Optimizing Conditions Suited for Stress Determinations in Q-Space Focusing Configurations

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During the last decade a new concept of high-resolution focusing configuration has been developed, [1], [2], [3], which proved to be an alternative to the existing conventional configuration. According to these general principles a crystal neutron diffractometer focusing configuration was realised, with the following general characteristics:

- the absence of the Soller collimators
- the use of the bent crystals in asymmetric reflexion as monochromators
- a take-off angle of the monochromatic beam around 90^{o}
- high resolution obtained for all values of the scattering angles by exploiting the focusing effects
- use of a plate-like sample properly rotated during the diffraction pattern raising to fulfill the focusing condition

If such a focusing configuration is to be used for stress determinations, special problems arise. As, for a given scattering angle, thin peaks are obtained only for a certain position of the sample, severe limitations appears in choosing the scattering angle or in amount of information possible to be obtained.

A convenient solution is to limit the dimensions of the sample zone for which strain determinations are realised. That means not only the use of corresponding diaphragms but also getting real-space focusing at sample position.

In conclusion if strain determinations are to be realized using focusing configuration both real space focusing at sample position and the phase-space focusing getting thin diffraction peaks must be obtained. The corresponding focusing conditions are deduced in this paper for three neutron diffractometer configurations: crystal diffractometer, 2 crystals diffractometer and time-of-flight diffractoemeter using steady-state neutron source.

1. Crystal neutron diffractometer

1.1 **1 crystal monochromator unit**

The considered configuration is given in fig.1. The Bragg constraints are given by:

$$\gamma_0 + \gamma_1 = \frac{2l_m}{R_m} sign\left(\theta_m + \chi_m\right) \tag{1}$$

The configuration geometry gives:

$$L_0\gamma_0 = l_m \sin(\theta_m + \chi_m) - l_0$$
$$L_1\gamma_1 = l_s \cos(\theta_s + \chi_s) + l_m \sin(\theta_m - \chi_m)$$
$$L_2\gamma_2 = l_d - l_s \cos(\theta_s - \chi_s)$$
(2)

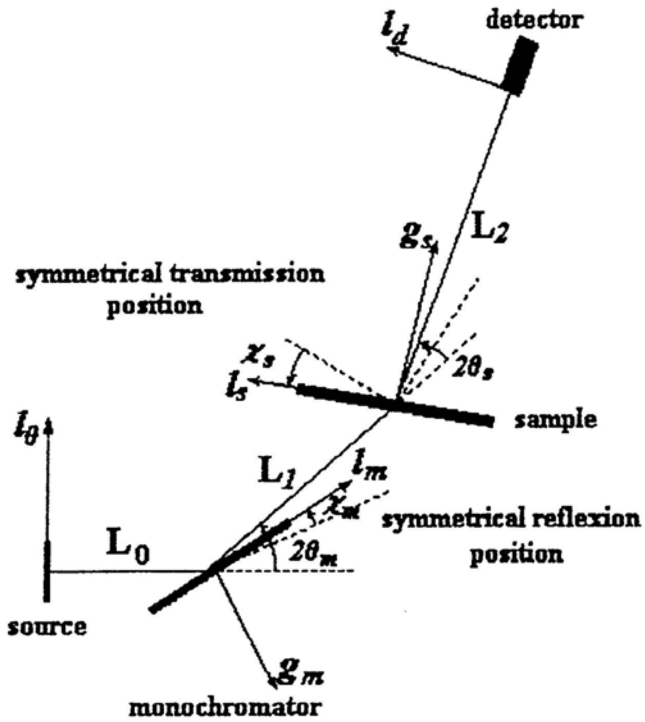

Fig.1 Experimental setup for an one crystal diffractometer

where θ_m and χ_m are the monochromator Bragg angle and the cutting angle respectively, l_i (i= 0, m, s, d) are the widths in the horizontal plane of the source, monochromator sample and detector respectively , R_m is the radius of curvature of the monochromator and Li (i=0, 1, 2) are the distances between source and monochromator, between monochromator and sample and between sample and detector respectively; γ_i are angular variables in the horizontal plane, representing deviations from the most probable values and sign(α) = abs $(\alpha)/\alpha$.

