

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

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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 $50 \times 50 \mu\text{m}^2$ 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 $0.3 \mu\text{m}$ GaAs cup. The structures were studied before and after implantation with 150 keV He ions at room temperature and 180°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

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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 $\text{Al}_x\text{Ga}_{1-x}\text{As}$ 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 120°C . The doses varied from 2×10^{16} to $6 \times 10^{16} \text{ cm}^{-2}$. The measurements included taking local rocking curves using small $50 \times 50 \mu\text{m}^2$ 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

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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.

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Keywords: diffuse scattering, defect structures, defect clusters

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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 sample 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 range. 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

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

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