13-Defects, Microstructures and Textures

We will discuss these techniques, showing their possibilities and limitations. For instance we will show how it is possible to correct a varying background which often exists in the topographs, due to extended strains, and which severely prevents from observing small defects in the black areas of the image or enhance the visibility of an anisotropic feature. It is also possible to study an anisotropic texture in the images. Fourier and entropy techniques are complementary. We will compare their results and try to build a strategy for image analysis.

Two kinds of treatments may be considered. On-line analysis for standard features such as background correction, off-line treatment to extract special features. The scientist, having the knowledge of the contents of a topograph, is the only person able to choose between the various means of analysis. Thus a full investigation of a given topograph is a long process which must be applied to selected images only after a first rapid analysis.

PS-13.02.19 BRAGG-CASE IMAGES OF STACKING FAULTS. By Wojciech Wierzchowski, Institute of Electronic Materials Technology, Wólczynska 133, 01-919 Warsaw, Poland and Moreton Moore*, Department of Physics, Royal Holloway, University of London, Egham, Surrey TW20 0EX, England.

Bragg-case synchrotron double-crystal images of stacking faults have been studied in a synthetic diamond. The topographs taken on the tails of the rocking curve showed well pronounced interference fringes arising from the stacking faults: the first such observation in Bragg diffraction geometry. The fringes were strongly dependent upon the angular setting, being invisible at the rocking curve maximum but gaining in contrast and becoming more closely spaced further from the maximum. These experimental images were compared with predictions of plane-wave dynamical theory and a reasonably good correspondence was obtained when the finite beam divergence was taken into account. It was found that the theoretical fringe sequences depended upon the type of stacking fault, and confirmed that the stacking faults observed were of intrinsic type.

PS-13.02.20 DOMAIN WALLS IN FERROELECTRICS. By M. Takagi* and S. Suzuki. 1-10-6,Tsurumaki,Setagaya,Tokyo. Sanyo Tsukuba RC.Tsukuba,Japan. Images of imperfections which arise from the dynamical diffraction effect are observed on X-ray topographs of perfect or nearly perfect crystals. If a mosaic spread of a specimen crystal is a few minute of arc (which is ten times as large as that of perfect crystals), intensity in a Lang section topograph is uniform and the intensity is proportional to the integrated intensity of the Bragg reflection. Images of antiparallel domain walls and of the regions in the intermediate states of polarization reversal have been observed on the section topographs of ferroelectric $NaNO_2$ and thiourea crystals with such a mosaic spread. Structure of domain walls and of the intermediate state regions have been determined from dependence of the contrast of the images on the indices of Bragg reflection hkl. Studies of domain walls for $NaNO_2$ and thiourea, and of the intermediate state for $NaNO_2$ have already been reported and additional studies have been made on the polarization reversal of thiourea and on change in images of domain walls of $NaNO_2$ near the Curie temperature T_c. Results of these series of studies have made clear the structures of 180° domain walls and the polarization reversal procedure. Atomic positions in positive domain and those in negative domain shift relatively. For a perovskite-type crystal such as $BaTiO_3$, the relative shifts are as small as the amplitudes of thermal vibration, so that the two opposite domains are expected to be connected smoothly at an antiparallel domain boundary without any special layer. For some ferroelectrics such as $NaNO_2$ and thiourea the amount of the relative shift is as large as 0.5 ~ 1 Å. For such ferroelectric crystals, thick 180° domain walls which connect the two opposite domains without lattice strain are expected. The structures of domain walls determined are as have been expected. Fig.1(a) is the c-projection of the unit cell of $NaNO_2$ and (b) is that of domain walls where NO_2 radicals are rotated by about 50° or 130° around the c-axis from the original orientation. Fig.2 is the projection of the unit cell of ferroelectric thiourea, where full circles and the dotted circles represent the atomic positions in the positive and the negative domains respectively. The domain wall structure of thiourea determined is a modulated superstructure with long periods along the c-axis. In the structure, direction of thiourea molecules gradually varies along the c-axis between the two directions shown in Fig.2. 180° domain walls of $NaNO_2$ and thiourea are about 1 μm thick and in the domain wall structure atoms and molecules are at the halfway positions between the two opposite domains. On application of d. c. electric fields to $NaNO_2$ and thiourea, polarization reversal takes place via intermediate states. Structure of the intermediate state resembles the structure of domain wall.

The structure of domain walls of thiourea resembles that of the higher temperature phase above T_c, and topographic observation on $NaNO_2$ at T_c suggests the same correlation for $NaNO_2$. These structural correlations would be applied for any ferroelectric for which the atomic shift between the two opposite domains is far larger than the amplitudes of thermal vibration.

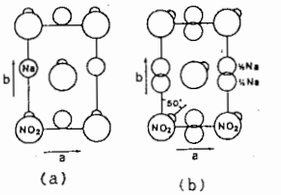

Fig.1

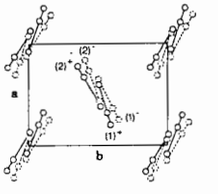

Fig.2

PS-13.02.21 STRUCTURE FACTORS OF LAYER SYSTEMS – EXAMPLE: BRAGG REFLECTORS (GaAs/AlAs)/GaAs. By R. Koehler* and B. Jenichen**; *MPG–AG Roentgenbeugung, Berlin, **Paul–Drude–Institut, Berlin, Germany.

Shifts of the atomic positions inside a layers system have a strong influence on the diffracted intensities even for high order satellites and, hence, have to be described correctly. At these high orders the Fourier components of the term exp(–ihu) (h: diffraction vector; u: shift in the atomic positions as compared to a reference lattice) might be negligible but neighboring high Fourier orders of the electric susceptibility $\chi_h(r)$ are combined with low orders of the exponential. For that reason the concentration profile inside a layer stack of a quasi binary compound cannot be calculated straightforward from the diffraction curve.

On the other hand due to intermixing of Fourier orders the structure factors also depend on the phases of the Fourier components. If the satellite reflections are well separated a simulation procedure based on the integrated intensities of the satellites and on the Fourier transform of the mo-