If l_{seff} is the effective sample width (the part of the sample irradiated by the neutrons) in the direction normal to the beam incident on the sample, using (1) and (2) one obtains:

$$l_{seff} = l_m \left[\frac{2L_1}{R_m} sign(\theta_m + \chi_m) - \sin(\theta_m - \chi_m) - \frac{L_1}{L_0} \sin(\theta_m + \chi_m) \right] + l_0 \frac{L_1}{L_0}$$
(3)

The minimum value of l_{seff}, i.e. the minimum width of the beam at the sample position, is obtained cancelling the l_m coefficient. It is obtained:

$$R_m = \frac{2L_1 sign(\theta_m + \chi_m)}{\sin(\theta_m - \chi_m) + \frac{L_1}{L_0}\sin(\theta_m + \chi_m)} \qquad (4)$$

The relation (4) is the real space focusing condition giving the monochromator radius of curvature for which the contribution to the beam width at the sample position given by the monochromator length is compensated.

If we want to have a thin diffraction line for the 2θ value of the scattering angle, the "Q space" focusing condition should be fulfilled, [1], [2], [3] also:

$$R_m = \frac{a}{2a-1}\frac{2L_1 sign(\theta_m + \chi_m)}{\sin(\theta_m - \chi_m)} \quad with\ a = -\frac{\tan\theta_s}{\tan\theta_m} \qquad (5)$$

The value given by the (4) condition depends only on θ_m and χ_m while that given by (5) depends on θ_m , χ_m and θ_s. In order to have the best **conditions for the stress** measurements, both (4) and (5) have to be fulfilled. These two conditions are satisfied, for a given value of θ_m, only for a certain value of the scattering angle given by**:**

$$\tan\theta_s = \frac{\tan(\theta_m)}{1 - \frac{L_1}{L_0}\frac{\sin(\theta_m + \chi_m)}{\sin(\theta_m - \chi_m)}} \qquad (6)$$

1.2. 2 crystals monochromator unit

The considered configuration is given in fig.2. The Bragg constraints are given by:

$$\gamma_0 + \gamma_1 = \frac{2l_{m1}}{R_{m1}} sign(\theta_{m1} + \chi_{m1})$$

$$\gamma_2 + \gamma_1 = \frac{2l_{m2}}{R_{m2}} sign(\theta_{m2} + \chi_{m2}) \qquad (7)$$

The configuration geometry gives:

$$\begin{aligned} L_0\gamma_0 &= l_{m1}\sin(\theta_{m1} + \chi_{m1}) - l_0 \\ L_1\gamma_1 &= l_{m1}\sin(\theta_{m1} - \chi_{m1}) + l_{m2}\sin(\theta_{m2} + \chi_{m2}) \\ L_2\gamma_2 &= l_s\cos(\theta_s + \chi_s) + l_{m2}\sin(\theta_{m2} - \chi_{m2}) \\ L_3\gamma_3 &= l_d - l_s\cos(\theta_s - \chi_s) \end{aligned} \qquad (8)$$

where θ_{m1}, θ_{m2} and χ_{m1}, χ_{m2} are the monochromator Bragg angles and the cutting angles respectively for the two crystals, l_i (i= 0, m1, m2, s, d) are the widths in the horizontal plane of the source, monochromator crystals, sample and detector respectively , R_{m1}, R_{m2} are the radii of curvature of the crystals and Li (i= 0,1,2,3) are the distances between source and the first crystal, between the two crystals, between the second crystal and sample and between sample and detector respectively.

