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Fixed exit DC-monochromator of *general position* for Side Beam Line

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Abstract

We develop an idea of fixed exit double-crystal monochromator of general position, *in which the lines of entering and exit beams (both being fixed) do not lie in one plane, i.e., are in general position.*

Both cases of identical and not identical crystals are considered, and exact solutions are obtained. Special attention is paid to the case of small lattice mismatch between first and second crystal (e.g. due to temperature difference) and small "skew" (that is to say, an angle between skew lines of entrance and exit beams is much less than unity).

We derive also some useful formulations describing beam profile change after two reflections (whose reflection planes are non-parallel). At last, possible designing approach for such a skew DC-mono is briefly discussed.

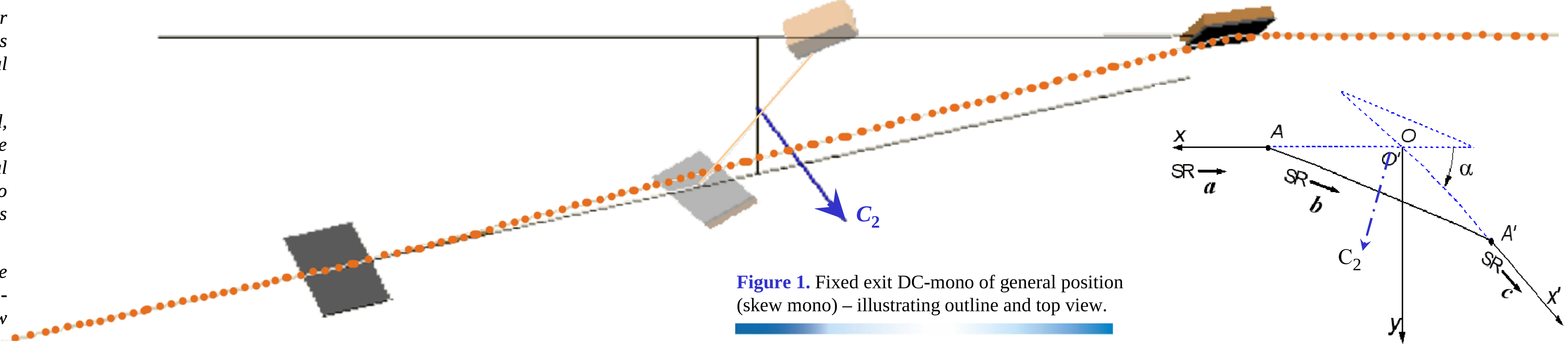


Figure 1. Fixed exit DC-mono of general position (skew mono) – illustrating outline and top view.

1. Introduction

Side beam lines of synchrotron radiation use as a rule single crystal monochromator providing monochromatic beam of a fixed energy (or energy can vary only in a very small range) [1]. The new functionality of energy tuning in a side beam line could be an important quality or feature raising user value of a side beam line (and multiplying the use of an insertion device and storage ring as well). The possible way to attain this feature is a fixed exit double crystal monochromator of *general position* (or skew DC-mono where lines of entering and exit beams do not lie in one plane) considered in this paper. As we will show, this gives the opportunity that the first and the second crystal to be not identical.

Therefore, such a crystal pair as Di(111) [Di is for diamond] and Ge(220), or Si(hkl) and Ge(hkl) could be used – without third optical element (mirror or multilayer) required in plane arrangement in order to compensate the lattice mismatch between crystals [2]. The desire to use not identical crystals is explainable by the fact that the first and the second crystals are working under very different thermal loads and should meet different requirements (especially when the second crystal is in use for sagittal focusing).

As we will see, in (slightly) skew monochromator with equal crystals, small changes of lattice spacing because of thermal expansion of the first crystal could be compensated through small corrections in crystals' positions and orientations. We believe that radiant cooling of (or heat abstraction from) the first crystal could be preferable in some conditions, especially having in view forthcoming synchrotron radiation sources of forth generation.

