profile analysis and TEM observations has been established [1].

[1] Couvy H., Frost D., Heidelbach F., Nyilas K., Ungár T., Mackwell S., Cordier P., *European Journal of Mineralogy*, 2004, **16 (6)**, 877-889.

Keywords: dislocation structure, microbeam analysis, high resolution X-ray diffraction

P.17.04.4

Acta Cryst. (2005). A**61**, C449

X-ray Synchrotron Studies of AlGaAs Based Laser Structures

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Modern semiconductor lasers include a complicated layered structures with quantum wells and insulated buried layers introduced by selective implantation with He or H ions. The strain and defects induced by implantation may disturb the action of the laser. In present studies the most important methods of characterization were white beam Bragg case section topography and recording of rocking curves with a small 50×50 μm^2 probe beam.

The investigations were performed in a special multilayers containing two relatively thick layers of AlGaAs separated by a thin layer with smaller Al concentration, covered by 0.3 μm GaAs cup. The structures were studied before and after implantation with 150 keV He ions at room temperature and 180º C. It was possible to reproduce the character of experimental rocking curves in numerically simulated using the Takagi-Taupin theory. In the computations we included the change of chemical composition and a strain profile being a sum of strain connected with epitaxial layers and the point defect distribution obtained with TRIM95. The necessary modification of the point defects distribution was flattening of the top part.

The section topographs revealed stripes due to successive epitaxial layers and the strain modulation fringes due to the buried layer. In case of selective implantation the topographs revealed some contrasts due to strains at the edges of the implanted areas.

Keywords: defects, semiconductor structures, diffraction

P.17.04.5

Acta Cryst. (2005). A**61**, C449

Strain Profiles in the Insulated Buried Layers Obtained by He Implantation in AlGaAs

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The insulated buried layers formed by 150 keV He ions to $Al_xGa_{1-x}As$ with various concentration of Al were studied with synchrotron diffraction methods. Some samples were studied with HRTEM. The implantations were performed at RT, 80 and 120º C. The doses varied from 2×10^{16} to 6×10^{16} cm^{-2}. The measurements included taking local rocking curves using small 50×50 μm^2 probe beam. The rocking curves exhibited characteristic interference maxima and enabled the analysis of the strain profiles by fitting the theoretical rocking curves obtained by numerical integration of the Takagi-Taupin equations. The white beam synchrotron back reflection topography revealed a sequence of strain modulation fringes similar to the main interference maxima in the rocking curves. The evaluated profiles exhibited the deformed region close to the surface indicating that the deformation is mainly caused by the point defects produced by incident ions and the recoils. The other feature increasing with the temperature of implantation was the flattening of top part of the strain maximum corresponding to the insulating buried layer. This flattening was more distinct for lower concentration of Al. The HRTEM patterns revealed characteristic small gaseous inclusions appeared in the most deformed region in the samples implanted with the highest applied doses.

Keywords: strain, ion implantation, diffraction

P.17.04.6

Acta Cryst. (2005). A**61**, C449

Huang Diffuse Scattering by Mesoscopic Interstitial Defects in BCC Metals

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Microstructural evolution of materials in the extreme environment of a fusion or an advanced fission power plant is driven by migration of defects produced by irradiation. If the energy of collision cascades is low, only point defects (vacancies and single interstitial atoms) are generated. Agglomerating point defects form dislocation loops and voids. Huang diffuse scattering (HDS) is used for the determination of structure of single interstitial defects generated by irradiation.

We show that in addition to single interstitial atom defects, mesoscopic defect clusters containing two or more interstitial atoms give a strong contribution to the observed HDS patterns. The occurrence of clusters of interstitial atoms in e-irradiated bcc iron was proved in a recent study of resistivity recovery curves. The effect of interstitial atom clusters on HDS has not yet been investigated. The size of these clusters is comparable with the lattice constant making the infinitesimal dislocation loop approximation underlying the existing treatment of HDS not applicable. We show that the fact that the core of a mesoscopic interstitial cluster is fully three-dimensional has a strong effect on the long-range elastic strain field, and this masks the symmetry-related features of HDS associated with single interstitial atom defects. The new findings may help resolving the conflict between predictions of density functional calculations and the existing interpretation of experimental observations of HDS in bcc metals of the VIth group of the periodic table.

