07.8–6 THE CONCENTRATIONS IN HETEROEPITAXIAL SILICON ON SAPPHIRE. C Dineen, K S Knight, T Peters, M Pitt and J C Robertson, GEC Research Laboratories, Hirst Research Centre, Wembley, UK.

The surface of heteroepitaxial silicon grown on sapphire substrates exhibits a haze-like appearance. It has been noted that device yield and performance can be correlated with the degree and extent of haze observed on the silicon. Considerable effort has therefore been expended on developing quantitative optical procedures for the assessment of haze. Little has been reported on work aimed at establishing the structural origin of haze.

This contribution describes recent results on the determination of twin concentrations in hetero-epitaxial silicon on sapphire by XRD. Details of the instrumentation employed will be given. It is shown that a correlation exists between twin concentrations and measurements of haze.

07.8–7 THE STRUCTURE OF MBE GROWN $(Ga_{1-x}Al_xAs)n_1$ $(GaAs)n_2$ / GaAs (001) SUPER LATTICES AS DETERMINED BY MEANS OF X-RAYS DIFFRACTION TECHNIQUES. By J. Kervarec, M. Baudet, P. Auvray and A. Regreny, Centre National d'Etudes des Télécommunications, 22301 LANNION FRANCE

The study of the physical properties of the superlattices $(Ga_{1-x}Al_xAs)n_1$ $(GaAs)n_2$ / GaAs (001) requires the knowledge of their structural parameters n_1, n_2 and x and of their crystalline perfection.

For this purpose, two experimental techniques are used a standard powder goniometer and a double crystal diffractometer. The diffraction diagrams directly yield the super period and the average Al concentration in the superlattices The value of x is determined by refinement between observed and calculated structure factors. The results are even more accurate when the number of observed satellite peaks for a given periodicity is greater ; this number depends at the same time on the Al composition x, the n_1 / n_2 ratio, the periodicity and its dispersion and the characteristic features of the interfaces.

This method is illustrated by a few examples. The consequences of various defects (dispersion in n_1 and n_2, super period gradient, Al diffusion) on the X-ray diagrams will be discussed.

07.8–8 КАЛИНИНСКИЙ ГОСУДАРСТВЕННЫЙ УНИВЕРСИТЕТ
КАЛИНИН, СССР

УДК 548.55

СМИРНОВ Ю.М.

ВЫРАЩИВАНИЕ МОНОКРИСТАЛЛОВ БОЛЬШИХ РАЗМЕРОВ ИЗ РАСПЛАВОВ

Монокристаллический германий обладает хорошими оптическими, механическими и химическими свойствами и находит применение в приборах, работающих в инфракрасной области спектра [I].

Нами изучались возможности получения монокристаллов германия с большой площадью поперечного сечения. В результате были последовательно получены монокристаллы с диаметрами I60, 200 и 300 мм [2-3]. Решение уравнения, предложенного в работе [4]

$$\alpha\beta^2x^5-\beta^2x^4-2\alpha\beta x^3+2\beta x^2+\gamma^2\alpha x-1=0,$$

где x – соотношение радиусов кристалла и расплава,

α, β, γ – функции свойств вещества и условий процесса роста, показало, что диаметр растущего кристалла обратно пропорционален квадрату температурного градиента в расплаве. Проверка этого результата проводилась на монокристаллах германия. Расчеты показали, что для выращивания монокристаллов диаметром 500 мм величина градиента температур в расплаве не должна превышать 40 $К \cdot м^{-1}$, что трудно выполнимо.

Тем не менее точное соблюдение температурного и кинематического режимов процесса роста, позволило вырастить монокристаллы германия диаметрами 400–500 мм и весом более 40–50 кг.

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07.9–1 CHARACTERIZATION OF THE $BaLaGa_3O_7$ SINGLE CRYSTALS GROWN BY CZOCHRALSKI METHOD. By G.Jasiolek, M.Berkowski and Wl.Piekarczyk, Institute of Physics of Polish Academy of Sciences, Warszawa, Poland.

The single crystal samples cut from the Czochralski growth $BaLaGa_3O_7$ crystals have been the subject of our investigations (Wl.Piekarczyk,M.Berkowski,G.Jasiolek, submitted to the J.Crystal Growth). The samples were prepared in the slice form with the surfaces parallel or perpendicular to the growth axis of the crystals, [001]. These samples were extracted from the part of the crystals with the convex crystallization front as well as from the part with the flat front. The morphology of the samples were revealed by the X-ray topography and the SEM techniques. These techniques permitted to detect few regions of the crystals which differ from surroundings. Particular attention was paid to the melt -back region as well as to the skin and core regions of the crystals. The observations of the changes of the lattice parameter "c" up to 0.0003nm were carried out using photographically modified Popovic method (J.Appl Crystall., (1971),4,240). The lattice parameters mapping along one of the crystals has been done using Bond method (Acta Cryst.,(1960),13,330). The concentrations of the gallium, barium and lanthanium as well as the level of distribution homogeneity of these elements were measured in the different regions of the crystals using the Electron Microprobe Analyzer. The increase of the gallium concentration was confirmed in the core region of the crystals. A slight increase of the barium concentration was observed in this region, too. It was found that the distribution of lanthanium is homogeneous in the whole crystal. The barium and gallium distributions are homogeneous out of inter-regions. Vickers microhardness was measured in the selected regions of the crystals, for the different orientations of the specimen

