Трехкристальная рентгеновская дифрактометрия

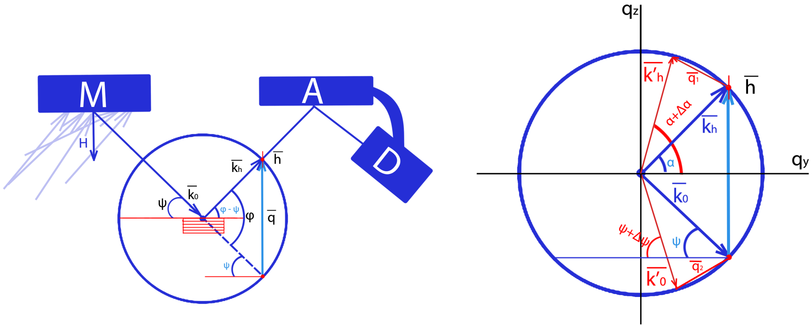
I. Atknin[1,2,3] F. Chukhovsky[2] N. Marchenkov[2,3]

[1]Department of optics, spectroskopy and physics of nanosystems
Moscow State University

[2]X-ray analysis technique and synchrotron radiation laboratory
Shubnikov Institute of Crystallography, Russian Academy of Sciences.

[3]National Research Centre "Kurchatov Institute"
Department of Nano-, Bio-, Info-, and Cognitive Sciences and Technologies

qz and qy [1]



q - the deviation of the scattering vector, h - the reciprocal lattice point. The left figure – illustrates the case when the specimen angle, $\boxed{\psi}$, and the analyser angle, $\boxed{\phi}$, are set so as to satisfy the Bragg condition.

qz and qy [1]

q_1 :

$$\frac{q_y}{|k|} = \cos\alpha - \cos(\alpha - \Delta\alpha) \tag{1}$$

$$\frac{q_z}{|k|} = \sin(\alpha + \Delta\alpha) - \sin\alpha \tag{2}$$

q_2 :

$$\frac{q_y}{|k|} = \cos\psi - \cos(\psi - \Delta\psi) \tag{3}$$

$$\frac{q_z}{|k|} = \sin(\psi + \Delta\psi) - \sin\psi \tag{4}$$

where:

$$\sin(a + b) = \sin(a) \cdot \cos(b) - \sin(b) \cdot \cos(a)$$

$$\cos(a + b) = \cos(a) \cdot \cos(b) - \sin(b) \cdot \sin(a)$$

$$\cos\Delta\alpha = \cos\Delta\psi = 1$$

$$\sin\Delta\alpha = \Delta\alpha$$

$$\sin\Delta\psi = \Delta\psi$$

qz and qy [1]

$$\frac{q_{1y} + q_{2y}}{|k|} = \frac{q_y}{\mathbf{k}} = -\Delta\alpha \cdot \sin\alpha + \Delta\psi \cdot \sin\psi \tag{5}$$

$$\frac{q_{1z} + q_{2z}}{|k|} = \frac{q_z}{\mathbf{k}} = \Delta\alpha \cdot \cos\alpha + \Delta\psi \cdot \cos\psi \tag{6}$$

where

$$\alpha = \phi - \psi$$

$$\Delta\alpha = \Delta\phi - \Delta\psi$$

for the result we have

$$\frac{q_y}{|k|} = \Delta\psi \cdot \sin\psi - (\Delta\phi - \Delta\psi) \cdot \sin(\phi - \psi) \tag{7}$$

$$\frac{q_z}{|k|} = \Delta\psi \cdot \cos\psi + (\Delta\phi - \Delta\psi) \cdot \cos(\phi - \psi) \tag{8}$$

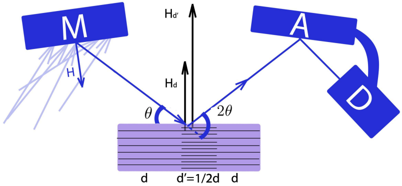
for symmetric reflection:

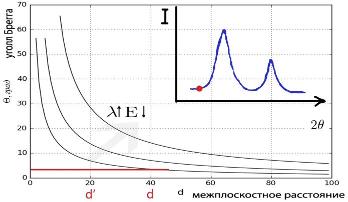
$$\psi = \theta_B$$

$$\phi - \psi = \theta_B$$

$\theta - 2\theta$ scan. Separation of lattice tilts and $\boxed{\text{strains}}$

Any region of the specimen which also has lattice parameter $\boxed{d}$ but is tilted with respect to the original region will never provide scattering which reaches the detector;

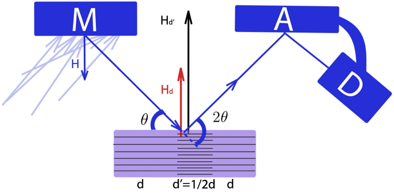


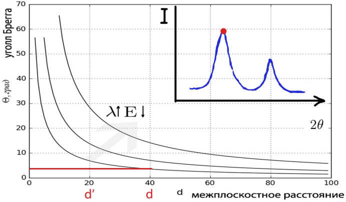


However, another region of the sample with lattice parameter $\boxed{d}$ may come to a position where the Bragg angle is satisfied.