This work was funded by the UK EPSRC and by EURATOM.

Keywords: diffuse scattering, defect structures, defect clusters

P.17.04.7

Acta Cryst. (2005). A**61**, C449

XRD Peak Profiles in the Case of the Lognormal Crystallite Size Distribution

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Since the lognormal distribution of a crystallite size in a powder simple is the most realizable one in practice, determination of the size distribution parameters (the median and logarithmic standard deviation) from X-ray diffraction peak profile characteristics (FWHM or integral width and shape factor) is an important problem of structure analysis.

Langford *et al*. [1] have shown in principle that the size distribution can be determined directly by a profile fitting method. However, their evaluation restricted to a small variance of the distribution.

In this paper, effect of the lognormal distribution parameters on the peak profile is examined without any assumption of the parameter rage. For that the diffraction peak intensity profiles from lognormally distributed spherical crystallites is simulated and analyzed thoroughly.

Unique correlation between the distribution parameters and the XRD peak characteristics was found to exist within a wide range of the parameter values.

[1] Langford J.I., Louer D., Scardi P., *J. Appl. Cryst.*, 2000, **33**, 964.

Keywords: powder, crystallite size distribution, XRD

P.17.04.8

Acta Cryst. (2005). A**61**, C449-C450

Evolution of Nanostructure States of Cu-powders Prepared by Ball Milling

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By HREM it was shown that the nanostructure states of Cu-powder prepared by ball milling is characterized by the presence of a high density of dislocations and twin faults. For the determination of microstructure parameters of Cu-powder the method of analysis of the X-ray powder diffraction pattern was developed [1].

The microstructure evolution of Cu-nanostructured powders depending on the ball milling conditions (namely, frequency of shocks, kinetic energy of shocks, the ratio between normal and tangential components of shock under constant time of the milling) was investigated. It is shown that the frequency of shocks in the range of 6-17 Hz does not affect on microstructure characteristics. The dislocation and twin densities are functions of the kinetic energy of shocks and the dislocation and twin densities change in non monotonous way when the energy of shocks increases. The ratio between normal and tangential components of shock is dominant factor that determines the ratio between edge and screw of dislocations.

[1] Ustinov A., Olikhovska L., Budarina N., Bernard F., *Diffraction analysis of the microstructure of materials*, Eds. E.J. Mittemeijer, P.Scardi, 2003, 333-359.

Keywords: nanostructured materials, ball-milling, X-ray powder diffraction pattern

P.17.04.9

Acta Cryst. (2005). A**61**, C450

Defects in γ Irradiated Cz-Si Annealed under High Pressure

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The effect of uniform stress on creation of oxygen - related defects in annealed Czochralski grown silicon, with point defects introduced by γ irradiation, is investigated. The (111) oriented Cz-Si samples with interstitial oxygen concentration, c_o = 9.5x10^{17} cm^{-3} were irradiated by γ rays (E=1.2 MeV, dose 1000 Mrad). Next the samples were treated for 5 h or 10 h at 920, 1270 and 1400 K under hydrostatic Ar pressure (HP) equal to 1.1 GPa. The kind, dimension and concentration of defects were estimated from X-ray diffuse scattering data. While the concentrations of point defects were similar for irradiated and non irradiated Cz-Si, X-Ray diffuse scattering was stronger after the HP treatment of γ irradiated samples. The temperature dependent effect of HP at annealing is specific for γ irradiated Cz-Si. The changes in diffuse scattering intensity are accompanied by the changed concentration and dimension of point defects conglomerates; the average defect dimension is below 100 nm. HP affects oxygen precipitation in γ irradiated Cz-Si mostly through its effect on the creation and transformation of *V*O and V_mO_n complexes, the last ones acting as the nuclei for oxygen precipitation.