Such a not-planar approach to DC-mono setup opens up evident possibility to have a set of skew monochromators shedding rays of different energy on the same sample.

2. Skew DC-monochromator (with fixed exit)

Let us consider two skew lines in Figure 1, x and x', which indicate incoming and outgoing light beams and serve as guide lines (or rail guides) for two ideal mirrors placed at points A and A'. It is possible to orientate the first mirror in such a way that to throw reflected light spot to the point A'; in turn, the second mirror can be oriented to redirect double-reflected light beam along outgoing line x'.

If mirrors are not ideal, but instead some ordinary crystals serve to reflect x-rays, then their angles of reflection (Bragg angles) should be coordinated to match their pass bands. This requirement leads to one equation for x and x' having a form $F(x, x')=0$. So the crystal positions should be coordinated according to this equation.

Let the minimal length between skew lines x and x' (i.e., between points O and O', see Figure 1) is taken as a unit of length: $h=1$. Then we obtain the following coordinates for the points A and A':

$$A=(x,0,0), \qquad A'=(-x'\cos\alpha,\ x'\sin\alpha,\ 1); \tag{1}$$

here x (and x') is a length measured from the origin O (and O'), that is a length of the line segment A-O; angle α is a skew angle formed by projection of skew lines along the segment O-O'.

Using (1) we find the unit vectors along parts of beam trajectory, see Figure 1:

$$\vec{a}=(-1,\ 0,\ 0), \quad \vec{b}=\frac{(-x-x'\cos\alpha,\ x'\sin\alpha,\ 1)}{\sqrt{x^2+x'^2+2xx'\cos\alpha+1}}, \quad \vec{c}=(-\cos\alpha,\ \sin\alpha,\ 0) \tag{2}$$

The equations for Bragg angle θ and roll angle φ (conceived as the angle between reflection plane,

$$\{\vec{a},\ \vec{b}\}, \quad (0,\ x'\sin\alpha,\ 1)\in\{\vec{a},\ \vec{b}\},$$

and xz–plane) of the first crystal are now obtained easily using Eq. (2):

$$2\sin^2\theta=1-(\vec{a}\cdot\vec{b})=1-\frac{x+x'\cos\alpha}{\sqrt{x^2+x'^2+2xx'\cos\alpha+1}}, \qquad \tan\varphi=x'\sin\alpha \tag{3}$$

Similar equations are valid for primed angles of the second crystal (it is necessary just to replace primed and unprimed values excepting α). Pass bands of two crystals will be matched if

$$\lambda=\lambda', \text{ where } \lambda=2d\sin\theta,\ \ \lambda'=2d'\sin\theta',$$

or

$$\sin^2\theta=q^2\sin^2\theta', \quad \text{where } q=d'/d. \tag{4}$$

Here d and d' are lattice spacing of first and second crystal, respectively.

This match condition fixes x' as a function of x (or vice versa). However, there are values of parameters α and q, that solution of Eq. (4) is absent. For example, in the case of $\alpha=0$, $q\neq1$ substitution of these values to Eq. (4) leads to the equation which obviously has no solution (well, in real numbers):

$$\sqrt{(x+x')^2+1}=x+x'.$$

On the other hand, the special case $\alpha=0$, $q=1$ admits any combination x, x' as solution of match condition, Eq. (4); this is a feature concerned with additional symmetry of whole system – translations along parallel lines x, x' (which lie now in one plane). It is due to this extra-symmetry that one crystal of the pair can be fixed as it takes place in usual fixed-exit double-crystal monochromator (in nondispersive setting). It is obvious, however, that this special case with its extra-symmetry is not stable with respect to small deviation $\delta d=d-d'$ (due to temperature difference between crystals and their thermal expansion).

