

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.

[1] Toraya, H. and Okuda, T., *J. Phys. Chem. Solids*, 56, 1317-1322 (1995).

[2] Toraya, H. Proceedings for European Powder Diffraction Conference (EPDIC) IV (1995) (submitted).

[3] Jarvinen, M., *J. Appl. Cryst.*, 26, 525-531 (1993).

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].

1. J. Groseh, J. Morral and D. Schneider, editors: 1995 Carburizing and Nitriding with Atmospheres, Conf. Proc. 6-8 Dec 1995, ASM International, Materials Park OH, USA. 1995.

2. D. Gerardin, H. Michel and M. Gantois, *Script. Met* 11(1977)557.

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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 hetero 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. Their 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. Vaillonis, 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, $(\text{Sr,Ca})\text{CuO}_2$, films as well as $\text{Bi}_2\text{Sr}_2\text{Ca}_{n-1}\text{Cu}_n\text{O}_y$ 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 $\text{Bi}_2\text{Sr}_2\text{Cu}_1\text{O}_y$ and $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_5\text{O}_y$ phases as intergrowths in the $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_y$ film matrix. For $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_y/\text{Bi}_2\text{Sr}_2\text{Cu}_1\text{O}_y$ 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. $\text{CuO}_2\text{-CuO}_2$ and $\text{CuO}_2\text{-SrO}$ 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-