**In Situ Alignment Procedure for X-ray Topography**

**BY RICHARD A. FORMAN AND SANTOS MAYO**

*Semiconductor Materials and Processes Division, National Bureau of Standards, Gaithersburg, MD 20899, USA*

*(Received 21 August 1984; accepted 22 November 1984)*

**Abstract**

A simple method for *in situ* alignment of samples in a double-crystal X-ray topography system is described. This method permits a specific crystallographic axis to be made coincident with the sample rotation axis used to set the Bragg angle. Surface reflections from approximately orthogonal crystallographic planes are required and tables of such planes suitable for alignment of cubic crystals are given. This procedure allows rapid setup for the other accessible surface reflection or transmission topographs.

In the study of semiconductor materials by X-ray topography, one often desires topographs of a specimen using different reflecting planes and a particular monochromatic radiation. This is necessary, for example, in studies of the depth behavior of epitaxial (Rozgonyi & Miller, 1976) or implanted layers or for studies of dislocation patterns (Halliwell, Childs & O'Hara, 1973). When the topographs desired are for surface reflection geometry, the alignment of the crystal is usually simple, as the reflected X-ray photon flux is relatively large. Image intensifiers, counter tubes, or X-ray vidicons have conventionally been used for these alignments with final adjustments sometimes made using the photographic image of the entire topograph. Alignment for transmission topographs is generally more difficult due to the lower diffracted X-ray intensity available.

In III–V semiconductors, for example, transmission topography is normally used to study the dislocation density patterns (Kamejima, Shimura, Matsumoto, Watanabe & Matsui, 1982; Yasuami, Mikami & Hojo, 1983). We have found it difficult to align typical commercial GaAs wafer samples in the transmission configuration often because of the limited photon flux. We have developed a simple geometric procedure whereby the final sample-crystal alignment is easily obtained using two (nearly) orthogonal crystal planes that produce surface reflections. This guarantees a complete *in situ* orientation of the specimen in the X-ray topography system; the sample alignment for a transmission topograph is then quite easily obtained. This method is closely related to existing techniques for single-crystal diffractometry, but these have not previously been applied to topography (Furnas & Harker, 1955).

Specimen alignment by Laue techniques with later transferal to the topography system is commonly done. We have found that alignment, in the topography system, by this method can only be done to within approximately 1°. This is not sufficient for some of the sharp rocking-curve widths encountered in high-quality semiconductor crystals. Further, the Laue alignment examines only a very small portion (typically less than 1 mm diameter) of the crystal, whereas our method provides an integration over either the topography beam size or the detector size. This has proven very useful for crystals with small-angle grain boundaries.

Our topographic apparatus is a version of the widely used double-crystal topography system developed by Kuriyama and collaborators (Boettinger, Burdette, Kuriyama & Green, 1976; Kuo, Emamian & Bilello, 1984). In this system a fine-focus X-ray tube is used as a radiation source and the first (asymmetrically-cut) crystal produces a monochromatic horizontally magnified image of the source. With this system the monochromatic beam width is determined by the first-crystal asymmetry and its physical dimensions; typically, the second crystal (under study) can easily be illuminated over about 50 mm width (at the incident angles normally used), as desired for most commercial semiconductor wafers. As we have implemented the apparatus, the diffraction plane defined by the singly diffracted monochromatic radiation is horizontal and in the aligned condition topographs are taken from specimen Bragg reflections of vertical crystallographic planes (Furnas & Harker, 1955; Boettinger, Burdette, Kuriyama & Green, 1976).