2.1. Identical Crystals

In the case of equal crystals, when $d=d'$, we have easy solution of Eq. (4):

$$x=x',\ \theta=\theta',\ \varphi=\varphi'$$

and hence [see Eqs. (3), (4)]

$$\sin\theta=\sqrt{\frac{1}{2}-\frac{x(1+\cos\alpha)}{\sqrt{8x^2(1+\cos\alpha)+4}}}, \quad \tan\varphi=x\sin\alpha. \tag{5}$$

This solution keeps the symmetry C_2 with symmetry axis being the bisector of adjacent angle, $\pi-\alpha$; see Figure 1.

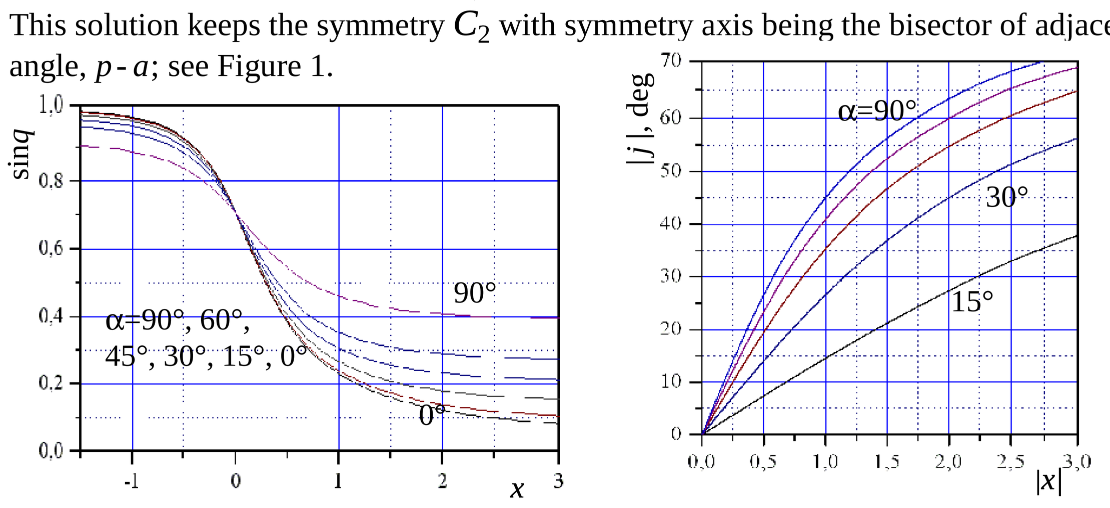


Figure 2a and **2b** show $\sin\theta\,(x)$ and $\varphi\,(x)$; Eq. (5) is in use with different values of α.

Considering limits $x\to\pm\infty$ in Eq. (5), one can find the possible range of Bragg angle depending on the skew angle α:

$$\theta_-=\theta_{min}=\alpha/4,\ \ \theta_+=\theta_{max}=\pi/2-\alpha/4,\ \ \Delta\theta=(\pi-\alpha)/2, \tag{6}$$

So we see that an increase in skew angle α leads to decrease in the range of available Bragg angle. In general case ($q\neq1$), this range will also depend on q; above-mentioned absence of solution of Eq. (4) in the case $q=1$ means that this available range is empty.

2.2. Not identical Crystals

In general case, Eq. (4) yields [using Eq. (3)]

