THE DEVELOPMENT OF SPECTRAL TOMOGRAPHY USING OF CRYSTAL-ANALYZER SCHEME

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Motivation

- Nowadays laboratory microtomographs usually use continuous energy spectrum X-ray tubes and detectors without both spatial and energy resolution. Therefore, the main efforts in this area are focused on the search for methods that allow taking into account or using the polychromatic nature of X-ray sources.

- In the incident polychromatic radiation, low energy quanta are mainly absorbed more strongly by the sample under study. Thus, with increasing the sample thickness, the high-energy component of the radiation in the beam recorded at the output begins to prevail. The so-called "beam hardening" occurs. The conventional methods of tomographic reconstruction can only process linearized projection data. Attempts to linearize the problem if the linearity conditions are not met at the physical level generate additional reconstruction artifacts, such as the "cupping effect". To reduce inaccuracies in the reconstructed structure of the object, several essentially different approaches are used.
Polychromaticity of the beam. Solutions

SOFTWARE

- developing of special reconstruction algorithms taking into account the polychromaticity incorporated into the mathematical model.

HARDWARE

- energy dispersive detectors;
- “sandwich detectors”;
- second source-detector systems;
- X-ray beam filters;
- X-ray optics elements.
In spectral tomography a number of different types of images can be formed, including the low- and high-energy spectral images, mixed images that combine these two data sets, material-specific images, and energy-specific images.

The general principle of selecting pairwise reciprocal lattice (RL) for $K_\alpha$ and $K_\beta$ lines simultaneous diffraction

Schematic construction to find the conditions for the simultaneous diffraction of the $K_\alpha$ and $K_\beta$ lines of an X-ray tube for a selected pair of points in the RL crystal space: (a) intersection of the Ewald spheres for $K_\alpha$ and $K_\beta$ lines by the diffraction plane for the $K_\alpha$ line; (b) a torus formed by the rotation of the Ewald spheres around an axis passing through the RL point $H^{(\alpha)}$; (c) rotation of the $K_\beta$ Ewald sphere around $H^{(\alpha)}$ to get diffraction from the RL point $H^{(\beta)}$; (d) same as (c), but top view.
The practical implementation of the algorithm

\[
\begin{align*}
\langle \vec{h}_\alpha \cdot \vec{k}_{\alpha,\beta} \rangle &= a_1 c_1 + a_2 c_2 + a_3 c_3 = \cos \alpha = \sin \theta_{Br} K_\alpha = \frac{\lambda K_\alpha}{2d_{111}} \\
\langle \vec{h}_\beta \cdot \vec{k}_{\alpha,\beta} \rangle &= b_1 c_1 + b_2 c_2 + b_3 c_3 = \cos \beta = \sin \theta_{Br} K_\beta = \frac{\lambda K_\beta}{2d_{111}} \\
\vec{k}_{\alpha,\beta} &= (c_1, c_2, c_3) \\
d &= |\vec{k}_{\alpha,\beta}| \cdot \sin \beta \sin(\angle A), \text{ or } d = |\vec{k}_{\alpha,\beta}| \cdot \sin \alpha \sin(\angle B) \\
c_1^2 + c_2^2 + c_3^2 &= 1 \\
\vec{n} &= [\vec{h}_\alpha \times \vec{h}_\beta]. \\
n_1 c_1 + n_2 c_2 + n_3 c_3 &= d \sin \gamma \\
d &= |\vec{k}_{\alpha,\beta}| \cdot \cos \left( \frac{\vec{k}_{\alpha,\beta} \cdot \vec{n}}{|\vec{k}_{\alpha,\beta}| |\vec{n}|} \right) \\
\begin{bmatrix}
0 \\
0 \\
1
\end{bmatrix} &= 
\begin{bmatrix}
\cos \alpha & -\sin \alpha & 0 \\
\sin \alpha & \cos \alpha & 0 \\
0 & 0 & 1
\end{bmatrix} \times
\begin{bmatrix}
1 & 0 & 0 \\
0 & \cos \gamma & -\sin \gamma \\
0 & \sin \gamma & \cos \gamma
\end{bmatrix} \times
\begin{bmatrix}
c_1 \\
c_2 \\
c_3
\end{bmatrix}
- \text{ the example of matrix for the XZ rotations}
\end{align*}
\]

Spectral tomography. The scheme with crystal-analyzer Si(111)

The method for adjusting a crystal-analyzer to separate two characteristic lines from the spectrum of a conventional X-ray tube. The set of tomographic data (projections) for two monochromatic $K_{\alpha_1}$ and $K_{\beta}$ lines can be obtained.
The results of separation of two characteristic lines

Experimental results of separation of two characteristic lines from the incident polychromatic beam of the molybdenum anode in comparison with the Laue-grams calculated by LauePT* software.

