ESRF	**Experiment title:** An XRD study of symmetric tilt grain-boundary interfaces in metals and semiconductors	**Experiment number:** SI630
Beamline: ID32	**Date of experiment:** from: 06-sept-00 to: 15-sept-00	**Date of report:** 28-feb-01
Shifts: 12	**Local contact(s):** Tian-Lin LEE	*Received at ESRF:*

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Report:

The aim of the experiment was the determination of the atomic structure of symmetric tilt grain boundary interfaces. A comprehensive data set comprising 20 Bragg rods was measured from a silicon bicrystal.
The Si Σ13 (22.6°/[001]) bicrystal was grown by the Czrochralski method using *two* carefully prealigned seed crystals. The interface is a fully relaxed special angle grain boundary at which the interface planes are exactly {510} planes and the interface forms a regular 2-dimensional crystalline structure. This is in contrast to an arbitrary tilt grain boundary where the interface structure is incommensurate. An important consequence of the precise orientation of this Σ13 interface is that the two crystals share 1 in 13 Bragg peaks. In fact all of the Bragg rods associated with the interface contain Bragg peaks from *both* crystals. This makes such a sample fundamentally different from a surface or an incommensurate interface.

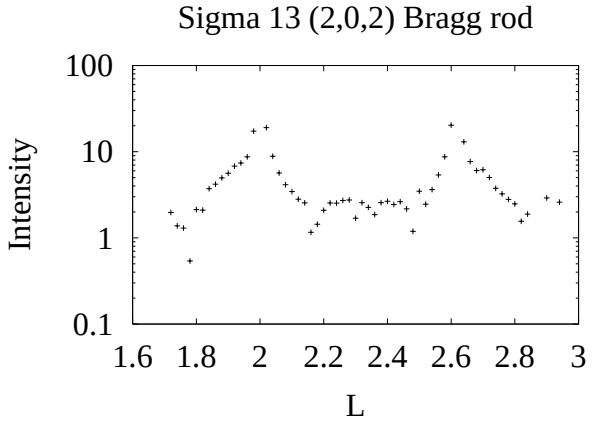

Figure 1

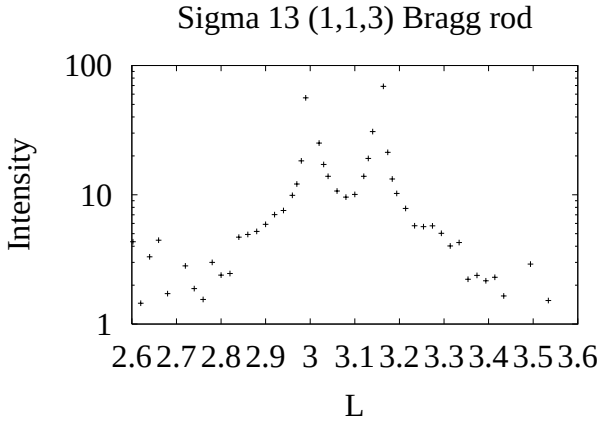

Figure 2

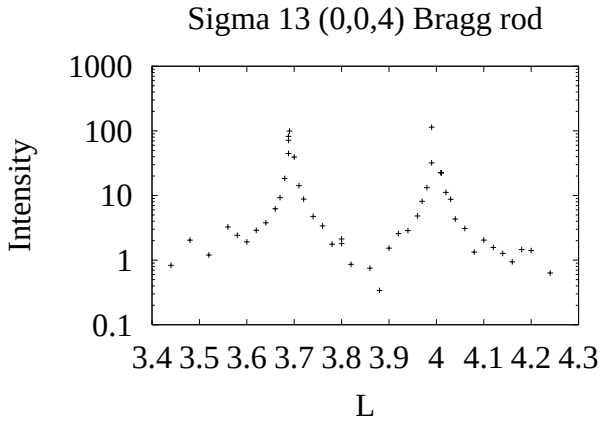

Figure 3

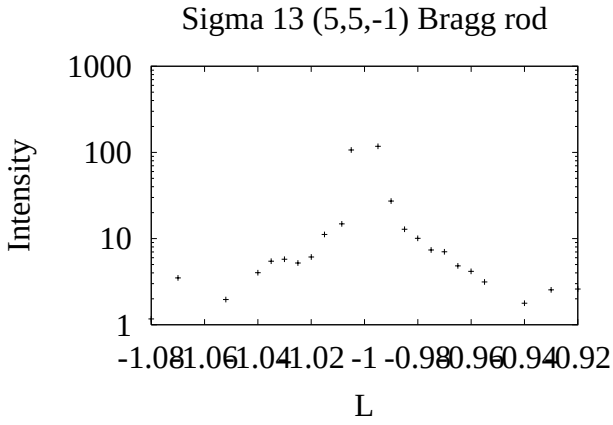

Figure 4

Examples of the measured Bragg rods are shown above. Figures 1, 2 and 3 show rods containing two Bragg peaks, corresponding to the two crystals. The tails due to the interface overlap exactly and well defined rods were observed. It can be seen that the rods contain features due to the structure of the interface.

Particularly interesting data were measured from (the 1 in 13) Bragg peaks that belong to both crystals. For some such reflections, the Bragg peak was point-like and no Bragg rod scattering could be found. For others such as the $(5,5,\overline{1})$ shown in Figure 4, an extremely narrow Bragg rod was observed. These data are particularly important in determining the geometry of the interface and the translation of one crystal with respect to the other. A missing Bragg rod implies that the crystal planes associated with the reflection are uninterupted at the interface. This is an important constraint on the final model structure.

Analysis is still underway to fit the rods and determine the interface structure.