$\theta - 2\theta$ scan. Separation of lattice tilts and $\boxed{\text{strains}}$

Any region of the specimen which also has lattice parameter $\boxed{d}$ but is tilted with respect to the original region will never provide scattering which reaches the detector;

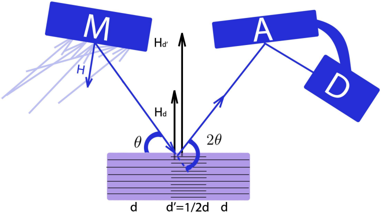


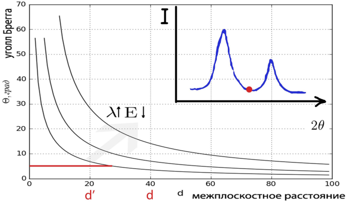


However, another region of the sample with lattice parameter $\boxed{d}$ may come to a position where the Bragg angle is satisfied.

$\theta - 2\theta$ scan. Separation of lattice tilts and $\boxed{\text{strains}}$

Any region of the specimen which also has lattice parameter $\boxed{\text{d}}$ but is tilted with respect to the original region will never provide scattering which reaches the detector;

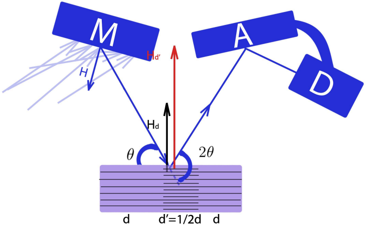


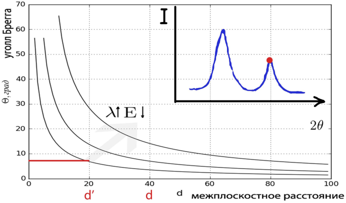


However, another region of the sample with lattice parameter $\boxed{\text{d}}$ may come to a position where the Bragg angle is satisfied.

$\theta - 2\theta$ scan. Separation of lattice tilts and $\boxed{\text{strains}}$

Any region of the specimen which also has lattice parameter d but is tilted with respect to the original region will never provide scattering which reaches the detector;

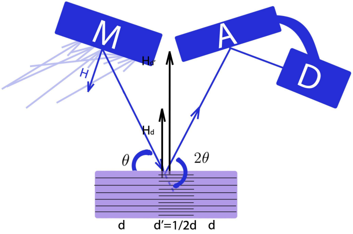


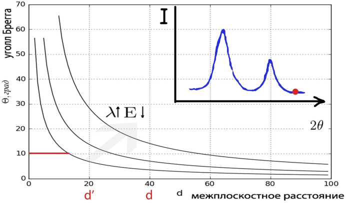


However, another region of the sample with lattice parameter $\boxed{\text{d}}$ may come to a position where the Bragg angle is s§tisfied.

$\theta - 2\theta$ scan. Separation of lattice tilts and $\boxed{\text{strains}}$

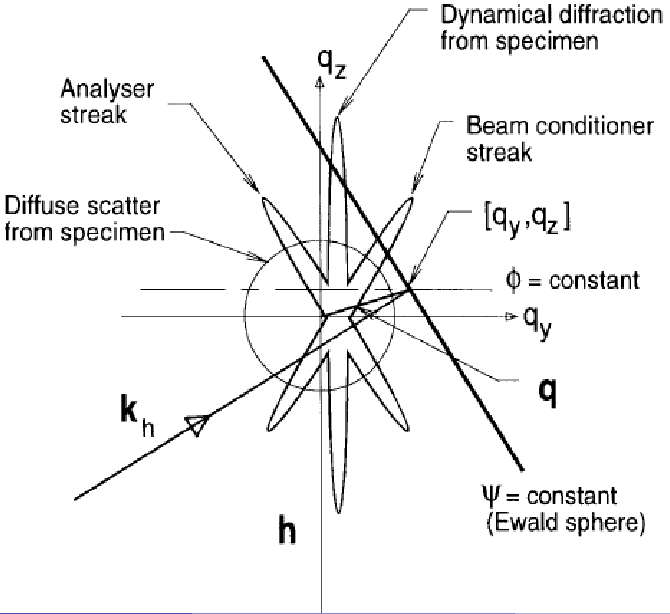
Any region of the specimen which also has lattice parameter $\boxed{\text{d}}$ but is tilted with respect to the original region will never provide scattering which reaches the detector;





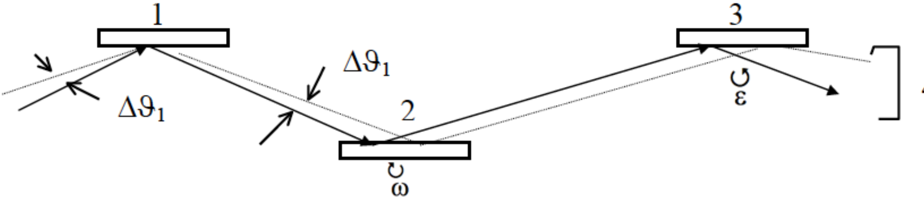
However, another region of the sample with lattice parameter $\boxed{\text{d}}$ may come to a position where the Bragg angle is satisfied.