The study of pineal gland calcified concrements

Test object (calibration grid)

The parameters of experiment:
Mo X-ray tube: accelerating voltage 40 kV and current 40 mA;
A silicon crystal-analyzer with a thickness of 540 μm;
1 - system of slits;
2 - sample in the study (TEM gold grid);
3 - aluminum filter;
4 - CCD-camera (Ximea XiRay11).

Mathematical correction of projections

\[ p^\text{norm}_*(x_{\text{det}}, y_{\text{det}}) = \frac{I^0_*(x_{\text{det}}, y_{\text{det}}) - I^\text{dark}_*(x_{\text{det}}, y_{\text{det}})}{I^0_*(x_{\text{det}}, y_{\text{det}}) - I^\text{dark}_*(x_{\text{det}}, y_{\text{det}})} \]

(a) Image in transmission mode; (b) \( K_\alpha \) image \( p^\text{norm}_{K_\alpha} \); (c) \( K_\beta \) image \( p^\text{norm}_{K_\beta} \); (d) \( K_\alpha \) image after projective correction \( p^{\text{proj}}_{K_\alpha} \); (e) \( K_\beta \) image after projective correction \( p^{\text{proj}}_{K_\beta} \).

A three-channel image of the calibration grid. The red channel contains \( p^{\text{norm}}_T \), the green channel contains \( p^{\text{proj}}_{K_\beta} \), and the blue channel contains \( p^{\text{proj}}_{K_\alpha} \).
Mathematical correction of projections. MicroSD card measurements

(a) Normalized images of the chip section; (b) $P_{K\alpha}^{\text{norm}}$ image; (c) $P_{K\beta}^{\text{norm}}$ picture; (d) after projective correction $P_{K\alpha}^{\text{proj}}$; (e) after projective correction $P_{K\beta}^{\text{proj}}$.

This image allows to conclude that the proposed procedure to compensate for the geometric distortions caused by the crystal-analyzer installed in the optical path is correct. But…
The influence of crystal-analyzer thickness and high Miller`s indexes

MicroSD section images:
(a) for \{111\} reflections obtained for a crystal 330 µm thick.
(b) for \{220\} reflections obtained for a crystal 330 µm thick.
(c) for \{220\} reflections obtained for a crystal 540 µm thick.

Therefore, the first thickness oscillation of the rocking curve is also involved in the formation of a diffraction image with a relatively thick crystal-analyzer (540 µm). If a thinner crystal (330 µm) is used, the dual image is already less defined, since the first thick oscillation will be further along the angle (a, b). When reflections with high Miller’s indexes are using it is possible to avoid the effect of thick oscillations (b, c)
Conclusions

- In the present work, the method for adjusting the crystal-analyzer to separate jointly two characteristic lines from the spectrum of a conventional X-ray tube for simultaneous registration of tomographic projections is proposed.

- The experimental implementation of the proposed method using radiation of molybdenum anode ($K_{\alpha 1}$, $K_\beta$ – lines) and silicon Si(111) crystal-analyzer in Laue-geometry is presented.

- An algorithm for the geometric correction of projection distortions was built. Furthermore, work began on building a model of tomographic projections based on the dynamic theory of X-ray diffraction in crystals, which will allow quantitative analysis.

- In addition, the use of a crystal-analyzer as an energy separator of the primary beam together with polychromatic synchrotron X-ray radiation opens new opportunities for research to contrast almost any substance in the sample. In this case, the crystal can be tuned to obtain reflections before and after the absorption edge of a particular chemical element.

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Work in progress

Thank you for your attention!

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