From the two relations (7) results:

$$\gamma_2 - \gamma_0 = \frac{2l_{m2}}{R_{m2}} sign(\theta_{m2} + \chi_{m2}) - \frac{2l_{m1}}{R_{m1}} sign(\theta_{m1} + \chi_{m1})$$

If the expressions of γ_2, γ_0, from (8) are introduced in this relation, on obtains:

$$l_{seff} = l_{m2}\left[\frac{2L_2}{R_{m2}} sign(\theta_{m2} + \chi_{m2}) - \sin(\theta_{m2} - \chi_{m2})\right] + l_{m1}\left[-\frac{2L_2}{R_{m1}} sign(\theta_{m1} + \chi_{m1}) + \frac{L_2}{L_0}\sin(\theta_{m1} + \chi_{m1})\right] + l_0\frac{L_2}{L_0}$$

The minimum value of l_{seff}, i.e. the minimum width of the beam at the sample position, is obtained cancelling the l_{m1}, l_{m2} coefficients. It is obtained:

$$R_{m1} = \frac{2L_0 sign(\theta_{m1} + \chi_{m1})}{\sin(\theta_{m1} + \chi_{m1})} \tag{9}$$

$$R_{m2} = \frac{2L_2 sign(\theta_{m2} + \chi_{m2})}{\sin(\theta_{m2} - \chi_{m2})} \tag{10}$$

The relations (9), (10) are the real space focusing conditions giving the crystals radii of curvature for which the contribution to the beam width at the sample position given by the corresponding crystal length is compensated.

If we want to have a thin diffraction line for the 2θ value of the scattering angle, the "Q space" focusing conditions should be fulfilled also:

$$R_{m1} = \frac{a_m L_1}{a_m - 1}\frac{sign(\theta_{m1} + \chi_{m1})}{\sin(\theta_{m1} - \chi_{m1})} \quad with\ a_m = -\frac{\tan\theta_{m2}}{\tan\theta_{m1}} \tag{11}$$

$$R_{m2} = -\frac{L_1}{a_m - 1}\frac{sign(\theta_{m2} + \chi_{m2})}{\sin(\theta_{m2} + \chi_{m2})} \tag{12}$$

In order to have the best conditions for the stress measurements, both (9) and (11) respectively (10) and (12) have to be fulfilled. From (9) and (11) one obtains:

$$\frac{2L_0}{L_1} = \frac{a_m}{a_m - 1}\frac{\sin(\theta_{m1} + \chi_{m1})}{\sin(\theta_{m1} - \chi_{m1})} \tag{13}$$

From (10) and (12) one obtains:

$$\frac{2L_2}{L_1} = -\frac{1}{a_m - 1}\frac{\sin(\theta_{m2} - \chi_{m2})}{\sin(\theta_{m2} + \chi_{m2})} \tag{14}$$

Both (13) and (14) are fulfilled for a certain relation between θ_{m1}, θ_{m2}, χ_{m1}, χ_{m2} given by:

$$\frac{L_0}{L_2}\frac{\tan\theta_{m2} - \tan\chi_{m2}}{\tan\theta_{m1} + \tan\chi_{m1}} = \frac{\tan\theta_{m2}}{\tan\theta_{m1}}\frac{\tan\theta_{m2} + \tan\chi_{m2}}{\tan\theta_{m1} - \tan\chi_{m1}} \tag{15}$$