A scattering map in reciprocal space.



Total intensity

$$\mathrm{I}(\varepsilon, \omega, \Delta\theta_1) = \int_{-\infty}^{\infty} \mathrm{R}_1(\Delta\theta_1)\mathrm{R}_2(\Delta\theta_1 + \omega)\mathrm{R}_3(\Delta\theta_1 + 2\omega - \varepsilon) \cdot \mathbf{d}\Delta\theta_1 \quad (9)$$



CASE A $\boxed{|\omega| \gg \Delta\theta_{\mathrm{B}}}$

where, $\Delta\theta_{\mathrm{B}}$ - full width at half maximum, abbreviated as FWHM

- $\Delta\theta_1 = 0$ – the condition for maximum intensity from the monochromator

$$\mathrm{I}(\varepsilon, \omega, 0) = \int\limits_{-\infty}^{\infty} \mathrm{R}_1(0)\mathrm{R}_2(\omega)\mathrm{R}_3(2\omega - \varepsilon) \cdot \mathbf{d}\Delta\theta_1$$

Maximum intensity for the specimen is $\varepsilon = 2\omega$ (take in to account the condition $|\omega| \gg \Delta\theta_{\mathrm{B}}$) - $\boxed{\text{MAIN PEAK (MP)}}$

$$\mathrm{I}_{\mathrm{MP}}^{\max} = \mathrm{R}_1(0)\mathrm{R}_2(\omega)\mathrm{R}_3(0) \cdot \mathbf{d}\Delta\theta_1$$

The MP intensity is defined by the intensity $\mathrm{R}_2(\omega)$ on the ROCKING CURVE tail for the specimen

CASE A $\boxed{|\omega| \gg \Delta\theta_B}$

- $\Delta\theta_1 = -\omega$ - the condition for maximum intensity from the specimen
  c Maximum intensity is $\varepsilon = \omega$ -
  $\boxed{\text{PSEUDO-PEAK (PP) or MONOCHROMATOR PSEUDO-PEAK}}$

$$\mathrm{I}_{\mathrm{PPM}}^{\max} = \mathrm{R}_1(-\omega)\mathrm{R}_2(0)\mathrm{R}_3(0) \cdot \mathbf{d}\boldsymbol{\Delta}\theta_1$$

The PP intensity is defined by the intensity $\mathrm{R}_1(-\omega)$ on the ROCKING CURVE tail for the monochromator

CASE B $\boxed{|\varepsilon| \gg \Delta\theta_{\mathrm{B}}}$

- $\Delta\theta_1 = 0$

$$\mathrm{I}(\varepsilon, \omega, 0) = \int\limits_{-\infty}^{\infty} \mathrm{R}_1(0)\mathrm{R}_2(\omega)\mathrm{R}_3(2\omega - \varepsilon) \cdot \mathbf{d}\Delta\theta_1$$

There are two conditiond to have maximima

- $\omega = 0$ - $\mathrm{R}_3(-\varepsilon)$ $\boxed{\text{ANALYSER PSEUDO-PEAK}}$ - realize on the ROCKING CURVE tail for the analyser

$$\mathrm{I}_{\mathrm{PPA}} = \mathrm{R}_1(0)\mathrm{R}_2(0)\mathrm{R}_3(-\varepsilon) \cdot \mathbf{d}\Delta\theta_1$$

- $\omega = \varepsilon/2$ $\boxed{\text{MAIN PEAK}}$

$$\mathrm{I}_{\mathrm{PPA}} = \mathrm{R}_1(0)\mathrm{R}_2(\varepsilon/2)\mathrm{R}_3(0) \cdot \mathbf{d}\Delta\theta_1$$

CASE B $\boxed{|\varepsilon| \gg \Delta\theta_{\mathrm{B}}}$

- $\Delta\theta = -\varepsilon$

$$\mathrm{I_{PPM}} = \mathrm{R_1}(-\varepsilon)\mathrm{R_2}(\omega - \varepsilon)\mathrm{R_3}(2\omega - 2\varepsilon) \cdot \mathbf{d}\boldsymbol{\Delta}\theta_1$$

the condition for maximum intensity $\omega = \varepsilon$
The pseudo-peak is defined by the intensity on the ROCKING CURVE tail for the monochromator

$$\mathrm{I_{PPM}^{max}} = \mathrm{R_1}(-\varepsilon)\mathrm{R_2}(0)\mathrm{R_3}(0) \cdot \mathbf{d}\boldsymbol{\Delta}\theta_1$$

CASE C $\theta/2\theta$ - scan $\boxed{\varepsilon = 2\omega}$

incipient questions

Here I will ask you for some questions.

References

[1] Bowen D.K., Tanner B.K. High resolution X-ray Diffractometry and Topography p.169