<table>
<tr><td rowspan="1"> </td><td colspan="2">Experiment title:
Compliant Universal Substrates: an x-ray diffraction study of the strain relief mechanism</td><td>Experiment number:
SI521</td></tr>
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<tr><td>Shifts: 21</td><td colspan="2">Local contact(s):Carmela Aruta</td></tr>
<tr><td colspan="4">Names and affiliations of applicants (* indicates experimentalists):
Paul Howes, University of Leicester *
Colin Norris , University of Leicester *</td></tr>
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Report:

A number of difficulties were encountered with alignment of the compliant universal substrate interface samples and no useful data were measured. We have highlighted the steps that need to be taken to ensure success in future measurements of samples of this type.

Successful preliminary measurements were, however, made of a backup sample containing another semiconductor interface.

GaAs twist bonded samples

A number samples were prepared by joining clean GaAs(001) surfaces to form twist grain boundary interfaces. In attempting to measure the x-ray diffraction signal from the dislocation array at the interface, a number of difficulties were encountered. The attenuation of the x-ray beam by the top GaAs crystal was severe and it proved impossible to find Bragg peaks associated with the substrate crystal. A further problem became apparent during the experiment. The surfaces of the commercial quality GaAs(001) wafers used to prepare the samples were not accurately aligned with the (001) crystal axis. This made locating Bragg peaks for crystallographic alignment difficult and time consuming.

Without crystallographic alignment of *both* crystals the geometry of the interface could not be defined and meaningful measuremnts of the interface structure were impossible. For future experiments of compliant universal substrates one should ensure that:

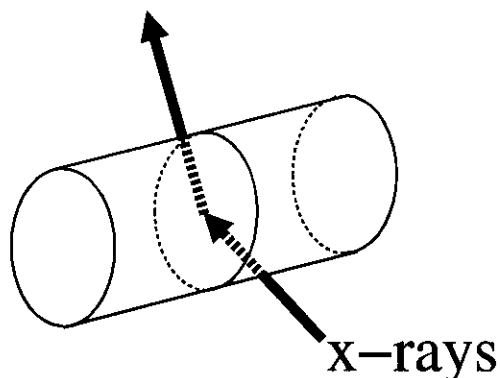
1. The GaAs wafer substrates should be accuately cut to within 0.1 degrees of the (001) crystallographic direction.
2. The top crystal should be carefully thinned to 100 microns or less with a chemical-mechanical polish.

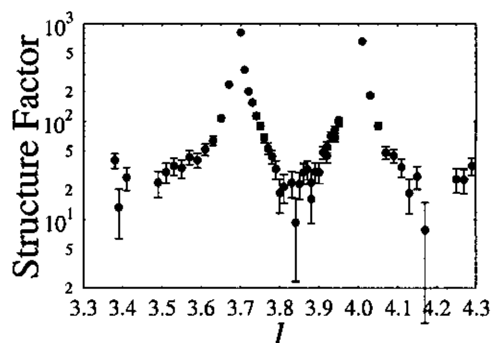
Silicon-silicon symmetric tilt boundary

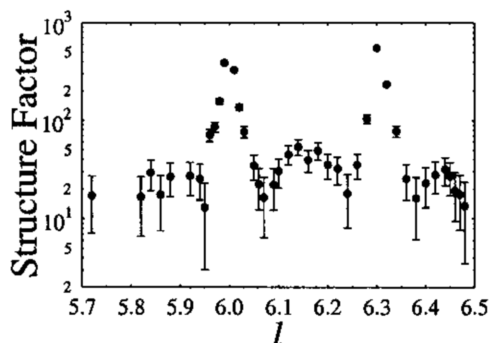
A backup sample containing a Σ13 (22.6°/[001]) symmetric tilt grain boundary was measured. The sample was grown from molten silicon by the Czochralski method using two seed crystals carefully prealigned using XRD. The interface contains {510} planes. Another portion of the same bicrystal sample has been previously studied by TEM.

The Σ13 boundary is an example a low energy, special angle grain boundary interface. The interface structure has a regular unit cell with a volume 13 times as large as the bulk unit cell. There is an exact cooincidence in reciprocal space of 1 in 13 of the Bragg points. A consequence of this is that all of the crystal truncation rods (CTRs) associated with the interface contain Bragg peaks from both crystals.

Two CTRs were measured using a cylindrical sample with a 2 mm diameter in a transmission geometry.







Other x-ray diffraction studies of interfaces have measured fractional order Bragg rods due to interface superstructure or satellite peaks due to long-range strain at *incommensurate* (ie, not special angle) interfaces. We believe that this is *the first measurement of CTRs due to a special angle crystalline grain boundary interface.* The CTRs contain information about the atomic structure of the regular unit cell at the interface. Analysis of the data is underway.

We expect that a full determination of the crystal structure of this interface will require measurement of many more CTRs than the two measured in these preliminary studies and this will be the subject of a future beam time application