X-ray topography

By: Anders Lundskog

Introduction

X-ray topography is a powerful and non-destructive technique for defect imaging (and the defects belonging strain field). The name topography arise from the fact the diffracted image reassemble a geographical topographic map, with pronounced protrusions and elevations contours. However, in x-ray topography the diffracted image derive from the structure of the material, therefore is the interpretation of the diffracted picture is not as straight forward as the case of a geographical topographical map. In this paper, we will discuss some important fundamental features of x-ray topography.

X-ray topography can be performed in various ways. The sample can be illuminated by either a synchrotron source or by a simple x-ray tube. The beam can be either monochromatic (consist of a single wavelength) or polychromatic (consist of several wavelengths i.e. white beam). In principle can simple x-ray topography be performed by a simple Bragg-Brentano goniometer, however, this is not very practical. Scanning an entire wafer for a certain diffraction angle may take several hours/days due to the low intensity. In the case of a synchrotron source, all possible reflections can be collected on a photographic film (or a modern 2D – CCD camera) during a single exposure of a few seconds. Using a synchrotron source and a photographic film is therefore much more convenient. In addition, synchrotron source typically has higher collimation degree of the x-rays, leading to sharper and more distinct diffraction peaks which increase the ultimate resolution of the topographical picture.

The sample can be illuminated in either a reflection (Bragg) or transmission (Laue) –geometry. Reflection geometry is often preferred when information of a thin film is desired since it emphasizes the microstructure of the crystal surface. Transmission geometry the topography displays the bulk microstructure of the crystal. Typical information which can be excluded from topographic pictures includes:

- Dislocation density and its belonging distribution
- The distribution of inhomogeneous strain
- Subgrain structures including missorientations
- Dislocation depth mapping
- Phase separations and much more.

Today x-ray topography is applied in multiple research fields today such as metallurgy, semiconductors, entire electronic devices, polymers, and organic materials such as proteins.
Physical principles
When the beam hits a crystalline sample (could be single or poly-crystalline), Bragg diffraction occurs. In the case of reflection geometry, some incident beams are reflected on specific crystal planes which are determined by the Bragg condition:

$$\lambda = 2dsin(\theta_B)$$

The angle, $\theta_B$, $d$, and $\lambda$ is known as the Bragg angle, the lattice plane spacing, and the beam wavelength respectively. For a monochromatic source, only certain lattice plane spacing’s and Bragg angles can be fulfilled by Bragg’s law simultaneously which gives rise to Laue spots. The concept for a single crystal is shown in Figure 1.

![Figure 1: a) Experimental setup for a Laue camera. b) Laue spots from a single crystal.](image)

When neglecting the divergence of the beam, the spots are perfectly uniform for a perfect crystal. However, if the crystal is strained by for example a defect or a grainboundary, streaks appear instead of spots due to the variations in lattice spacing. In the presence of multiple dislocations, grainboundaries etc an intensity pattern on each Laue point will appear. The intensity pattern is known as the x-ray topography of the illuminated sample area. In other words x-ray topography is the fine structure of the Bragg spot.

As mentioned earlier, can either a mono or a polychromatic beams can be used in x-ray topography. When using a monochromatic beam, only one topograph is recorded at a time. The recorded topograph is determined by Bragg’s law. Bragg’s law is in principle always fulfilled when using polychromatic beams. There is always one wavelength in the incident spectrum for which the Bragg angle for a certain set of lattice planes and Bragg angles (see equation 1). However, polychromatic beams still produce a fine structure of the Laue spots. There are two different kinds of contrasts which can be identified in a polychromatic x-ray topographical picture, orientation and extinction -contrast.

Orientation contrast
Orientation contrast is based upon Bragg’s law. Orientation contrast arises when misorientations of subdomains are large enough. In white-beam topography, all misoriented subdomains will be diffracting simultaneously (each at a different wavelength). The exit angles of the diffracted beams will different, leading to overlapping regions of enhanced intensity which results in contrast differences.
Extinction contrast

Extinction contrast on the other hand is much more complex compared to the orientation contrast. The extinction contrast is based upon the dynamical theory of x-ray scattering. In the dynamical theory of x-ray scattering interactions between incident and diffracted waves within the crystal are considered. In the kinematical theory of x-ray scattering (orientation contrast is based on the kinematical theory), each atomic site is considered as an independent scattering source. Extinction contrast is only observed in high quality single crystals.

Defect visibility

A dislocation is characterized by its propagation direction and Burgers vector. If the defect is aligned with a certain direction, it may not give any contrast on an x-ray topograph. The criteria of visibility are defined as:

\[ g \cdot (b \times l) \neq 0 \]

where \( g \), \( b \) and \( l \) are the diffraction vector, burgers vector and propagation direction respectively. The diffraction vector is dependent on the experiment geometry. In a symmetric Bragg geometry of an on-axis 4H-SiC taken in the (0001) direction for example, the diffraction vector is defined as \([0001]\). Edge dislocations will not be visible in this type of scan hence the criterion above is not fulfilled. Screw dislocations on the other hand will be visible. When analyzing polychromatic x-ray topographs, the picture should be interpreted the following way:

- White regions correspond to low scattering regions. On a photographic film, these areas will not be exposed thus appear white.
- Dark regions correspond to defective regions on the sample. This is due to the scattering power of imperfect regions is greater than from a perfect surrounding matrix.
- Uniform contrast areas are high quality crystal regions.

Figure 2 shows a 4H-SiC epilayer polychromatic topograph taken in (0001) Bragg geometry. A micropipe is a hollow core dislocation, thus showing white contrast in Figure 2. Threading screw dislocations are denoted as TSD, and basal plane dislocations are denoted as BPD.

![Figure 2: SWBXT (Synchrotron white beam X-ray topography) picture of a 4H-SiC epilayer taken in back reflection mode.](image)
Sources