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Simulation of the Sample Alignment Process for the White Beam Tomography

A H Ozdiev[1], Dr. S N Liventsov[2]

[1]Department of General Physics, Institute of Physics and Technology, Tomsk Polytechnic University, Russia, Tomsk, 30 Lenin Avenue, 634050
[2]Department of Electronics and Automation of Nuclear Plants, Institute of Physics and Technology, Tomsk Polytechnic University, Russia, Tomsk, 30 Lenin Avenue, 634050

E-mail: ozdiev@tpu.ru

Abstract. Nowadays growth of synthetic crystals is a very prospective direction of research activity. However, it is well known that in synthesized crystals there are still many defects and the main idea is to synthesize crystal of ideal form and structure. But in purpose to remove defects first you have to characterize them. This paper describes the method for the characterization of such defects and mainly concentrates on the problem of sample alignment procedure, offering the way to avoid misalignments.

1. Method description

The idea is to use combination of topography and tomography (topo-tomography) with application of the white beam.

1.1. Topography and tomography

In order to characterize defects X-ray topography can be used. Topography is a 2D imaging of some area of analyzed object in purpose to find the defects. It can be implemented with using of monochromatic or white beam. Tomography is 3D imaging of scanned object with possibility to analyze it slice by slice. Combining those two methods allows not only find the defects, but presents them in 3D-view. In case of dislocations [1] described method helps to know how they are located inside crystal. This method already was implemented with monochromatic beam [2], but in current work the white beam have been used.

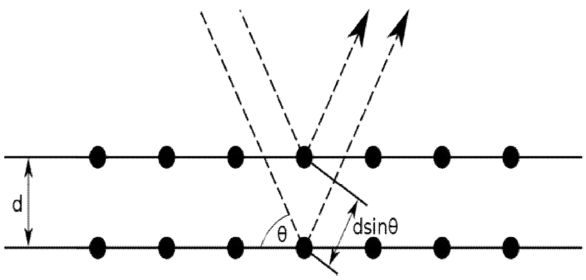

Figure 1. Schematic of Bragg's condition

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X-ray topography is a method of obtaining images of defects in crystals by X-ray diffraction. This is the non-destructive method for characterizing and monitoring of the real structure of the material. Due to its high sensitivity to defects in the crystal lattice, this method makes it possible to analyze sample of quite big thickness and area. The sensitivity of X-ray topography to the presence of defects in the crystal lattice connected with the local deformation of the lattice in the location of the defect, for example, dislocations. The reflection of the beam from the deformed region of the crystal is different from the reflection of the beam from perfect part of crystal. This difference allows finding the defects.

To get the diffraction, the Bragg condition (Figure 1) has to be fulfilled. Bragg diffraction occurs when electromagnetic radiation or subatomic particle waves with wavelength comparable to atomic spacing’s are incident upon a crystalline sample, are scattered in a specular fashion by the atoms in the system, and undergo constructive interference in accordance to Bragg's law [3]. For a crystalline solid, the waves are scattered from lattice planes separated by the interplanar distance d.

$$2d \times sin\theta = n\lambda \tag{1}$$

where n is an integer determined by the order given, and λ is the wavelength. A diffraction pattern is obtained by measuring the intensity of scattered waves as a function of scattering angle. Very strong intensities known as Bragg peaks are obtained in the diffraction pattern when scattered waves satisfy the Bragg condition.

Tomography (Figure 2) is a generating of three-dimensional image of the inside of an object from large series of two-dimensional X-ray images or projections taken around a single axis of rotation. In the end from tomographic reconstructions obtains 3D volume of object, which is possible to analyze slice by slice [4].