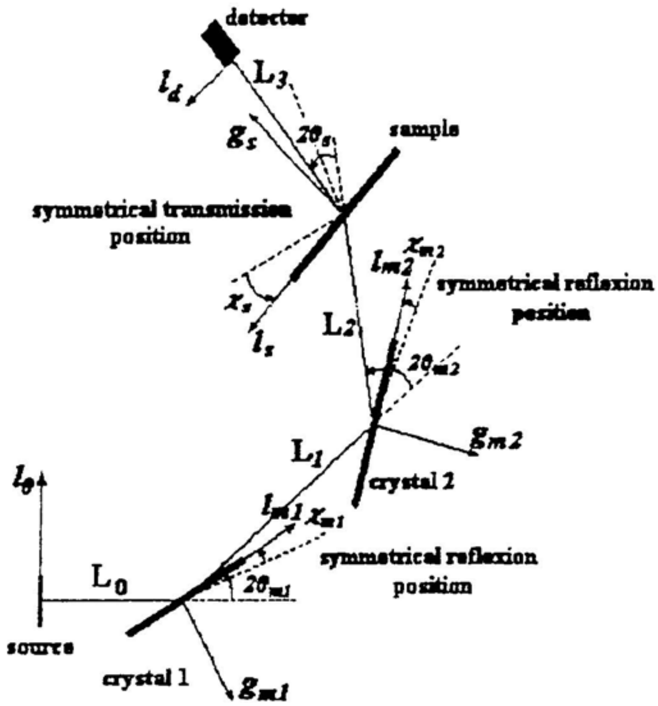

Fig.2 Experimental setup for a two crystals diffractometer

2. TOF diffractometer with steady state source (with chopper)

The considered configuration is given in fig.3. The corresponding constraints are given by:

$$t_0 = \frac{\gamma_1}{\omega} \qquad \gamma_0 = -\gamma_1 \tag{16}$$

The configuration geometry gives:

$$\begin{aligned} L_0\gamma_0 &= l_{ch} - l_0 \\ L_1\gamma_1 &= l_s\cos(\theta_s + \chi_s) - l_{ch} \\ L_2\gamma_2 &= l_d\cos\chi_d - l_s\cos(\theta_s - \chi_s) \end{aligned} \tag{17}$$

Li (i=0, 1, 2) are the distances between source and chopper, between chopper and sample and between sample and between sample and detector respectively; t_0 is the moment when the neutron passes the chopper center while ω is the chopper angular velocity, l_i (i= 0, ch, s, d) are the widths in the horizontal plane of the source, chopper sample and detector respectively, γ_i are angular variables in the horizontal plane.

If l_{seff} is the effective sample width (the part of the sample irradiated by the neutrons) in the direction normal to the beam incident on the sample, using (16) and (17) one obtains:

$$l_{seff} = l_{ch}\left(-\frac{L_1}{L_0}+1\right)+l_0\frac{L_1}{L_0} \tag{18}$$

The minimum value of l_{seff}, i.e. the minimum width of the beam at the sample position, is obtained cancelling the l_{ch} coefficient. It is obtained:

$$L_1 = L_0 \tag{19}$$

The relation (19) is the real space focusing condition for which the contribution to the beam width at the sample position given by the chopper length is compensated.

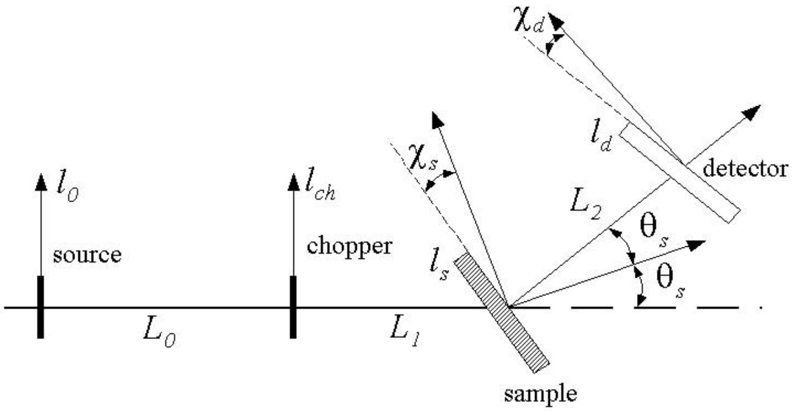

Fig.3 The experimental setup for a steady state source TOF diffractometer

The “Q space” focusing conditions should be fulfilled also:

$$\tan\theta_s = -\frac{m\omega}{hk_0}(L_1+L_2) \tag{20}$$

(21)

where ω is the chopper angular speed, m is the neutron mass, h is the Plank constant, χ_d is the detector inclination angle and L is $L_1 + L_2$.

The condition involving the sample angular position is not important; only the sample dimension in the horizontal plane (the dimensions of the sample region for which the residual stress is determined) should not exceed 5 mm.

References

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et**3] I. Ionita, A.D. Stoica, M. Popovici, N.C. Popa, Design for a focusing high-resolution neutron crystal diffractometer,** ***Nucl. Instr. and Meth.***, **A 431, 1999, pp509-520.**
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