 Brno, Czech Republic

The X-ray reflectivity and diffuse scattering measurements at grazing incidence after a thermal treatment were performed on the [10x(2.65nmW/9.15nmSi)] and [9x(1.7nmW/5.4nmSi)] multilayers. The samples were prepared by electron-beam evaporation in the Balzers 500 UHV apparatus onto oxidized Si(100) substrates covered with 500 nm of SiO2. The measurements were performed on the Stoe high-resolution diffractometer equipped with a double-crystal GaAs monochromator using CuKα1 radiation. The rapid thermal annealing was performed in a halogen lamp furnace. The reflectivity was measured also in-situ during long-time linear and isothermal annealings using a laboratory-made apparatus. The results of the reflectivity and diffuse scattering measurements were simulated within the Fresnel optical computational code and distorted-wave Born approximation, respectively, using various interface conformity models. The rms interface roughness is unchanged or even decreases up to the 500°C/20s annealing, the sharpening of the interfaces being accompanied by a large shift exceeding 1 nm caused by the Si diffusion into W without disturbing the multilayer structure itself. The conformity of the interface profiles and fractal behaviour found in the as-deposited state is lost after the thermal treatment and the lateral interface correlation length increases by more than one order of magnitude. An extensive interdiffusion above 500°C is observed leading to the breakdown of the multilayer after the 750°C/40s annealing. Various dynamical scattering effects at grazing incidence are discussed, too.

PS12.02.11 THE DETERMINATION OF CRYSTAL STRUCTURE AND TEXTURE PARAMETERS OF POLYCRYSTALLINE THIN FILMS USING MULTIPLE DIFFRACTION DATASETS. H. Toraya, Ceramics Research Laboratory, Nagoya Institute of Technology Asahigaoka, Tajimi 507, Japan

Polycrystalline thin film/powder samples often exhibit the texture (preferred orientation) effect. The intensity correction for texture effect is, however, apt to induce the correlation with other parameters, and makes a result of crystal structure analysis less reliable. In the present study, a new procedure using multiple differaction datasest for the determination of crystal structure and texture parameters of polycrystalline thin films is proposed.

A sample used for the present study was a polycrystalline $Bi_3Fe_5O_{12}$ thin film. A wide-angle two-axis thin-film diffractometer based on a parallel-beam optics was used for data collection. Multiple diffraction datasets were obtained by using an asymmetric 2 θ scan technique at various fixed incident angles ranging from 1° to 30°. An individual profile fitting technique was used for pattern decomposition. In asymmetric diffraction, the scattering vector does not coincide with the polar axis of the specimen. Thus each of these datasets exhibited the different degree of texture effect. In previous studies, a Rietveld refinement technique was applied separately to individual diffraction datasets [1,2].

In the present study, all integrated intensity datasets observed at different incident angles were simultaneously used for the least-squares determination of crystal structure and texture parameters of the specimen.

The function of symmetrized harmonics expansion [3] was used to correct the intensity for preferred orientation. The accuracy of refined parameters was improved compared to the result obtained by using single scan datasets. The present technique will be applied to powder specimens with preferred orientation effect.

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PS12.02.12 EPSILON-GAMMA PRIME TRANSFORMATION IN NITRIDED Fe AND STEEL: STRUCTURE CHARACTERIZATION. P. S. Schabes-Retchkiman, G. Hinojosa* and J. Oseguera*, Instituto de Fisica, U.N.A.M., Apdo. Postal 20-364, Mexico, D. F. 01000, MEXICO, *ITESM-CEM,DGI, Apdo. Postal 18, Atizapan, Mexico 529926, MEXICO.

Thin layers formed by means of thermochemical nitriding treatments, of the surface of metals, particularly iron and steel, produce big enhancements in their mechanical and tribological properties. The origin of the improvement in iron and steel stems from the formation of a compact nitride compound surface layers and a diffusion zone of nitrogen interstitially dissolved in ferrite [1]. The top layers may be composed of epsilon and gamma' (carbo)nitrides. Above the eutectoid transformation point, an epsilon compact nitride layer is formed, and a transformation of the nitride into epsilon+gamma' during the sample's cooling occurs. In this work we have set out to study the epsilon to gamma' transformation, particularly by high-resolution transmission electron microscopy.

Glow discharge plasma nitriding was performed. In these experiments, pure iron and steel samples were nitrided. The results obtained in this work show that desaturation of the epsilon nitride during slow cooling produces equilibrium between the epsilon and gamma' phases. This reaction results in the formation of alternating plates of the given phases. HREM of the structures observed has confirmed that the transformation epsilon to gamma' is displacive confirming the model suggested by Gerardin et al [2].