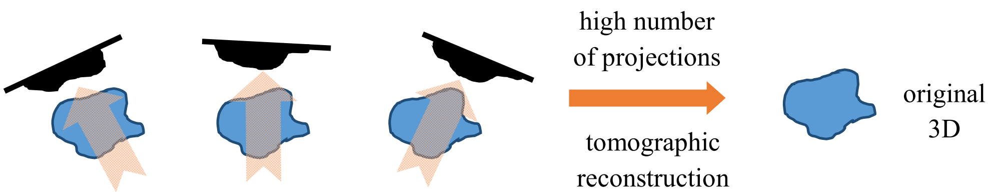

Figure 2. Basic principle of tomography

1.2. Principle of the method

In contrast to the monochromatic case, in which accurate sample adjustment is often necessary in order to reach diffraction conditions, the Bragg equation is always and automatically fulfilled in case of a white X-ray beam: whatever the angle at which the beam hits a specific lattice plane, there is always one wavelength in the incident

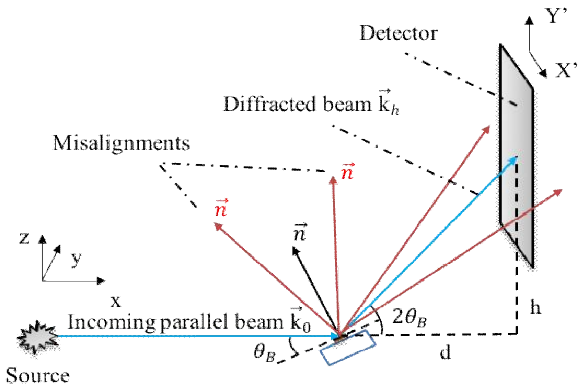

Figure 3. Misalignments

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spectrum for which the Bragg angle is fulfilled just at this precise angle (on condition that the spectrum is wide enough).

So, Bragg's law works in each rotation angle, it means that in each rotation angle possible to get 2D-projection. But the problem is to adjust the orientation of the sample without any misalignments (Figure 3). Because if the sample is not aligned, the projections move during rotation, which does not allow 3D reconstruction. Misalignment in our case means that the diffraction normal to lattice plane of sample is not parallel to rotation axis. This is the main problem – problem of neutralizing of misalignments [5].

To solve the problem was used the experimental setup. This setup allows adjusting position and orientation of the sample in the space. Setup consist of several main and important parts namely source of beam, tilts, which change the orientation of the sample and the detector, which allows to find diffracted beam. Directions of position changing of sample for tilts 1 and 2 are shown on Figure 4. Directions of position changing of sample for tilts 3 and 4 are parallel and perpendicular, accordingly.

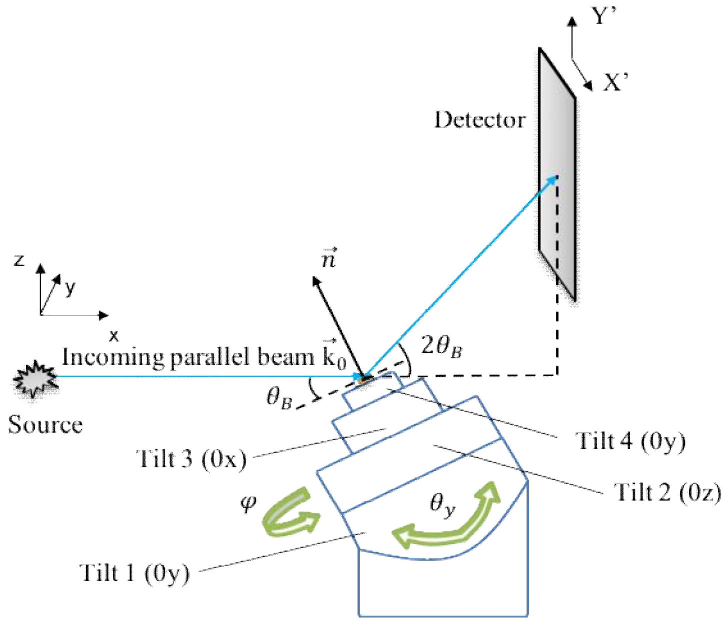

Figure 4. Misalignments

2. Simulation

To simulate the position of diffracted beam on the detector the coordinates of hit has to be calculated. Necessary calculations were made in Wolfram Mathematic 8.0.