surfaces. Its value of (4.0 ± 0.1)GPa was found for the (001) oriented specimens. The glide systems of the investigated crystals basing on the {100} planes and <110> directions were detected by the microhardness anisotropy observations. The dislocation densities were estimated at the level lower than $10^4 cm^{-2}$ by the etch pits technique and the X-ray method. For the investigated crystals the X-ray $L_{\alpha 1}$, $L_{\beta 1}$, $L_{\beta 2}$ and $L_{\beta 4}$ emission spectra of Ba^{+2} and La^{+3} (A.A.Dakhel, Jpn.J.Appl.Phys.,(1982),21,1521) were obtained. They were compared with the same lines for BaF_2 and LaF_3 crystals. These investigations were carried out using the lithium fluoride (200) analysing crystal. The positions and the half-widths of these lines were defined. For example, it was confirmed that the half-width of the $L_{\beta 4}$ line increases from (11.3±0.5)eV for lanthanium fluoride up to (16.0 ± 0.5)eV for lanthanum ions in the $BaLaGa_3O_7$ single crystals. The information about some optical properties of the $BaLaGa_3O_7$ crystals was reported in (W.Wardzynski et all.,Physica B+C, (1984),123B,2).
Autors of the present work belive that their investigations permitted to select the best conditions for the $BaLaGa_3O_7$ single crystals growth process, and, on the other hand, to reveal the real structure of the crystals

07.9–2 OXIDATION BEHAVIOUR OF MAGNETITE, INVESTIGATED BY MEANS OF X-RAY ANALYSIS.

By M. Alavi, Chemistry Dept., Univ. Isfahan

Quantitative X-ray analysis, using soft radiation, results in information about the species and amount of oxidation products of so-called active magnetite.
For the formation of Fe_3O_4 the starting material α-Fe_2O_3 is applicated, which is to be reduced at 460-550°C by H_2/N_2. The active magnetite formed will be converted into maghemite, γ-Fe_2O_3 either directly after formation or after keeping a certain time at room temperature.
Contrary to the aged Fe_3O_4 which forms γ-Fe_2O_3 besides α-Fe_2O_3, the active Fe_3O_4 oxidizes to α-Fe_2O_3 completely. While cooling in an oxidizing atmosphere, the magnetite primarily formed shows an anomaly in Fe_3O_4 decrease between 290 and 350°C. An explanation is given by Faraday's passivation theory: temporarily an oxide skin is formed around the Fe_3O_4 grain which is hindering a further bulk oxidation.

07.9–3 Calculation of Single-Crystal Electrostrictive Coefficients from Time-Resolved X-Ray Diffraction Measurements

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The electrostrictive coefficients Q_{11}, Q_{12} and Q_{44} of high permittivity ceramics ($Pb(Zr,Ti)O_3$, $BaTiO_3$) can be measured separately with a time-resolved x-ray diffraction technique (Göbel, Adv. in X-Ray Anal., Vol 24, 1981; Zorn, to be published in Ferroelectrics). Electrostrictive lattice distortions are induced by an electrical ac-field and are measured as a function of polarization with x-ray diffraction. In a polycrystalline ceramic the electrostrictive distortions of crystallites are hindered by their neighbouring crystallites. This is obvious above all at high fields, where observed shifts in diffraction peaks are overlayed by asymmetric line broadenings. The broadenings must be taken into account for calculation of close-to-single-crystal electrostrictive coefficients. This is done with a least squares fit program. The program convolutes the diffraction peak at field zero with a predicted lattice constant distribution at high fields. By adapting the lattice constant distribution, the convoluted profile is fitted to the measured profile. Extrapolation leads to the lattice constants of stress free crystallites in the stressed ceramic.
In dilatometric measurements unreleased stresses lead to low electrostrictive coefficients. Time-resolved x-ray diffraction shows these stresses and therefore allows a correction of the result. It is a method to measure electrostrictive coefficients, which are close to single-crystal values, on materials that cannot be obtained as single-crystals.

07.9–4 THE MICROSTRUCTURE OF UNIDIRECTIONALLY SOLIDIFIED Ni-W EUTECTIC COMPOSITE. By S.F. Dirnfeld and D. Shectman, Dept. of Materials Engineering, Technion, Israel Institute of Technology, Haifa, Israel.

The microstructure of unidirectionally solidified (UDS) specimens of a Ni-W eutectic composition consists of W-fibres in a Ni(W) solid solution matrix which contains semi-coherent Ni_4W precipitates of the D_{1a} type. The growth axis of the W fibres and the orientation relationship between the phases in the as grown condition as well as after creep experiments at elevated temperatures were studied by transmission electron microscopy. Selected area diffraction patterns indicate that the growth axis (checked on three different fibres) is that of the <111> family. The analysis of the diffraction patterns taken from the boundary region of the Ni(W) and W phases shows that the orientation relationship between the phases is of the Bain type, so that <100> of the W fibres in parallel to the <100> of the Ni(W) matrix. It was found that the matrix of the as-grown specimens solidified at relatively high solidification rate (R>0.9 cm/hr) contains equiaxial Ni_4W precipitates of D_{1a}-type (face centered tetragonal structure) with the same orientation relationship as in Ni_4Mo (Okomoto and Thomas, Acta Met. (1971), 19, 825). The Ni_4W precipitates in specimens solidified at lower R are plate-like in shape with identical orientation relationship as mentioned before. The boundary between the two phases Ni_4W and Ni(W) solid solution consists of dislocation networks to compensate for the incoherency between the two structures. The fault structure of the W fibres shows low density of dislocation and no subboundaries were detected. A specimen that was subjected to creep for 95 hours at 960°C, shows strained areas. The boundary between the W fibres and the matrix is highly stressed at elevated temperature due to the difference in the thermal expansion coefficients and the different ductility of the two phases,