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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We acknowledge support by CONACyT grant 3334-A. Technical support by L. Rendon is also appreciated.

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-

ness of the film. Such morphological changes were not observed on the PMMA film when the samples were continuously kept in the liquid nitrogen for a few hours. The changes in the morphology could be attributed to the release of thermal stresses developed during the plasma polymerisation of MMA, coupled with entrapping of gases, which cause thermal strains during the repeated cryo-thermal cycles.

PS12.02.16 DEPOSITION, MOLECULAR ORGANIZATION AND FUNCTIONAL ACTIVITY OF IgG LANGMUIR FILMS A.Tronin[1], T.Dubrovsky[2] [1]Institute of Crystallography, Leninsky 59, Moscow 117333, Russia [2]Bakh Institute of Biochemistry, Leninsky 33, Moscow 117071, Russia

Monolayers formed at the air-water interface and covalently immobilized on solid supports were studied by means of ellipsometry, time resolved fluorimetry, nanogravimetry and immunology testing. The model of the film molecular packing has been put forward, according to which the molecular orientation depends on the surface pressure. At the pressure below 20 mN/m the molecules are oriented parallel to the surface, when compressed up to 35 mN/m the molecules take perpendicular position, with their Fab fragments oriented preferentially outside the film. Within the range 20 mN/m<<35 mN/m the molecular inclination angle increases monotonically from 0 to 90. The pattern of the orientation-pressure behavior for transferred monolayers is almost the same showing that the film molecular structure does not change upon deposition onto the solid activated substrate. Complex structures of protein A sublayer-Langmuir film of IgG have been obtained and studied as well. The problem of protein monolayer stability has been addressed, and partial unfolding of the protein globule has been suggested to be an origin for high molecular surface activity. The dependence of immunological activity of IgG films on the packing parameters has been studied.

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PS12.02.17 TECTONIC SETTING AND CHARACTERS OF RAS SHAIT PODIFORM CHROMITE, EASTERN DESERT, EGYPT. Nadi A. Saad, Department of Geology, Faculty of Science, University of Alexandria, Egypt

The chromite deposits of Ras Shait area occur in an ophiolite complex as isolated lenses, pods, nodules or as disseminated grains mainly enclosed in serpentinites and talc carbonates. Incomplete sequence of the ophiolite complex is recorded in the studied area. Metamorphic peridotites and the overlying foliated gabbro are the main units, while sheeted dykes and massive basalts are encountered as limited exposures. The peridotite and associated chromite mineralization display features characteristic of the Alpine-type. The Ni/Co and MgO/SiO_2 ratios of the serpentinites and talc carbonates, beside their petrographic characteristics suggest that the parental rocks were harzburgite-lherzolite. The main opaque constituents in the studied area is chromite and its alteration products (ferritchromite and chromian magnetite). Ilmenite, titanomagnetite and rutile are present in subordinate amounts. Pyrite, chalcopyrite and pyrrhotite are rare. The associated gangues are antigorite, lizardite, talc, magnesite, calcite, fuchsite and kaemmererite. The microprobe analysis of the zoned chromite grains shows chemical compositional variations from the core to the rim and reveal that the alteration zones of chromite crystals are enriched in Fe and Ni and depleted in Al, Mg and Mn. This alteration is concomitant with the serpentinization process which affected the ultramafic masses. A plate tectonic model is proposed to explain the genesis of Ras Shait chromites. The ophiolite complex, with its associated chromite, are considered to be a mass of oceanic lithosphere obducted over continental crust. During obduction, the original chromite layers were subjected to intense tectonic disturbances with the result that the chromite deposits were dismembered and variously rolled giving the present pod form.

PS12.02.18 INTERFACE ROUGHNESS CORRELATIONS IN Ge/Si/Si1-xGex QUANTUM WELL HETEROSTRUCTURES. Y. Yamaguchi, P. M. Reimer, J.H. Li, O. Sakata, H. Hashizume, Tokyo Institute of Technology

We examine roughness correlations between interfaces in a simple Ge/Si/Si1-x Gex heterostructure as a function of Si layer thickness. Recently it has been found [1] that the photoluminescence (PL) spectra from quantum wells (QW) of Ge/Si/Si1-xGex (with x less than 0.4) can be strongly perturbed by growing several Ge-rich monolayers on top of a Si layer which tops the QW. No PL perturbation is observed for Si thicknesses greater than about 1000 nm, and the perturbation saturates for Si thicknesses less than about 30 nm.

We collected x-ray diffuse scattering data at glancing angles from solid-source MBE grown Ge/Si/Si1-xGex heterostructures on Si (100) substrates, with a variety of Si layer thicknesses. Using techniques described in another session (see the presentation by P. M. Reimer, et. al.) we modelled and fit parameters to find in-plane and inter-layer roughness correlations as a function of Si layer thickness. Parameters may be compared with recent results from multilayers on Si (111) substrates (see the presentation by J.H. Li, et. al.).

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PR12.02.19 STRUCTURE OF ULTRATHIN FILMS Ni/Au(001) AND Au/Ni(001): A STUDY USING MOLECULAR-DYNAMICS SIMULATION. O.V.Lysenko (Volf), A.A.Katsnelson, A.E.Moroz, V.S.Stepanyuk, O.S.Trushin. Physics Department, Moscow State University, Russia.

Growth of the ultrathin films Ni on substrate Au(001) and Au on substrate Ni(001) at room temperature are studied by means of molecular- dynamics simulation using Lennard- Jones potential.

From structural Ni/Au(001) and Au/Ni(001) data can be deduced: The first epilayer Au exhibits fcc Au(111) film. Larger radius of Au atoms (by 16%) in comparison to Ni atoms gives rise to the orientation change of this layer relatively to substrate. If positions of Au atoms correspond to (111) lattice plane than greater number of ordering particles of Au coincides with positions of Ni atoms. The structure of the second epilayer is the same of the first one.

In process of Ni atoms adsorption on substrate Au(001) Ni atoms are placed upon interatomic hollow of substrate topmost layer. Besides, due to smaller radius of Ni atoms, they do not touch each other. Moreover, part of peaks of pair correlation function for the first epilayer is asymmetrical. The atomic positions in the next layers are characterized by lots of defects, but basic lattice plane type is the same of topmost layer of substrate. In this case interatomic distances Ni-Ni are smaller than ones in substrate Au-Au by 3-4% (but not by 16%) as in case Au/Ni(001). The weak diffusion of Ni atoms into substrate Au is observed.