2.1. Mathematical model

For calculation were used following formulas and mathematical expressions:

Tilts: rotation around 0y, angle θ_y; rotation around 0z, angle φ; rotation around 0y, angle β for $\theta_y = 0$, $\varphi = 0$; rotation around 0x, angle α for $\theta_y = 0$, $\varphi = 0$. $n' = (R'_y.\ R'_x) \times n_0$, where $R'_y(\beta)$ – matrix of rotation around 0y, tilt 3 and $R'_x(\alpha)$ – matrix of rotation around 0x, tilt 4. Initial normal:

$$n_0 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{2}$$

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Misalignments includes in the system by random initialization of α and β. Such as: α = (a1-a2), where a1 is random part and a2 is adjustable part. β = (b1-b2), b1 –random, b2 – adjustable. The normal for the whole system:

$$n = (R_y(\theta_y).\ R_z(\varphi)).n' \tag{3}$$

where n' – normal for tilts 1 and 2; R_y – matrix of rotation around 0y, tilt 1; R_z– matrix of rotation around 0z, tilt 2. Diffracted beam:

$$k_n = k_0 - 2n(k_0.n) \tag{4}$$

Then from X, Y and Z components of diffracted beam S-parameter and hit coordinates can be calculated:

$$S = \frac{d}{k_{nx}} \tag{5}$$

d – distance to the detector; $X = S \times k_{ny}$ - X coordinate of hit; $Y = S \times k_{nz}$ - Y coordinate of hit.

On the figure 5 presented a user interface, which is simulating the experimental adjusting procedure. The green point is the diffracted beam, the white field is the detector, the scale bars are in cm. By changing of α and β angles user can change incline orientations of the sample. By changing of angle φ changes the rotation angle. Changing of θ_y angle allows changing Bragg angle. Also it possible to change position of detector by adjusting of X' and Y' coordinates in detector CS. Corresponding script is presented in figure 6.

