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Quick determination of included angles distribution for miscut substrate

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ABSTRACT

A simple method which can be performed with general laboratory facility is described for quickly determining the included angles distribution (including miscut angle) between the crystal plane and sample plane for a miscut substrate. This method is based on the rocking curve measurement of High-resolution X-ray diffraction (HRXRD). After easily measuring and calculating values of two included angles (θ_1 and θ_2) between the crystal plane and sample plane at two arbitrary mutually perpendicular azimuths of the sample plane by HRXRD, all included angles at arbitrary azimuths of the miscut substrate can be quickly calculated. Further, the value of miscut angle (θ_{max}) can be determined and its specific azimuth position on sample plane can be also easily found. Besides, since original azimuthal measurements of θ_1 and θ_2 may be situated on different positions of the sample plane, the possible condition is finally classified as four types. And then, the curves of miscut angle and azimuthal orientation under four different conditions are described in detail, respectively and their computational formulas are also distinguished carefully.

1. Introduction

For the single crystal substrate, the sample plane is not always parallel to the crystal plane. Usually, terraces can be formed because of the existence of included angles of different sizes between the sample plane and crystal plane, which may result from the manufacturing process of wafers or experimental procedure of material. It is found that the ordered terraces are sometimes crucial for the monatomic formation and epitaxial growth of thin film [1–3]. The maximum included angle between the sample plane and crystal plane is defined as the miscut angle expressed as θ_{max}. During the growth processes of thin films, the miscut angle of substrate can directly lead to deviations of the actual implant angles from the intended nominal values and then impact the growth of crystalline thin films [2,4]. On one hand, obviously, the miscut angle can influence the crystallinity of thin film growing on the top of the substrate and then lead to a lot of crystal defects on the interface. On the other hand, people may intentionally utilize vicinal substrate surfaces as ideal templates for selective deposition of film materials, where nucleation and formation of terraces can be induced by adsorptions of some metals at high temperatures [5–7]. For example, Liu and Nogami made it possible to produce a parallel array of nanowires by growing thin layers of rare-earth silicides on a single-domain vicinal Si (001) surface [8]. In addition, on 4° misoriented Si (001) substrate, Apostolopoulos et al. successfully grew Y_2O_3 nanometer films which exhibit a low degree of mosaicity, a small proportion of twinned regions and sharp interfaces [9]. Therefore, many thin films grown on vicinal Si substrates show a significant improvement compared to those grown on the exact silicon surfaces [10–12]. Moreover, the value of miscut angle is also an extremely important parameter for many devices applications [13,14]. For instance, anisotropic crystals with expected excitation and propagation properties need to be within a few arc minutes of the desired crystal surface during the preparing process of optical and acoustic devices [14]. However, the miscut angle may be unavoidable for wafers during cutting and polishing process in some cases.

In view of above reasons, the determination for value and crystal orientation of miscut angle is extremely essential in order to eliminate or effectively utilize the influence of miscut angle. However, owing to the test condition limitations, some high-precision measurements (e.g. X-ray diffractometer) are not usually available during the industrial fabrication procedure [15]. In the laboratory, the miscut angle is not always measured since people sometimes consider that the value itself is not too big or that the value is exactly the one they asked to the wafer processing company. Even if miscut angle is measured, a total of 360° rocking curves could not be often measured for the reason that the values of included angles between the crystal plane and sample plane are varied with different orientations. Thus if there are no detailed mathematical procedures to calculate the value of miscut angle, the merely measured

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angle will not be convincing. The main reason is that it is uncertain about whether the measured angle is actual miscut angle.

As we know, X-ray diffraction (XRD) is an effective approach of choice for nondestructive, rapid characterization of specific crystal plane for some single crystal specimens [14]. Therefore, rare papers in the past presented that the miscut angle of wafers can be measured by the extremely asymmetric Bragg diffraction method [16–20]. Generally, it can't be exactly known that the azimuth orientation of included angle for miscut substrate during the initial measurement process of substrate (especially for some small substrates which were cut to pieces). Therefore, if the initial azimuth orientation is different, the sign and the value of included angle would be also different. The sign of included angle could be plus or minus and the values of included angles are varied with different azimuth orientation. The distribution trends of included angle under different initial measurement conditions need to be understood and the corresponding computational formulas need to be developed for quick determination.

In our work, a very simple and quick method based on the rocking curve measurements of HRXRD for determining the included angles distribution (including miscut angle) was further developed. The value of miscut angle and its specific orientation on sample plane can be fast accurately determined by this method. The values of other included angles at arbitrary azimuths could be also calculated out easily by measuring two included angles (i.e. θ_1, θ_2) which are situated on two mutually perpendicular azimuth positions of the sample plane. Additionally, since azimuthal orientation measurements of θ_1 and θ_2 may be situated on different positions of sample plane, namely, the signs of θ_1 and θ_2 may be positive or be negative, which could result in existences of four kinds of different conditions. Finally, different variation trends of arbitrary included angles along with the azimuthal orientation of sample plane under four conditions will be described in detail and their specific computational formulas will be also distinguished carefully.

