

**P.12.01.1***Acta Cryst.* (2005). **A61**, C409**Phase and Stress Analysis of Porous Titania Layer with Two-dimensional XRD**Bob B. He<sup>a</sup>, Kewei Xu<sup>b</sup>, <sup>a</sup>*Bruker AXS, Madison, WI, USA.* <sup>b</sup>*School of Materials Sci. & Eng., Xian Jiaotong University, Xian 710049, PRC.* E-mail: bhe@bruker-axs.com

The surface modification of titanium by micro-arc oxidation under various voltages was performed to form a porous titania layer which may improve the biocompatibility of titanium implants. The phases and residual stresses of the porous layers were measured with two-dimensional X-ray diffraction. The results show the porous layers contain anatase (TiO<sub>2</sub>) and rutile (TiO<sub>2</sub>). The content of rutile (TiO<sub>2</sub>) increases with increasing voltage. At 450V, anatase peaks almost disappear and many new peaks appear in the profile, some of them are identified as polymorphous CaTiO<sub>3</sub>. The residual stresses in the porous layers are compressive and increase with increasing voltage.

This presentation also introduces the recent progress in two-dimensional X-ray diffraction using the above application as an example for microstructure and residual stress analysis. The two-dimensional X-ray diffraction provides far more information than the conventional X-ray diffraction. Phase identification can be done by integration over a selected range of diffraction rings. The integrated data gives better intensity and statistics, especially for those samples with texture, large grain size, thin film or small quantity. Stress measurement using two-dimensional detector is based on a direct relationship between the stress tensor and the diffraction cone distortion.

[1] Huang P., Xu K., He B., Han Y., *Mat. Sci. Forum*, 2005, **490-491**, 1552. [2] He B., Xu K., Wang F., Huang P., *Mat. Sci. Forum*, 2005, **490-491**, 1.

**Keywords:** porous materials, stress, two-dimensional XRD**P.12.01.2***Acta Cryst.* (2005). **A61**, C409**Three-Beam Diffraction Anomalous Fine Structure of Thin Films**Hsueh-Hung Wu, Yen-Ru Lee, Hsin-Hung Chen, Wen-Shien Sun, Shih-Lin Chang, *Department of Physics, National Tsing Hua University, Hsinchu, Taiwan, 300, R.O.C.* E-mail: d893308@oz.nthu.edu.tw

Different from the usual two-beam DAFS (diffraction anomalous fine structure), we have recently developed the multi-beam DAFS (MDAFS) for observing the local structural environment of resonant atoms. With three-beam diffraction data for different photon energies, the visibility  $R_v$  of the intensity asymmetry related to the phases of structure-factor triplets involved in the three-beam diffraction can be determined. Analysis based on the dynamical diffraction theory and XAFS gives fine structures of DAFS spectra. In this paper, the three-wave diffractions of (100) *CdTe* thin films epitaxially grown on the (100) *InSb* substrates are measured for different photon energies covering all the  $L$  edges of the constituent atoms. The crystallographic phase of structure-factor triplets and the resonance phase shifts influenced by the substrate could be analyzed to give the interface structures in relation to the *CdTe* and *InSb*. Using this MDAFS technique, we have also extracted the information about the fine structures of *Cd* and *Te* around the interface.

**Keywords:** structure, thin film, DAFS**P.12.01.3***Acta Cryst.* (2005). **A61**, C409**X-ray Study of Titanium Coatings Made in Shaped Charge Jet Condition**Alexey Alexeyev<sup>a</sup>, Sergey Gromilov<sup>a</sup>, Sergey Kinelovsky<sup>b</sup>, Irina Kireenko<sup>a</sup>, <sup>a</sup>*Nikolayev Institute of Inorganic Chemistry. Novosibirsk, Russia.* <sup>b</sup>*Lavrent'ev Institute of Hydrodynamics. Novosibirsk, Russia.* E-mail: alexeyev@gorodok.net

To improve hardness and corrosion resistance of a titanium surface, one technique of its treatment is the introduction of C, N and B into the metal crystal lattice. A technique for the application of coatings to titanium surfaces by a cumulative jet is suggested [1].

