Modeling of polygonal half-loops dislocations in silicon single crystal using X-ray diffraction topo-tomography data

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Abstract. Topo-tomographic methods for identifying defects in semiconductors are the most effective among X-ray methods. Combining experimental data with model calculations makes it possible to determine various parameters and properties of crystal structures. In this work, using X-ray diffraction topo-tomography, images of the dislocation half-loop in Si (111) crystal were obtained. The Takagi-Taupin equations have been used to modeling the topograms. A quantitative comparison of the images made it possible to determine the direction of the Burgers vector.

1. Introduction

Much work related to the study of semiconductor materials is focused on the study of the defect structure. It is known that defects in the crystal structure concern the properties of the material. For example, Seibt (2008) showed that the interaction of dislocations with silicon crystal impurities affects the energy yield of charge carriers [1]. In turn, silicon is a widespread material used in solar cells. In addition, Wang (2018) investigated the semiconductor monolayer ZrS2 and found that the accumulation of defects can cause the metallic properties of the layer, and defects of several atoms can increase the magnetic moment of the material [2]. Modern methods of defect identification deserve no less consideration. Today, the most common methods are laminography [3], reciprocal-space mapping methods [4], and X-ray topo-tomography [5], which is more popular.

Despite the successes achieved in the experimental detection of defects, there remains a need for an accurate quantitative assessment of their parameters. For this, one can use the experiment's simulation and apply its results to interpret the experimental data. This approach is justified by the number of works devoted to modeling the single defects and dislocation structures in single crystals [6, 7] and grain boundaries in polycrystals [8]. However, the determination of the direction of the Burgers vector of a dislocation was still based on a drop in the intensity of the diffraction image satisfying the condition \((h \cdot b) = 0\). Here \(h\) is the diffraction vector, \(b\) is the Burgers vector.

In this paper, we propose a method for determining the direction of the Burgers vector of a dislocation half-loop in a silicon crystal by quantitatively comparing experimental topograms obtained by X-ray diffraction topo-tomography and their model analogs.
2. Methods and objects

Experimental diffraction images (topograms) of the Si (111) crystal plate were obtained at the ID19 station of the ESRF synchrotron center (Grenoble, France). The data were recorded with a resolution of 0.96 μm at a radiation energy $E = 25.3$ keV. The sample was rotated in angle $\varphi$ around the diffraction vector $h$ [220] by 360° with a step of 3.6°. At $\varphi = 0°$, the plate is parallel to the detector surface. One of the obtained topograms is shown in Figure 1a. To simulate the experiment, the best-quality topogram was selected in terms of contrast, noise level, and the absence of extraneous crystal defects near the selected dislocation half-loop. A 3D model of this half-loop was reconstructed from a series of topograms, and two parameters were extracted that will be used in modeling: the length of the middle dislocation and its distance to the nearest surface of the silicon plate (the dislocation is parallel to the surface of the plate).

![Figure 1](image1.png)

**Figure 1.** a) Topogram of a dislocation half-loop (resolution 0.96 μm). b) Thompson’s tetrahedron, built on slip planes {111} [9]. Possible configurations of half loops are marked with bold lines.

As is known, in a silicon crystal, as in crystals with a diamond-like structure, directions of dislocations of the <110> type are possible, forming the edges of the so-called Thompson tetrahedron (Figure 1b). Since the four-point bending of the crystal around the [111] axis was used in our sample to generate dislocations, only two types of dislocation half-loops are possible, consisting of three sections with the directions [110], [011], [101] (Figure 2) and [010], [101], [011]. In the first case, the Burgers vector can have the directions [011] and [101], in the second case - [101] and [011], which also follows from the condition of the sample deformation.

![Figure 2](image2.png)

**Figure 2.** Schematic representation of a dislocation half-loop in the Si (111) plate ($n$ is the normal vector to the plate surface).

The topograms were simulated using the Takagi-Taupin equations based on the dynamic theory of diffraction [10]:

$$\frac{2i}{k} \frac{\partial D_0(r)}{\partial s_0} = \chi_0 D_0(r) + C \chi_h D_h(r) \exp(-ihu(r))$$

$$\frac{2i}{k} \frac{\partial D_h(r)}{\partial s_h} = (\chi_0 - \alpha) D_h(r) + C \chi_h D_0(r) \exp(ihu(r))$$
The numerical solution of the equations was based on the program code, the algorithm of which was described in detail by Besedin (2014) in the article [11]. The solution of the equations is the amplitudes of the transmitted $D_0$ and diffracted $D_h$ waves in the volume of the crystal. The displacement fields $u(r)$ of each individual dislocation are cross-linked into a single expression to describe the entire half-loop. Since the radiation hits the detector after leaving the crystal, the intensity distribution on the output surface of the sample is taken as a topogram. However, for non-zero values of $\varphi$ the exit plane of the plate is not parallel to the surface of the detector, and this image does not correspond to the experimental image. For this, a correction is introduced to project the image along the direction of the diffracted wave.

As for the quantitative assessment of the experimental and model topograms, the following expression is proposed as the correspondence parameter:

$$R^2 = \left( \frac{\sum_{i=1}^{n} (I_{\text{exp},i} - I_{\text{calc},i})^2}{\sum_{i=1}^{n} I_{\text{calc},i}^2} \right)^{-1},$$

where $I_{\text{exp}}$ and $I_{\text{calc}}$ - intensity of experimental and model topograms, $n$ - the number of pixels in the image.

3. Results and conclusions

Model topograms were calculated for two Burgers vectors $[0\bar{1}1]$ and $[10\bar{1}]$ for a dislocation half-loop, the directions of which are shown in Figure 2. A similar topogram from experimental data and simulation results are shown in Figure 3.

![Figure 3](image-url) Diffraction images of the dislocation half-loop: on the left - experimental data, in the center - model with the Burgers vector $[0\bar{1}1]$, on the right - model with Burgers vector $[10\bar{1}]$.

The original larger topograms were manually aligned and cut with pixel precision, avoiding extraneous defects. Intensity values are scaled to a maximum of 100 arbitrary units. According to (1), the value of the $R^2$-factor is calculated. For the Burgers vector $[0\bar{1}1]$ $R^2 = 1.133$, for the Burgers vector $[10\bar{1}]$ $R^2 = 1.155$. Both values indicate good agreement between the model topograms, but the images show that the intensity from the middle dislocation in the experimental image is much weaker than from the side ones. The same is observed for the model topogram for the Burgers vector $[0\bar{1}1]$. In comparison with the topogram for another Burgers vector, the intensity from the middle dislocation is lower, and from the upper lateral one, it is higher. This means that the experimental topogram contains a dislocation half-loop with the Burgers vector $[0\bar{1}1]$. These results are confirmed by the data from the Laue X-ray diffraction experiment described in [7].

In the future, it is planned to use noise filtering to improve the signal-to-noise ratio, automatic alignment of experimental and model topograms, and also use more data at other values of the angle $\varphi$. 
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