Keywords: Cz-Si, γ irradiation, annealing stress

P.17.04.10

Acta Cryst. (2005). A**61**, C450

X-ray Diffuse Scattering on the First Type Defects in Semiconductors

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X-ray diffraction techniques give powerful tool for the investigation of the defect structure in crystals. For the case of I type defects (as interstitials, vacancies, dislocation loops etc.) in the lattice, main of these methods [1,2] are based on the analysis of the Huang and Stoks-Wilson scattered ranges, which contain information about the distortion field around the defect.

From our observations we conclude that described experimental procedures for determination of defects size and their concentration are trustworthy at the special case and can not be used for general one.

In this work we analyzed more basic case of the defect structure which include the simultaneously presence of defects giving lattice deformation of opposite signs. The effects following from the assumption that defect concentration should be described as a function of defects size are considered in details.

All diffraction measurements presented in this work were made using the triple-axes diffractometer Philips X'Pert MRD.

[1] Larson B.C., Schmatz W., *Phys. Rev. B.*, 1974, **10(6)**, 2307. [2] Patel J.R., *J. Appl. Cryst.*, **8**, 186.

Keywords: diffuse scattering, point defects, high-resolution X-ray diffraction

P.17.04.11

Acta Cryst. (2005). A**61**, C450

Structural and Microstructural Studies of Synthetic and Naturally Occurring Hydroxyapatites using Powder Diffraction

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Hydroxyapatite (HAP), the main constituent of mammalian hard tissue, is an important mineral reservoir for the metabolic activity of the organism. Structural and microstructural characterization of several naturally occurring HAP samples extracted from human tooth, goat bone, rabbit bone and synthetic HAP have been carried out using X-ray powder diffraction studies. Diffraction data were collected with a step scan mode at an interval of 0.02°(2θ) using a Bruker D8 Advance X-ray powder diffractometer equipped with a germanium crystal primary beam monochromator (CuK$\alpha_{1=}$ 1.5406 Å). Preliminary phase identification of the naturally occurring HAP samples using the ICDD data base indicated presence of small amounts of Calcite ($CaCO_3$) and Dolomite [$CaMg(CO_3)$], (2-4% each), in addition to the main HAP phase, $Ca_{10}(PO_4)_6(OH)_2$.The whole powder pattern decomposition of the naturally occurring samples indicated sharp (00l) reflections, is in agreement with the earlier reports of preferred orientation in HAP crystals along the c-axis. Rietveld analysis carried out incorporating the structural parameters of different constituents phases using the program TOPAS showed final R_{wp} values ranging between 9.9-111.5%. The average crystallize sizes in the samples vary between 500 to 400 nm. The refined P-O distances in the synthetic HAP sample differ significantly compared to these observed in the naturally occurring samples.

Keywords: hydroxyapatite, microstructure analysis, Rietveld refinement

P.17.04.12

Acta Cryst. (2005). A**61**, C450-C451

An X-ray Diffraction Study on Dislocation Microstructure of as-prepared Al-Al_2O_3 Composites

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Particle reinforced MMC of Al - α-Al_2O_3 were prepared in the powder metallurgy route with 20, 50 and 75wt% of Al powder. The line profile analysis of the composites was done in the Whole-Pattern Fitting procedure based on the Rietveld structure refinement codes. It also incorporates the microstructure refinement codes based on either phenomenological parameters [1] or physically based model [2]. Here the microstructures of α-Al_2O_3 containing Al-based composites were studied in terms of ab-initio quasi-composite model of dislocation cell structure [3] and ellipsoidal log-normal distribution of crystallite size.

Postproduction plastic deformation of the Al grains and hence stress relaxation of the composites have taken place during cooling from the sintering temperature (500°C). It was also noticed that in the composites with lower concentration Al, each reflection of Al could be fitted with two peaks indicating dissimilar fragments with different dislocation density and arrangements. The region of high (~10^{10} cm^{-2})