The procedure we have developed permits the simple and precise alignment of a sample's crystallographic axis with the (vertical) goniometer rotation axis used to set the diffraction angle. The first requirement for our procedure is that the incident monochromatic X-ray beam be horizontal. This is easily accomplished by proper monochromator (first crystal) alignment. We use an orthogonal cradle (two-circle) goniometer (Furnas & Harker, 1955) placed on top of a high-resolution rotation stage to hold the sample...
In Table 1 we have compiled a set of preferred reflection planes for alignment of commonly encountered cubic semiconductor crystal geometries. For illustrative purposes we have chosen the planes available for surface reflection geometry from silicon crystals using Cu Kα radiation, the most commonly available laboratory X-ray source. In the first column we have listed the normal to the wafer face; in the second column the high-symmetry axes that might be used for the Bragg rotation axis; in the third column the surface reflection planes and their interplanar angle used for alignment; and in the fourth and fifth columns the reflecting planes available (at Bragg
angles less than 80°) for this orientation, for reflection (Bragg) and transmission (Laue) cases, respectively.

The generalization to other radiations and lattice parameters is straightforward but tedious. The suitability of a given set of planes for this procedure depends on both the X-ray wavelength used and the lattice constant of the crystal to be aligned. A complete set of tables for silicon and the III–V compounds, using all readily available X-ray wavelengths, is in preparation and will be published elsewhere. In many of the cases shown, the internal planes used for alignment are not orthogonal, and iterations will be required. Crystallographic orientations were chosen to specify the reflecting planes completely. The table thus differs from earlier surface reflection compilations (Rozgonyi & Miller, 1976; Halliwell, Childs & O’Hara, 1973) in that the rotation axis is specified, which then defines the indices of the reflecting planes, and further the transmission cases are included.

As an example of the procedure, we show in Fig. 1 a semiconductor wafer mounted so that its nominal (001) face has an (upward) vertical axis of [100]. The crystal has been intentionally shown off orientation so as to display the alignment procedure. In Figs. 1(b) and (c), we show a cross section of the sample at the diffraction plane and a front view, respectively. The diffracted (off-horizontal) beams can be seen in these views. For illustrative purposes, we assume that the crystal is silicon and that Cu Kα radiation is used. In this geometry, the {044} surface reflections can be obtained from both the (011) and (011) planes. The crystal has been positioned so that the [001] axis, normal to the wafer face, approximately bisects the angle between the two orthogonal goniometer cradles. In this way the reflecting planes are nearly perpendicular to the goniometer axes. Orientation is performed using a wide-area X-ray detector centered on the diffraction plane to monitor the diffracted intensity for the two different crystal alignment positions. Alignment is accomplished by iterative adjustment of the Bragg rotation angle and only one of the two cradles depending on which specific plane is being examined. As can be seen from an examination of Fig. 1(a), the 044 reflection is maximized using one cradle (cradle b) and the 044 reflection is maximized using the other cradle (cradle a). Iteration between these reflections is required to remove the interactions between these circles produced by either misorientations of the vertical axis of the sample or from the inaccurate setting of the bisector of the cradle axes along the normal to the 001 plane. After a small number of iterations, the high-resolution Bragg rotation stage may be set for any accessible reflection or transmission topograph. We have usually found that no further adjustment of the cradles is necessary. The number of iterations required for alignment is minimized the closer the angle between the selected reflecting planes is to 90°. The final result of the procedure is to bring the doubly diffracted beam into the horizontal plane.

In an ideal case, like that described above, equivalent Bragg reflections are used, the surface reflection intensities for the two alignment positions will be approximately equal, and the angle between the beam and the detector remains the same; that is, the detector is not moved during the alignment. For some low-
symmetry situations, the detector position must be altered between the two alignment positions.

We note that not all theoretically possible topographs for a given wafer specimen surface (Halliwell, Childs & O’Hara, 1973) are shown in Table 1. Those few that are not shown do not occur when the stage rotation axis lies along a high-symmetry direction. If high-resolution circles were used in place of our orthogonal cradles, those reflections could also be easily set.

The procedure we have described allows the alignment of all crystallographic axes of a sample on a rotation stage utilizing only surface X-ray reflections. It is especially useful for rapid setup for the study of X-ray transmission topography. The relatively simple iterative procedure appears suitable for design of an automated topographic facility, since in general there is only one X-ray reflection maximum in the vicinity of a given sample orientation.

We would like to thank Dr M. Kuriyama and Dr M. I. Bell for numerous helpful suggestions.

References


