	Experiment title: Directly bonded silicon: an investigation of the interface atomic structure by x-ray diffraction	**Experiment number:**
ESRF		S1323
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Report:

Wafer bonding is an increasingly important tool in both microelectronics and micromechanics. For example, it can be used in the process of fabricating silicon-on-insulator (SIO) materials for sensors and actuators[1,2,3]. Si/Si bonding also provides a potent,ial replacement for epitaxiai growth. offering a simple, cheap and low-temperature process. There are two stages in interface bonding. The first occurs at room temperature in air where two mirror-smooth, clean, dry, dust-free surfaces are pressed together. Weak van der Waals-type bonds are formed across the interface. The interface is strengthened in the second stage by heat treatment resulting in much stronger silicon-silicon covalent bonding. Despite the technological potential of the technique, little is known in detail about the dependence of direct bonding on surface chemistry and morphology and the subsequent heat treatment.

Using synchrotron x-ray diffraction, we have studied bicrystal interfaces formed by the direct bonding and subsequent annealing of pairs of Si(001) wafers. The resulting interface can be seen as a giant grain boundary in which the inevitable misalignment gives rise to an array of screw dislocations at the interface.

One of the aims of the experiment was to characterize the bonded interface as a function of the fabrication process. We measured a comprehensive set of diffraction peaks from one Si(001) bicrystal sample interface with a, misorientation angle of $4.8°$. This diffraction is due to the ordered array of screw dislocations at the interface and allows the characterisation of the bonded interface. The satellite peak widths are sharp indicating a high degree of order (Fig. 1). This is because the interface crystallography is determined by the presence of two highly ordered silicon crystals on each side. The peak width may be thought of as being due to the correlation length of the grid of screw dislocations indicating that the grid is highly regular over a length scale of more than 1000 Å. Our observation of sharp peaks at irrational Miller index coordina.tes also confirms the prediction of Sutton[4,5] that the interface is quasicrystalline. A total of 15 superstructure peaks were measured.

The Bragg rods associated with some of the satellite reflections were also measured (Fig. 2). All of the satellite Bragg rods showed a single peak at the Z-value associated with the Bragg peaks of the nearest crystal truncation rods from the top and bottom crystals. The width of the peak indicates the depth of the strain field association with the interface. In the case of the 4.8" sample, this was around 40 A. The fact that the superstructure rods always peak at the same value as the associated CTR indicates that the relaxed material giving rise to the additional rods has basically the same structure as the bulk silicon. This means that the rods are largely due to the strained, bulk-like silicon in the regions between the dislocations, rather than due to scattering from the dislocation cores themselves.

The peak width as a function of Miller index, 1, was also measured for a number of other samples with different misorientation angles and it was found that the thickness of the interface decreases as the misorientation angle increases.

The general profile of the Bragg rods and also the dependence of the interfacial strain field thickness on the turn angle were both found to be in agreeme,nt with simple models of bicrystal interfaces based on a Keating energy minimization.
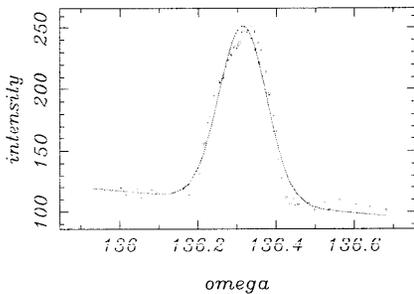

Fig. 1. Satellite peak near the two (022) Bragg peaks for a Si(001) bicrystal sample with a misorientation angle of 4.86". The width of the peak, 0.14°, corresponds to a correlation length of 1000 Å for the dislocation grid.
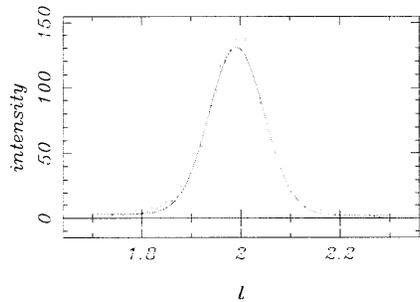

Fig. 2. The Bragg rod associated with the peak in Fig. 1. The width of the peak indicates that the interface region is of the order of 40 Å thick.

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