WHITEPAPER

Covalent Metrology X-ray Diffraction Offcut Measurement

The Impact of Semiconductor Wafer Offcut

Single crystal semiconductor wafers, i.e., silicon or sapphire, are the starting points for MOCVD and other types of epitaxial thin film growth used to produce devices. The highly polished wafer surfaces are usually nearly parallel to crystallographic planes with low indices in the materials, such as the (100) of Si. Typically, a small angular tilt (offcut angle) between the wafer surface and the crystallographic planes is intentionally introduced due to the resulting positive epitaxial film growth effects, which include lowered epitaxial film dislocation densities and improved chemical uniformity. XRD is the standard method to determine the offcut angle accurately and to monitor variations in large numbers of wafers.

XRD Offcut Determination

To determine the offcut of a substrate, XRD is used to precisely measure the change in Bragg angle (diffraction angle) as the rotational angle of the substrate is varied with respect to the incoming X-ray beam. If the Bragg angle varies with the substrate's rotational angle, this is indicative of a wafer with an offcut. A nonzero wafer offcut causes the Omega peak position to increase or decrease as the wafer is rotated, since the crystallographic planes are not perfectly parallel to the wafer surface. When the wafer is rotated such that the planes are tilted to the maximum value towards the X-ray beam, the Omega diffraction peak will be found at an angle lower than the Bragg angle by the magnitude of the offcut. For instance, a wafer with a 1° offcut oriented towards the X-ray beam will have an Omega peak position that is 1° less than the Bragg angle would predict. Likewise, if the offcut were the same magnitude but oriented in the opposite direction relative to the beam, the Omega peak would be at an angle 1° greater than the Bragg angle. As the wafer is rotated in the beam, the offcut causes the Omega peak to move from the minimum to maximum smoothly and the Omega peak shifts between these limits can be observed.

If the exact rotational position of the offcut was known, only one Omega scan would need to be collected along a direction parallel to the offcut. In reality the offcut direction is not known precisely, and pairs of Omega scans are collected usually parallel and perpendicular to the wafer flat or notch. By collecting four Omega peaks at 90° rotational (Phi) angles from each other, carefully aligning the wafer surface to the beam at each rotation, the overall offcut angle and Phi angle can be calculated regardless of the rotational position in the wafer. By measuring the set of four scans, instrument-dependent errors or wafer mounting artifacts are minimized or eliminated.

The offcut calculations are done using the method of Halliwell and Chua[1], in which four Omega scans are collected at 0°, 90°, 180°, and 270° Phi rotation. In the case where the wafer flat is parallel to the X-ray beam (at Phi rotations of 0° and 180°), the offcut component parallel to the flat is calculated as half of the difference of the Omega peak positions at 0° and 180°. Likewise, the component perpendicular to the flat uses the Omega peak positions at Phi values of 90° and 270°. In Figure 1, the axes are shown with the offcut components labeled as "Component V" – perpendicular to the flat – and "Component H" – parallel to the flat – and the tilt of the offcut is measured from the wafer surface normal towards the normal of the crystallographic planes. The offcut angle is calculated from the sum of the squares of the tangents of the components, and the Phi angle of the offcut is related to the ratio of the tangents of the components.

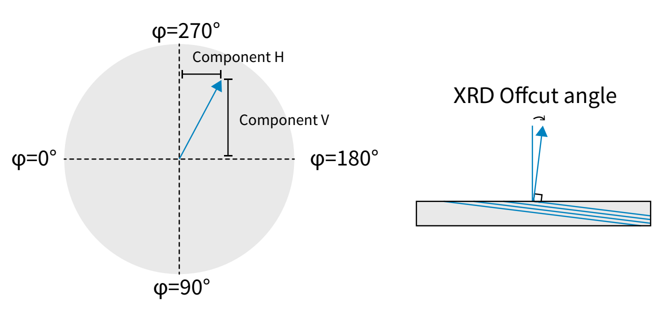

Figure 1. XRD orientation and offcut angle direction for Rigaku SmartLab measurements

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NIST SRM 1995 Certification and Covalent Metrology Results

Covalent's newest-generation Rigaku SmartLab XRD was used for the measurements. The SmartLab was setup in the Parallel Beam geometry with a High-Resolution Ge(220)x2 Incident-Side Monochromator, Receiving-Side Soller Slit (2.5°), and Hypix-3000 Hybrid Pixel Array Detector in 0D mode. The instrument broadening of the peaks was minimal and did not affect the maximum intensity positions of the peaks which were used for the calculations.