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PS12.02.13 MOLECULAR DYNAMICS STUDIES OF ULTRATHIN METALLIC FILMS GROWTH. A.E.Moroz, A.A.Katsnelson, O.S.Trushin, Department, of Solid State Physics, Moscow State University, Russia

We announce the results of our molecular dynamics (MD) simulation of the growth processes of metallic ultrathin films in molecular beam epitaxy procedures. In the case of the deposition of Co atoms to the Co(100) substrate we studied the homoepitaxy process. The Co/Co system was modelled at the substrate's temperature of 300 and 800 K. In both cases the atoms falling onto the substrate formed crystalline film and its structure was similar to the substrate's one. When the substrate's temperature was increased, the structure of the film was less ordered. The dynamics of the film growth was also observed. The Co atoms first formed two-dimensional islands on the surface and only later filled in the spaces between these groupings. We modelled the getero epitaxial process in the case of deposition of Ag atoms to the Co(100) substrate. The Ag atoms settled between the cobalt atoms and formed well-ordered structure. But if the Co atoms formed FCC plane lattice corresponding to the plane (100) then
Ag atoms formed FCC plane lattice corresponding to the plane (111). The system obtained was heated to 1500 K and cooled rapidly to 100 K. The two-dimensional pair correlation functions g(r) for Ag layers were calculated. Thier analysis indicates the absence of long-range correlations which are typical for well-ordered crystal layers. Whereas, the short-range order in the Ag film was detected. It corresponds to amorphous plane lattice appearance.

PS12.02.14 MICROSTRUCTURAL STUDIES OF SUPERCONDUCTING OXIDE THIN FILMS AND MULTILAYERS A. Vailionis, A. Brazdeikis, A.S. Flodström, Department of Physics, Materials Physics, Royal Institute of Technology, S-100 44 Stockholm, Sweden

Superconducting properties of the layered cuprate thin films and multilayers are known to be very sensitive to the microstructural quality such as intergrowth defects, interface roughness and substitutional disorder in a unit cell. An extensive structural analysis is often required before the physical properties are measured. We will present the microstructural studies of MBE-grown "infinite-layer" structure, (Sr,Ca)CuO_2, films as well as $Bi_2Sr_2Ca_{n-1}Cu_nO_y$ films and multilayers using x-ray diffraction (XRD) and extended x-ray absorption fine structure (EXAFS) techniques. To obtain a quantitative information of the thin film microstructure a general one- dimensional kinematic x-ray diffraction model has been applied to these complex layered oxides. Structure of Bi-based cuprates was determined by comparing the measured XRD spectra of the MBE-grown samples with the calculated x-ray diffraction profiles of the model structure. The interplanar distances and cationic substitutions within the unit cell and number of stacking faults were used as fitting parameters. The iterative fitting procedure revealed a substitutional disorder present in the average unit cell as well as stacking defects. The high-resolution transmission electron microscopy confirmed a presence of both $Bi_2Sr_2Cu_1O_y$ and $Bi_2Sr_2Ca_2Cu_3O_y$ phases as intergrowths in the $Bi_2Sr_2Ca_1Cu_2O_y$ film matrix. For $Bi_2Sr_2Ca_1Cu_2O_y/Bi_2Sr_2Cu_1O_y$ multilayers the randomly distributed stacking faults were distinguished from those localized at the interface. Local environment of the copper atoms in the layered unit cell was analyzed by EXAFS. The Cu-Sr, Cu-Ca, Cu-Cu distances and Cu-O bond lengths were determined from Cu K-edge absorption spectra. CuO_2-CuO_2 and CuO_2-SrO interplanar distances obtained from XRD data are compared with those from EXAFS data. The relations between structural quality and growth parameters are discussed. The origin of structural disorder is interpreted as being caused by growth kinetics that plays a major role in film formation.

PS12.02.15 LIQUID NITROGEN EFFECT ON THE MORPHOLOGY OF PMMA THIN FILMS ON YBCO. Amita Malik, M. Atreyi, Department of Chemistry, University of Delhi, Delhi, India, G. L. Bhalla, G. C. Trigunayat, Department of Physics & Astro-physics, University of Delhi, Delhi, India

High temperature superconducting YBCO was encapsulated with polymethylmethacrylate (PMMA) film by plasma polymerisation of methylmethacrylate (MMA). YBCO samples with encapsulating films of varying thickness (5-14 microns), obtained by varying the length of plasma polymerisation, were subjected to 50 cryo-thermal cycles, each consisting of keeping the sample in liquid nitrogen for 1 minute and then at ambient environment for 30 minutes. The changes in the morphology of PMMA after every 10 cryo-thermal cycles were examined by scanning electron microscope. It was generally observed that, the PMMA encapsulating film first develops inhomogeneities and then shrinks, with the extent of transformation depending on the number of cryo-thermal cycles and thick-