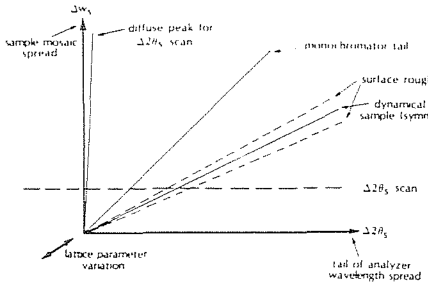
11.X-9 INVESTIGATIONS OF ASYMPTOTIC-BRAGG AND KINEMATICAL SCATTERING FROM ION-IMPLANTED AND OTHER SILICON SAMPLES USING AN X-RAY TRIPLE-AXIS DIFFRACTOMETER. By S.W. Wilkins and A.W. Stevenson, CSIRO Division of Materials Science and Technology, Locked Bag 33, Clayton, Victoria 3168, Australia; J. Harada, N. Kashiwagura, S. Kimura, M. Sakata and T. Tanaka, Department of Applied Physics, Faculty of Engineering, Nagoya University, Chikusa-ku, Nagoya 464, Japan and K. Ohshima, Institute of Applied Physics, Tsukuba University, Sakura, Ibaraki 305, Japan.

Triple-axis X-ray diffractometry offers the exciting possibility of cleanly separating dynamical, kinematical, instrumental and parasitic components of the scattering near a Bragg peak. In particular Eisenberger, Alexandropoulos and Platzman [Phys. Rev. Letts., 1972, 28, 1519-25] and later Iida and Kohra [Phys. Stat. Solidi (a), 1979, 51, 533-42] showed that for nearly perfect crystals dynamical and kinematical components of the scattering could be readily separated by scanning a perfect crystal analyzer. Examination of the theory for dynamical diffraction from a perfect crystal shows that the tail of the dynamical diffraction peak extends along the direction normal to the crystal surface. In the case of symmetrical Bragg reflection, the dynamical tail extends parallel to the scattering vector or, equivalently along the $\omega_s/2\theta_s$ scan line in $\Delta 2\theta_s$-$\Delta\omega_s$ space (where $\Delta 2\theta_s$ and $\Delta\omega_s$ are detector and sample angular sittings relative to Bragg condition). On the other hand, the kinematical component of the scattering can extend in various directions in k-space. For example, mosaic spread extends the Bragg scattering along a direction normal to the scattering vector in the plane of diffraction corresponding to the $\Delta\omega_s$ direction in $\Delta 2\theta_s$-$\Delta\omega_s$ space, while isotropic diffuse scattering leads to a broad peak centred on the line $\Delta\omega_s = \frac{1}{2}(1 - \cos^2\theta_B)^{-1}\Delta 2\theta_s$ in a $\Delta 2\theta_s$-scan. Instrumental factors can lead to a streak along $\Delta\omega_s = \Delta 2\theta_s$ corresponding to the rocking-curve tail of the monochromator being Bragg reflected by the sample and a streak along $\Delta 2\theta_s$ direction corresponding to $\Delta\lambda$-spread or to the tail of the analyzer crystal. These various features of the scattering are illustrated schematically in the figure below.



ANGULAR SPACE

In addition to cleanly separating instrumental characteristics, triple-crystal diffraction is a sensitive probe of sample properties, especially in the near surface region, [see e.g. Afanasev, Kovalchuk, Kovev and Kohn, Phys. Stat. Sol. 1977, 42, 415-22] and Cowley and Ryan, J. Phys. D. 1987, 20, 61-8]. In the present work, we present triple-crystal measurements on ion-implanted and other silicon samples which were carried out using the 6-circle Huber diffractometer on beam-line 4C at the Photon Factory. These results include observations of Bragg peaks over nearly 8 orders in magnitude and show that the method can provde valuable information on near-surface structure (such as strained layers and surface roughness).

11.X-10 SENSITIVITY OF X-RAY DYNAMICAL REFLECTING POWER TO THE STRAIN PROFILE IN HETEROSTRUCTURES. By C. Malgrange, Laboratoire de Minéralogie-Cristallographie, associé au CNRS et aux Universités Paris VI et Paris VII, 4 place Jussieu, Paris - France.

Many modern electrooptics devices make use of heteroepitaxial structures. In order to fully understand their optical and transport properties, it has often proved necessary to control a posteriori the actual parameters : composition, thickness and state of strain of individual layers. X-ray diffractometric techniques have become now widely used for this purpose since they are non destructive and rather simple to achieve. It is then necessary to determine the ultimate strain sensitivity of the technique.

Let us recall its principle : nearly plane wave X-ray rocking curves are recorded on a double crystal spectrometer and analyzed through a best fit procedure between experimental and computed profiles, the computation relying on Takagi-Taupin equations.

Among others, the example of a single heterostructure whose only imperfection is a strain distribution at the interface will be discussed.

In order to characterize the strain profile by a single parameter, a simple but nevertheless realistic strain model has been chosen : the ε_{zz} strain where z is a coordinate normal to the junction is taken equal to $f/(1+\exp(z-z_i)/C)$ where f is the misfit or relative lattice parameter difference between the epilayer and the substrate, z_i is the mid-position of the interface and C the parameter which describes the spreading of the strain (S. Bensoussan, C. Malgrange and M. Sauvage-Simkin, to be published in J. Appl. Cryst. 1987).

In the rocking curve, the features which proved to be the most sensitive to the strain are the intensities of the first subsidiary peaks on both sides of the epitactic layer main peak : the intensity assymetry between both subpeaks increases as the value of C increases. The variation of the ratio ρ of these peak intensities with the value of C has been studied in the case of $Ga_{1-x}Al_xAs/GaAs$ heterojunctions, a 400 reflection for two different wavelengths, as a function of the misfit f and the depth z_i of the junction. The sensitivity defined as the minimum detectable strain spreading is given in each case and proved to be enhanced as either the thickness of the layer decreases or the misfit increases. Writing Takagi-Taupin equations with suitable dimensionless parameters, it is shown that the conclusions can be extended to other reflections and wavelengths provided that the ratio χ_{hi}/χ_{hr} of the imaginary and real part of χ_h (respectively proportionnal to the absorption coefficient and the structure factor of the reflection) is kept below 10^{-1}. Some experimental results which have been analyzed with this method will be presented.