2. θ_1 and θ_2 determined by HRXRD rocking curve scan

Normally, the rocking curve scan in X-ray diffraction (XRD) is a very useful way to study perfection in both thin films and bulk of single crystals. In addition, the real peak can be also precisely positioned by the rocking curve. After comparing the real peak position to standard peak position of wafer, some crystal defects such as strain relaxation and dislocation can be studied carefully. With advantages of peak positioning and high precision, HRXRD using normal X-ray or synchrotron radiation X-ray can be used for measuring arbitrary included angles between the crystal plane and sample plane.

In regular Θ–2Θ scan, the scan direction is always along the normal of sample plane in the reciprocal space (as shown in Fig. 1). Nevertheless, when the miscut angle exists in the substrate, we will not get the maximum light intensity if the scan is still along the normal direction of sample plane. Obviously, the specific position of reciprocal point has changed due to the existence of miscut angle, i.e. from point A to point B in Fig. 1. The real reciprocal point (i.e. point B) can be only detected when the detector is fixed on the position of the Bragg reflection of standard peak firstly and then rock the sample independently (i.e. ω scan in Fig. 1). The rocking angle of the sample is precisely actual included angle between the sample plane and crystal plane at present azimuth, i.e. θ_x. In experiments, its value can be expressed by:

$$\theta_x = \omega - \Theta \tag{1}$$

where Θ is Bragg diffraction angle and ω is incidence angle in ω–2Θ scan.

Obviously, using above principle, the value of included angle at arbitrary azimuth of the substrate can be measured quickly and then be calculated easily. Therefore, as shown in Fig. 2, the included angle θ_1 situated on arbitrary azimuth of the sample plane (e.g. OA position) can be measured by this method and similarly, the value of another included angle (i.e. θ_2) on specimen surface (i.e. the OB position) can be also known by the same method. It needs to note that the sample is rotated by 90° on the horizontal azimuth, namely, OB is perpendicular to OA. As a result, a series of calculations can be done as follows by the two known included angles (i.e. θ_1, θ_2) at two mutually perpendicular azimuths of the sample plane.

3. Derivation process

For the convenience of calculation, a specific geometric figure, i.e. Fig. 3, could be used instead of Fig. 2. Further formulas derivation process and specific analysis are introduced at length as following.

3.1. Arbitrary included angle (θ_x) on the substrate plane

As shown in Fig. 3, the angle MON denoted as θ_x is a real included angle at arbitrary azimuth of substrate and the angle AON expressed as φ is an azimuth angle between θ_x and θ_1. Obviously, once two included angles at two arbitrary perpendicular azimuths of the sample plane, e.g. θ_1 and θ_2, are measured by above rocking curve of HRXRD method, θ_x can be determined as a function of azimuth angle (i.e. φ) and two known included angle (i.e. θ_1 and θ_2). The specific derivation procedure is as following:

In the triangle MNO of Fig. 3, the size of the angle MON (i.e. θ_x) can be given by tangents with MN and ON. Therefore, values of MN

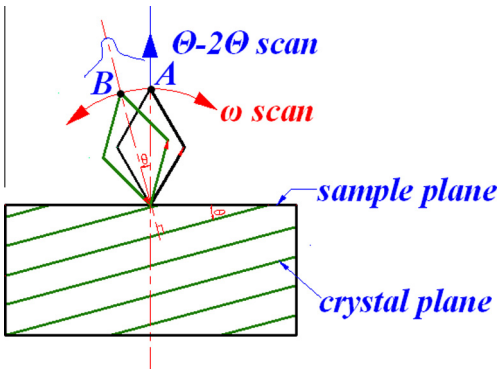

Fig. 1. Schematic of ω and Θ–2Θ scans along the crystal plane, the included angle between the sample plane and crystal plane is expressed by θ.

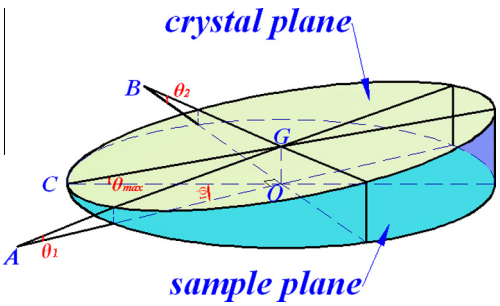

Fig. 2. Space diagram of included angles between the sample plane and crystal plane, θ_1, θ_2 are two included angles which are situated on OA and OB positions of sample plane, respectively and OA is perpendicular to OB. θ_{max} (i.e. miscut angle) situated on OC position is the maximum included angle between two planes.