Some coatings were studied on a DRON-RM4 diffractometer. X-ray phase analysis was performed using the POWDER CELL 2.4 software [2]. The atomic coordinates and thermal parameters were assigned according to the literature data. The characteristics, such as quantitative phase relations, unit cell parameters, profile parameters ( $u$ ,  $v$ ,  $w$ ), etc. were refined. The cubic and hexagonal modifications TiX, where  $X = C, N, B$ , were revealed in the samples investigated. The unit cell parameters  $a=4.23 - 4.31 \text{ \AA}$ ,  $a=2.97 - 2.98$  and  $c=4.75 - 4.80 \text{ \AA}$  were obtained for the cubic and hexagonal phases, respectively. The coating phase compositions appeared to be dependent on geometric characteristics of the cumulative device. The mean microhardness of the coating is 18 GPa, while the maximum value 39.5 GPa.

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**Keywords:** X-ray powder analysis, coatings, titanium compounds**P.12.01.4***Acta Cryst.* (2005). **A61**, C409**X-ray Investigation of Hydrogen Implanted GaAs**Kamila Orlińska<sup>a</sup>, M. Webb<sup>b</sup>, J. Domagała<sup>a</sup>, P. Vagović<sup>c</sup>, J. Bąk-Misiuk<sup>a</sup>, A. Kozanecki<sup>a</sup>, B. Sealy<sup>b</sup>, <sup>a</sup>*Institute of Physics, PAS, Warsaw, Poland.* <sup>b</sup>*University of Surrey, Guildford, UK.* <sup>c</sup>*Institute of Electrical Engineering SAS, Bratislava, Slovakia.* E-mail: orlin@ifpan.edu.pl

Smart-cut is a layer transfer technique, which offers a route to the monolithic integration of dissimilar materials. The technique exploits hydrogen implantation-induced exfoliation and wafer bonding to transfer thin layers of a semiconductor onto another material, which may have a different lattice constant. However, it is still unclear exactly how smart-cut is affected by different ion implantation parameters, especially for III-V materials such as GaAs. This work aims to investigate the role of the implant temperature and the dose rate on blistering in GaAs, in order to reconcile these findings, and to further the understanding of the smart-cut process.

Semi-insulating GaAs wafers were implanted with 190 keV H<sub>2</sub><sup>+</sup> ions, to a fluence of 5x10<sup>16</sup> H/cm<sup>2</sup>, at sample temperatures of 180K, 300K, 470K and 570K. The distribution of hydrogen and the implantation damage in the samples were studied by ion beam analysis and X-ray high-resolution diffraction. Information concerning the ion implantation damage and the strain distribution in the film was obtained by simulating the X-ray diffraction pattern. It was found that at higher temperature, hydrogen is mobile in the lattice and can rearrange into the plates, microcracks and bubbles, which are presented in blistered material, thus relieving the strain in the lattice. The dose rate was also found to be significant for the smart-cut process, as blistering and exfoliation are inhibited at low dose rates.

**Keywords:** smart-cut, X-ray diffraction, ion implantation**P.12.01.5***Acta Cryst.* (2005). **A61**, C409-C410**Grazing Incidence X-ray Diffraction Studies of Pharmaceutical Tablets**Mikko Koivisto, Vesa-Pekka Lehto, *Department of Physics, University of Turku, FI-20014 Turku, Finland.* E-mail: mikjuko@utu.fi

Grazing incidence diffraction (GID) is a technique not yet being used in the field of pharmaceutical physics widely. However, GID is a very potential alternative to the other surface sensitive techniques, e.g. various spectroscopic methods, used in the pharmaceutical materials analysis. With GID it is possible to monitor phase transitions on the surface of tablet as a function of time and depth, for example.

In the present study GID has been utilized to study the disorder of the tablet surface after the compaction. Three active pharmaceutical ingredients, namely tolbutamide, carbamazepine and chlorpropamide, were chosen to act as model tablet compounds. Several tablets were compacted using different compaction pressures. The prepared tablets were then analysed with GID with various incident angles in order to