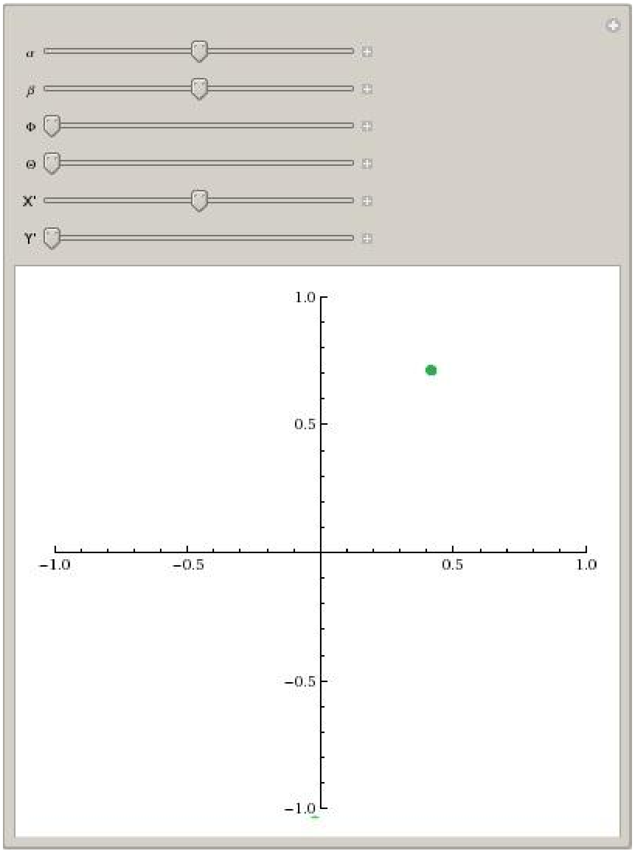

Figure 5. Simulation interface

```
α=alpha; (*Tilt angle*)
β=beta; (*Tilt angle*)
φ=phi; (*Rotation angle*)
Subscript[θ, y]=theta; (*Tilt angle*)
d=10; (*Distance to the detector*)
Subscript[k, 0]={1,0,0}; (*Initial beam*)
Print[Style["Source beam:",Blue, 14]]
Print["Subscript[k, 0]=",MatrixForm[Subscript[k, 0]]]
Ry1={{1,0,0},{0,Cos[α],-Sin[α]},{0,Sin[α],Cos[α]}}; (*Matrix of rotation aroung Ox for tilt #4*)
Rx1={{Cos[β],0,Sin[β]},{0,1,0},{-Sin[β],0,Cos[β]}}; (*Matrix of rotation around Oy for tilt #3*)
Print[Style["Matrix of rotation around 0x for tilt 4:",Blue, 14]]
Print["Subscript[R^', x]=",MatrixForm[Ry1]]
Print[Style["Matrix of rotation around 0y for tilt 3:",Blue, 14]]
Print["Subscript[R^', y]=",MatrixForm[Rx1]]
n2={0,0,1};
n=(Ry1.Rx1).n2; (*Normal n^'*)
Print[Style["Normal for system of tilts 3 and 4:",Blue, 14]]
Print["Normal n=",MatrixForm[n]]
Rz={{Cos[φ],-Sin[φ],0},{Sin[φ],Cos[φ],0},{0,0,1}};  (*Matrix of rotation around Oz for tilt #2*)
Print[Style["Matrix of rotation around 0z for tilt 2:",Blue, 14]]
Print["Subscript[R, z]=",MatrixForm[Rz]]
Ry={{Cos[Subscript[θ, y]],0,-Sin[Subscript[θ, y]]},{0,1,0},{Sin[Subscript[θ, y]],0,Cos[Subscript[θ,
y]]}};  (*Matrix of rotation around Oy for tilt #1*)
Print[Style["Matrix of rotation around 0y for tilt 1:",Blue, 14]]
Print["Subscript[R, y]=",MatrixForm[Ry]]
Subscript[n, L]=(Ry.Rz).n; (*Normal n*)
Print[Style["Normal for whole system:",Blue, 14]]
Print["Subscript[n, L]=",MatrixForm[Subscript[n, L]]]
Subscript[k, n]=Subscript[k, 0]-2 Subscript[n, L] (Subscript[k, 0].Subscript[n, L]); (*Diffracted
beam*)
Print[Style["Diffracted beam:",Blue, 14]]
Print["Subscript[k, n]=",MatrixForm[Subscript[k, n]]]
Print[Style["Components of diffracted beam:",Blue, 14]]
Print["X-component Subscript[k^x, n]=",Subscript[k^x, n]=Subscript[k, n][[1]]]; (*X component of
diffracted beam*)
Print["Y-component Subscript[k^y, n]",Subscript[k^y, n]=Subscript[k, n][[2]]]; (*Y component of
diffracted beam*)
Print["Z-component Subscript[k^z, n]=",Subscript[k^z, n]=Subscript[k, n][[3]]]; (*Z component of
diffracted beam*)
Print["Parameter s=",s=d/Subscript[k^x, n]]; (*Parameter S*)(*Coordinates of hit*)
Print[Style["Hit coordinates:",Blue, 14]]
Subscript[d, x]=s Subscript[k^y, n]; (*X coordinate*)
Subscript[d, y]=s Subscript[k^z, n]; (*Y coordinate*)
Print["X=",FullSimplify[Subscript[d, x]]];
Print["Y=",FullSimplify[Subscript[d, y]]];
(*Random missalignment angles*)
a12=RandomReal[{-10,10}];
a1=a12*Pi/180;
b12=RandomReal[{-10,10}];
b1=b12*Pi/180;
(*ρ=φ, a2=α, b2=β, σ=θ*)
```

