PR.17.00.17 INVESTIGATION OF THE DISLOCATION STRUCTURE PARAMETERS IN SINGLE CRYSTALS BY X-RAY METHOD. Sergey V. Ulshin and Olga P. Karasevskaya. Institute of Metal Physics,Ukrainian Academy of Sciences, 36,Vernadsky pr.,252142 Kiev,Ukraine

The basis for this method is the kinematic theory of X-ray scattering by non-ideal crystal with dislocations. This X-ray method allows to obtain three-dimensional intensity distribution from of I(q) in the cases of homogeneous and nonhomogeneous dislocation structure (DS), pole figure, average meanings of I(q) and their dispersion and to compare theoretical and experimental of I(q) for real crystals and identify DS.

But real crystals very often contain mixture of different DS with numerous parameters, that's why their analyze is complicated.In our paper we modeled several X-ray reflexes and found out that for crystals with different DS reflexes parameters strongly depend on their {hkl} and diffraction vector orientation. Therefore it is necessary to select reciprocal lattice sites, which can allow us to obtain the smallest error for structure parameters. The mathematical criterion for the choosing of the sum of sites which are suitable for investigation have been proposed by us. The investigations of I(q) in the cases of different types DS being in the crystal have shown that I(q) differs essentially for different sites and is very sensitive to types the DS. This makes it possible to develop the express-method for qualitative determination of the DS evolution during the process of single crystals deformation of new kind of the dislocations.

The parameters DS in BCC single crystals were studied. As a result of our experiments the change of the density of screw and edge dislocations {110},{112},{123}<111> and their distribution during the creep in the temperature interval (0,3-0,6) Tm established. At the high temperature creep multilevel DS is formed. The screw dislocations density really does not increase. At the initial stage of deformation correlation of the edge dislocations density 9:3:1 for the {110},{112},{123}<111> is formed.Than after 3-6% deformation depending on the single crystals orientation one sign surplus dislocation density essentially increases. At the low temperature creep dislocations density increase linearly with deformation.Correlation of the edge dislocations density 20:2:1 for the {110},{112},{123}<111> is formed.

Theory, Techniques And Instrumentation

PS17.01.01 SIMULATION OF SYNCHROTRON WHITE BEAM TOPOGRAPHS: APPLICATION TO THE STUDY OF PIEZOELECTRIC DEVICES . Y. Epelboin*, B. Capelle* & J. Détaint**, *LMCP, URA 009 CNRS, University P.M.Curie, Paris, France, **CNET, PAB, dept BAG/MCT/CMM, 92220 Bagneux, France

We present a new package which allows to simulate synchrotron white beam topographs for any kind of defect. It is split in two parts: a first program which computes the derivatives of the deformation and which must be written by the user for each model. A second general purpose simulation program takes these data and computes the image (Y. Epelboin, 1996, accepted in J. Appl. Cryst.). This program is valid for all studies. This allows to rapidly check new models for the defects without having to rewrite a whole simulation program.

A new algorithm for the integration of Takagi-Taupin equations has been written for massively parallel computers and multiple processors machines. It computes in parallel different lines of the image. The numerical method (C.A.M. Carvalho & Y. Epelboin (1993) Acta Cryst. A49, 460-467) has been modified to be able to vectorize the computation and to make it as efficient as possible. The simulation of an image needs from one up to three hours using one processor on a Cray C9x. It may be reduced by a factor equal to the number of available processors thus to less than one hour in all cases.

The study of the propagation of acoustic waves in piezoelectric devices is given as an example of the possibilities of this new program. The devices are circular plates from a quartz AT-cut crystal. The experimental topographs have been recorded by B. Capelle, J. Détaint & A. Zarka (1995). We consider an ideal case where the acoustic vibration mode is a pure thickness-shear mode. Two models have been investigated. describing the deformation inside the crystal either as exponentially decreasing cosine functions (Stevens & Tiersten, (1986) J. Acoust. Soc. Am. **79**, 1811-1826) or as a development with Bessel functions (Détaint & al. (1991) Proc. 45th Annu. Frequency Control Symp., pp 166-180).

The agreement between the experiments and the simulation is good except in the center of the resonator, which may be explained by imperfections in the geometry of the devices.

PS17.01.02 A NEW LIGHT MICROSCOPY TECHNIQUE FOR EXAMINING BIREFRINGENT MATERIALS. J.G. Lewis & A.M. Glazer, Clarendon Lab., Dept. Of Physics, Univ. Of Oxford, Oxford OX1 3PU, UK

A new imaging technique based around a polarising microscope is demonstrated (U.K. Patent Application Number BG9604785.7) [1]. Color coded images of optically birefringent materials are produced where colour represents | sin δ | (δ relative retardation) or ϕ the orientation of the cross section of the indicatrix of the specimen. Thus the contract seen in direfringent materials between the usual crossed polars setting is seperated out into its components. With this instrument the two values (ϕ and | sin δ |) can be easily quantified and monitored spatially with the resolution of a traditional light microscope.

Images of crystals, minerals and biological birefringent specimens are shown and analysed in both a qualitative and quantitative manner.

[1] Glazer, A.M. Lewis, J.G. & Kaminsky, W. *Nature* (awaiting publication).
[2] Wood, I.G. & Glazer, A.M. *J.Appl. Cryst.*, 133, 217-223 (1980).

PS17.01.03 X-RAY CHARACTERIZATION OF TEXTURE IN THIN FILMS USING A TWO DIMENSIONAL POSITION SENSITIVE DETECTOR P.D. Moran, Siemens Energy and Automation, Inc., Analytical Instrumentation, 6300 Enterprise Lane, Madison WI. 53719-1173, USA

By employing a low-noise, two-dimensional position sensitive x-ray detector it is possible to record pole figures in less than an hour from films that are as thin as 200 Angstroms. As well, "Area Detector" techniques allow one to accurately characterize sharply textured films, such as those seen in thin film optoelectronic and superconducting materials, with a resolution not practical with conventional point-detector based texture instruments. Third, by simultaneously collecting data from the substrate, one can also investigate the relationship of texture in the film to the crystallography of the substrate on which it was grown. The ability to accomplish these three tasks is primarily due to the ability of an area detector to simultaneously measure data from a large amount of reciprocal space at the same time. Of course, the measurements discussed above require different data collection and analysis strategies. The dependence of the strategy on the degree of texture present is discussed through practical examples of texture measurements from broadly and sharply textured thin films. Finally, the strategies employed using Area Detector techniques are examined through a comparison with the strategies that would be employed using a conventional point detector-based texture instrument to accomplish the same goals.

PS17.01.04 QUANTIFICATION OF STACKING FAULTS IN SYNDIOTACTIC POLYSTYRENE SINGLE CRYSTALS. Masatoshi Tosaka, Noritaka Hamada, Masaki Tsuji, Masahiro Fujita, Shinzo Kohjiya, Institute for Chemical Research, Kyoto University

Syndiotactic polystyrene (sPS) crystals have a unique character; i.e., they have inherent stacking faults in beta-form single crystals (orthorhombic $P2_1P2_1P2_1$, a=2.87nm, b=0.88nm, c(chain axis)= 0.51nm)[1]. In this study, we tried to determine the proportion of these faults from electron diffraction (ED) patterns and to investigate the dependence of the proportion on crystallization and annealing temperatures. The reli-