To demonstrate the high degree of accuracy of the SmartLab XRD system, a certified NIST Standard Reference Material wafer was used, SRM 1995 (CSI_3060104). The wafer was an Al_2O_3 single-crystal wafer with an (00.1) orientation, placed on the stage with the flat parallel to the X-ray beam. The wafer height with respect to the beam was optimized by reducing the direct beam intensity by half, then eliminating any tilt of the surface to the beam and reoptimizing the height. The detector was then moved to the diffraction position for the Al_2O_3 (00.6) reflection, 41.70°, and a fine-stepped Omega scan was collected around the Bragg angle. This procedure was repeated at the Phi positions of 0°, 90°, 180°, and 270°, with 0° and 180° Phi parallel to the wafer flat and 90° and 270° Phi perpendicular to the flat. The four Omega scans are shown in Figure 2, and it can be observed from the relative positions of the peaks that the offcut Phi angle will be between 180° and 270° degrees, indicated by the decreased Omega angles relative to the Bragg angle.

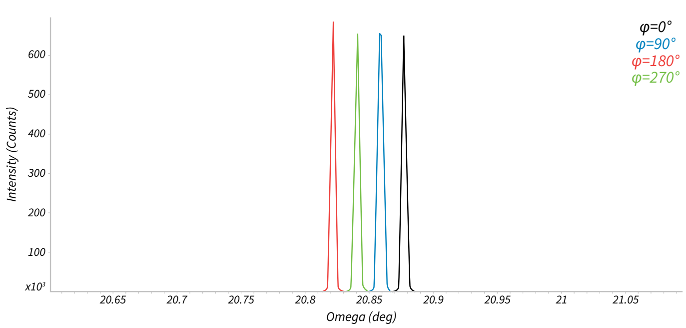

Figure 2. Overlay plot of the four Omega scans for the NIST SRM 1995 Al_2O_3 wafer

The collected Omega peaks were profile-fitted using Rigaku's SmartLab Studio II software. The peak shape was modeled using a split pseudo-Voigt shape and the background was modeled using a B-spline. The peak position was taken as the position of maximum intensity and the results are listed in Table 1, both as the overall offcut and as the offcut components parallel and perpendicular to the wafer flat. The offcut results are in excellent agreement with the absolute values listed in the NIST SRM 1995 certification, shown in Table 2, and the differences in the components are 0.007° or less. Absolute values for each measurement are listed due to the difference in XRD orientation axes between Covalent and NIST, which only affect the signs but not the magnitude of values. The orientation of the offcut determined by Covalent is shown in Figure 3.

Table 1. Results for NIST SRM 1995 Wafer Offcut

Phi Angle	Omega Peak Position	Offcut Angle	Offcut Phi	Parallel to flat	Perpendicular to Flat
0°	20.8772°	0.0290°	197.50°	0.0277°	0.0087°
90°	20.8586°				
180°	20.8218°				
270°	20.8412°				

Table 2. Comparison of Covalent Metrology Results to NIST-Certified Results

NIST SRM 1995 Results (Abs Values)		Covalent Offcut Results (Abs Values)	
Parellel to flat	Perpendicular to Flat	Parallel to Flat	Perpendicular to Flat
0.0206°	0.0098°	0.0277°	0.0087°

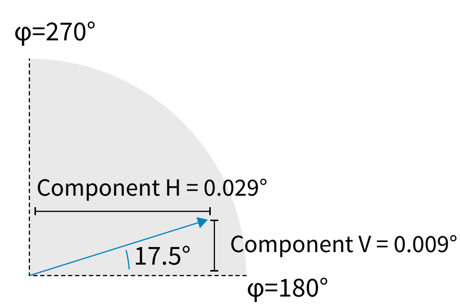

Figure 3. Measured offcut orientation and components of NIST SRM 1995 Al_2O_3 wafer

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Comment on Orientation Axes

The orientation axes used in this paper are common in XRD but are not the only axes used in practice. The XRD-determined offcut angles shown here were defined as the angle from the wafer surface normal towards the crystallographic plane normal. In manufacturing, it is not uncommon to encounter the reverse definition in which the offcut angle is defined as the angle from the plane normal to the surface normal. Although both definitions reference the same offcut magnitude, the sign of the offcut would not agree.

References

1. Halliwell, M.A.G., and Chua, *S.J. Journal of Crystal Growth 192* (1998) 456-461

Summary

Typically, a small offcut angle is intentionally introduced due to resulting positive effects on epitaxial film growth:

- Lowered epitaxial film dislocation densities
- Improved chemical uniformity

XRD is the standard method for measuring the offcut angle. This process involves:

- Analyzing the change in Omega diffraction peak position as the rotational angle of the substrate is varied with respect to the incoming X-ray beam. The Omega peak will shift proportionally to the magnitude of the offcut angle
- Measuring the Omega peak position at four Phi angles (0°, 90°, 180°, and 270°) to minimize or eliminate instrument-dependent errors or wafer mounting artifacts
- Computing the offcut angle using the standardized procedure of Halliwell and Chua[1]

Instrument Used

Rigaku SmartLab XRD
with SmartLab Studio II Analysis Software

About Covalent Metrology

Covalent Metrology is an advanced materials science and analytical services platform headquartered in the heart of Silicon Valley.

We succeed through a unique combination of cutting-edge analytical instruments and a world-class team of scientists: enabling us to provide our clients actionable, accurate and affordable data and insights to accelerate the development of product and technology innovations.

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