11. REAL AND IDEAL CRYSTALS

11.2-6 COMPARISON OF MOSAIC SPREADS MEASURED BY THREE DIFFERENTIAL METHODS. By L.P. Campos, C. Campos and S. Caticha-Ellis, Instituto de Fisica, UNICAMP, C.P. 6165, 13100, Campinas, SP, BRASIL.

Since mosaic spread is a commonly used parameter to assess crystal perfection, it is interesting to compare the results obtained when using different experimental methods. Three methods are dealt with in this work. The first two are well known, namely, the profile measurement followed by deconvolution from instrumental factors and the method based on multiple diffraction (Caticha-Ellis, 1969, ASLE, 666.). The third method used consists in the measurement of Bragg angle variation over the crystal by means of a fine beam with a small divergence. The measurements were performed along parallel rows of equally spaced points. A random distribution of $\delta$ indicates some type of crystal distortion such as those which are studied by methods reviewed by Hart (J. Cryst. Growth (1981), 55, 403). The three methods yielded results in good agreement for measurements made on the same germanium crystal plate and on pure and doped rutile crystals. The effects of surface damage on the mosaic spread was also measured as well as its variation with depth in the crystal.

Support from FAPESP, CNPq and FINEP is acknowledged.


(111) and (100) oriented Si wafers were implanted with 80 keV 31P$^+$ ions. The doses were 1x10$^{15}$, 6x10$^{15}$ and 30x10$^{15}$ atoms/cm$^2$ and the lowest one is just above the limit of amorphisation at room temperature. After successive heat treatments for 30 minutes at 630°C, 700°C, 800°C, 900°C and 1000°C respectively in Ar, the 422 rocking curves (RC) were measured with a double crystal goniometer, using CuK$\alpha$ radiation. The structure regrown at 630°C shows RCS with flanks typical for a contracted surface layer. Further treatments at higher temperatures result in disappearance of the oscillating structure of the flanks, depending on both dose and wafer orientation.

It was concluded that the regrown layer is oversaturated in phosphorus of substitutional position and the excess phosphorus was pushed out only partially during regrowth. As long as the temperature is not high enough, the system remains practically unchanged. At higher temperatures an out-diffusion of the phosphorus from substitutional position takes place. This process is faster for higher doses, probably due to the higher density of defects /traps/ formed by "pushing out" of atoms. The origin of the orientation dependence is not clear yet: it must be related to the difference in regrowth.


X-ray diffraction studies have shown that the 2H $\rightarrow$ 3C transformation in ZnS occurs by the non-random insertion of deformation faults occurring preferentially at two layer separations. The reverse transformation 3C $\rightarrow$ 2H can be accomplished by the movement of $\frac{1}{2}$ < 112 > Shockley partials on alternate (111) planes as depicted below:

- Initial structure (3C): A B C A B C A B C A ....
- A C B A B C A A C B A A ....
- A ....

resulting structure (2H): A B A B A B A B A B A ....

Lele and Pandey (Mater. Sci. Forum 3 (1982) 143) have developed a theoretical model for transformation in cobalt starting with an untwinned cubic crystal. Since cubic crystals of ZnS very often contain a random distribution of twin (growth) faults, we consider here the transformation of such crystals to the 2H phase.

We assume that the initial cubic crystal contains twin faults distributed randomly with a small fault probability $\gamma < 0.1$. During the transformation deformation faults nucleate preferentially at two layer separations with a probability $\beta$ which is much higher than the probability $\lambda$ of their occurrence at larger separations. The probability of deformation faults occurring on successive layers is assumed to be negligible. According to this model $\lambda$ corresponds to the probability of insertion of a fresh 2H nucleus in the twinned 3C structure and $\beta$ to the growth of these nuclei by non-random faulting. The diffuse x-ray intensity diffracted along the 10L reciprocal lattice row for transformation by such a model of non-random deformation faulting has been computed for various values of $\lambda$, $\beta$ and $\gamma$. The diffraction effects predicted theoretically are compared with experimental results and are found to be in good agreement.