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```
(*X coordinate function*)
X[ρ_,a2_,b2_,σ_]:=-((20 (-Cos[b1-b2] Cos[ρ] Sin[a1-a2]+Sin[b1-b2] Sin[ρ]) (Cos[ρ] Cos[σ] Sin[b1-b2]+Cos[b1-b2] (Cos[σ] Sin[a1-a2] Sin[ρ]-Cos[a1-a2] Sin[σ])))/(1-2 (Cos[ρ] Cos[σ] Sin[b1-b2]+Cos[b1-b2] (Cos[σ] Sin[a1-a2] Sin[ρ]-Cos[a1-a2] Sin[σ]))^2));
(*Y coordinate function*)
Y[ρ_,a2_,b2_,σ_]:=-((20 (Cos[a1-a2] Cos[b1-b2] Cos[σ]+(Cos[ρ] Sin[b1-b2]+Cos[b1-b2] Sin[a1-a2] Sin[ρ]) Sin[σ]) (Cos[ρ] Cos[σ] Sin[b1-b2]+Cos[b1-b2] (Cos[σ] Sin[a1-a2] Sin[ρ]-Cos[a1-a2] Sin[σ])))/(1-2 (Cos[ρ] Cos[σ] Sin[b1-b2]+Cos[b1-b2] (Cos[σ] Sin[a1-a2] Sin[ρ]-Cos[a1-a2] Sin[σ]))^2));
Manipulate[Graphics[{PointSize->Large,Green,Point[{X[ρ*Pi/180,a2*Pi/180,b2*Pi/180,σ*Pi/180]-x,Y[ρ*Pi/180,a2*Pi/180,b2*Pi/180,σ*Pi/180]-y(*-d*Tan[(Pi/90)σ]*)}]},Axes->True,AxesOrigin->{0,0}, PlotRange-> {{-1,1},{-1,1}}],{{a2,0,"α"},-90,90,.1},{{b2,0,"β"},-90,90,.1},{{ρ,0,"Φ"},0,360,90},{{σ,0,"Θ"},0,20,1},{{x,0,"X'"},-5,5,.1},{{y,0,"Y'"},0,10,.1}]
```

Figure 6. The script of the simulation of the alignment procedure

3. Conclusion

Since the method is a combination of topography and tomography, the alignment procedure aims to fulfil two conditions. First, Bragg's law has to work for each tomographic rotation angle of the mounted sample with a fixed Bragg angle (Figure 7). This is complicated by the fact that by using white beam Bragg's law is always fulfilled. The second conditions requirement of tomography, because to reconstruct the 3D volume of the sample, the image on the detector has to stay in the same position for all view angles of the sample.

Using slits the beam size was reduced so that diffracted beam can be displayed on the detector as a point. Misalignments can be neutralized by changing of incline orientation of the sample. It is possible to check by changing of rotation angle. If there are no misalignments changing of rotation angle will not cause changes in the hit coordinates on the detector. It was reached by turning always +/- 180° and trying to make the diffracted beam (point) stay at the same position on the detector, then the same operation was repeated for the 90° rotated case. And then back and iteratively the adjustment is improved. Developed algorithm was tested at the ANKA synchrotron facility [6].

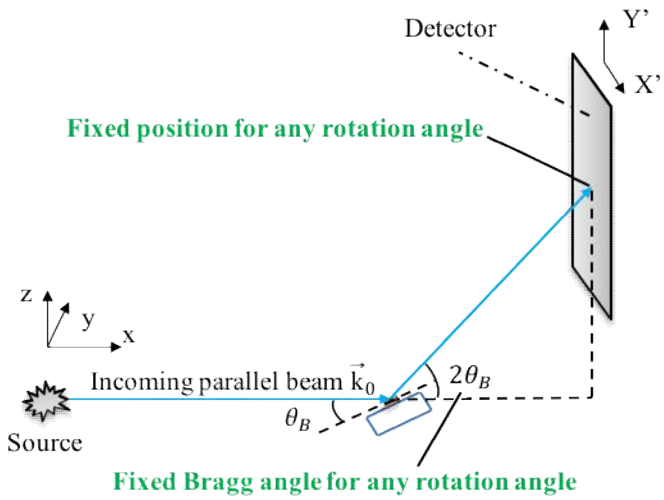

Figure 7. Alignment procedure

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References

[1] James Shackelford (2009). Introduction to Materials Science for Engineers (7th ed.)
[2] Wolfgang L. (2010) *Characterization of polycrystalline materials by X-ray diffraction tomography* (New York: Springer US)
[3] Bragg W. L., (1914) «The Diffraction of Short Electromagnetic Waves by a Crystal», Proceedings of the Cambridge Philosophical Society, 17, 43
[4] A. C. Kak and Malcolm Slaney, Principles of Computerized Tomographic Imaging
[5] Helfen L (2011) *Synchrotron and neutron laminography for three-dimensional imaging of devices and flat material specimens* (Berlin: Carl Hanser Verlag GmbH & Co. KG.)
[6] 2013 *ANKA instrumentation book* (Karlsruhe: ANKA Synchrotron Radiation Facility, Karlsruhe Institute of Technology, a member of the Helmholtz Association. IPS, Institute for Photon Science and Synchrotron Radiation)