

11.X-1 CALCULATIONS IN THE CRYSTALLINE STATE USING MOLECULAR MECHANICS. By M. Simonetta, Department of Physical Chemistry and Electrochemistry and C.N.R. Center, University of Milan, Via Golgi 19, 20133 Milano, Italy

Force field calculations can be used in three-dimensional crystallography as an aid in structure solution, and are particularly useful in the case of disordered crystals. When the molecules can be treated as rigid objects the study of thermal vibrations and rotations is quite feasible and the potential to be included in dynamic calculations is easily obtained. In two-dimensional crystallography the method is now more useful, since the alternative technique, multiple scattering theory in a trial and error procedure, is very time consuming and, at least for organic adsorbates on metal surfaces, not completely reliable. The results from molecular mechanics calculations can provide the screening to eliminate energetically unfavoured structures.

It will be shown that stress-induced anisotropy predicts "charged walls" properties which agree with experimental data, at distances from the boundary exceeding a fraction of a micron. In particular, the observed three-fold symmetry in the propagation of "charged walls" may easily be deduced from the present elastic model.

However, in the close vicinity of an implantation boundary, the complex spatial dependence of the various stress components imposes a three-dimensional treatment of implantation boundaries magnetoelastic properties.

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11.X-2 DETERMINATION OF STRESS/STRAIN PROFILES IN IMPLANTED FERRIMAGNETIC GARNET EPITAXIAL LAYERS BY PLANE WAVE X-RAY METHODS. By J. Miltat, Lab. de Physique des Solides, Bât.510, et LURE, Bât.209C, Université Paris-Sud, 91405-Orsay, France.

Ion implantation in ferrimagnetic garnet epilayers supporting bubbles has been primarily developed with the aim of overcoming bubble dynamic conversion, i.e. a process resulting in a drastically reduced bubble mobility. Besides, boundaries between implanted and non-implanted regions define propagation paths for the bubbles which are attached to the boundaries by so-called "charged walls". It is now widely accepted that stresses/strains around implantation boundaries control the morphology and the dynamic behaviour of "charged walls".

In order to allow for a full understanding of "charged walls" properties, stress/strain profiles around planar implantation boundaries have been derived according to the methodology below:

- 1) the dilation of the lattice, $\epsilon_{zz}^P(z)$, due to uniform implantation was first determined by means of plane wave rocking curve analysis according to X-Ray diffraction dynamical theory;
- 2) a model of the stress/strain distribution based on a distribution of edge dislocations with Burgers vectors $b(z) = f(\epsilon_{zz}^P)$ was then constructed;
- 3) the results of the strain calculation were compared to experimental data obtained by means of plane wave X-Ray imaging with varying incidence angles;
- 4) finally, the stress-induced easy magnetization directions were deduced from the stress calculations.

Results pertaining to garnet epilayers implanted with Neon or Hydrogen ions will be described and discussed.

11.X-3 A X-RAY TOPOGRAPHY INVESTIGATION OF THE MICRODEFORMATION OF ORIENTED BICRYSTALS OF SILICON

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Dislocation-free bicrystalline specimens of silicon were strained in creep conditions ($\tau \sim 20$ MPA, $T \sim 973$ K) in a tensile stage mounted on the two crystal spectrometer of the topography beam port of the LURE-DCI storage ring. Topographs were obtained in a few seconds, allowing an in situ observation of the ability of lattice dislocations to be transferred from one grain to the other across the boundary plane. After cooling under load, the observations were supplemented by conventional Lang topography and etch pit studies of the frozen-in dislocations.

Two kinds of symmetric tilt coincidence boundaries were studied: $\Sigma=9$, which corresponds to a misorientation angle $\theta=38,94^\circ$ around $[011]$, the boundary plane being (122) and $\Sigma=25$ ($\theta=16,26^\circ$ around $[001]$, boundary plane (175)).

In most cases, single dislocations were trapped in the boundary, without being able to cross it. A remarkable exception is, in $\Sigma=9$ bicrystals, for dislocations with a $a/2 [011]$ Burgers vector which is a vector of the Coincidence Site Lattice.

When helped by stress concentrations developed by pile-ups, other dislocations could cross the boundary. The correspondence between the slip systems activated in adjoining crystals is studied, and is discussed in terms of the known structures of the coincidence boundaries.