$$\sqrt{x^2+x'^2+2xx'\cos\alpha+1}=x+x'+k\,(qx-x'/q), \tag{7}$$

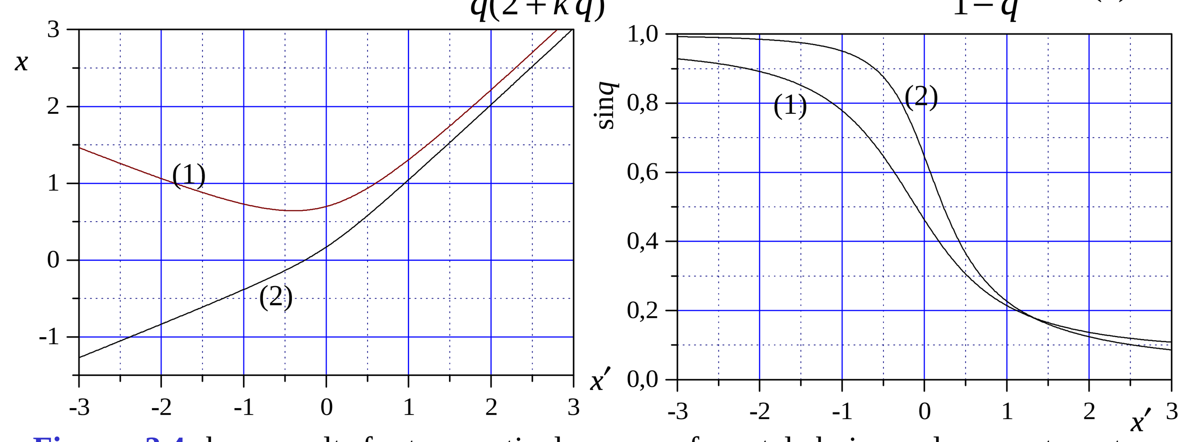
we introduce here parameter $k=(1-\cos\alpha)/(1/q-q)$. This equation (7) still has symmetry – namely with respect to the replacement: $x\leftrightarrow x',\ q\to1/q\ \ (k\to-k)$. Because of this symmetry we will assume further that $q<1$, and hence $k>0$.

Elimination of the radical in Eq. (7) leads to the following quadratic:

$$x^2k\,q(k\,q+2)-2k^2xx'-x'^2(2-k/q)k/q-1=0\,. \tag{8}$$

Using x' as independent (or control) variable, one can find the exact solution (only positive branch is correct – superfluous brunch arises because of previous radical elimination):

$$x=x(x';q,\alpha)=\frac{k\,x'+\sqrt{q(q+2/k)+4x'^2\cos^2(\alpha/2)}}{q(2+k\,q)}, \quad k=q\frac{1-\cos\alpha}{1-q^2} \tag{9}$$

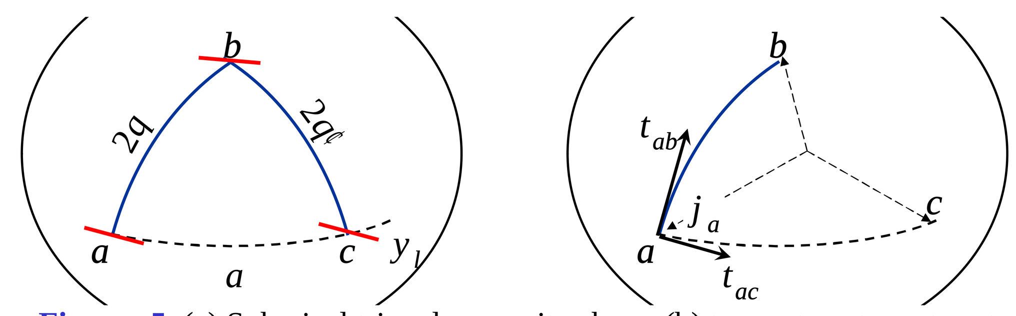


Figures 3,4 show results for two particular cases of crystal choice and parameter set:
(1) Diamond(111) and Ge(220): $q=0.971$, $\alpha=0.3$ (17.2°), $k=0.77$
(2) Identical crystals having different temperature: $q=1-5\cdot10^{-4}$, $\alpha=0.1$, $k=5$

3. Beam Profile issue

Let us assume that the initial white beam has fan-like form, and its width is much greater than its height. As a result of two reflections in skew monochromator, the beam profile line (and beam polarization as well, but it is some more complicated issue) will be turned on a small angle, ψ_l. Let us consider sphere of unit radius with the ends of vectors ***a***, ***b***, ***c*** (their starting points coincide with the centre of sphere), see Fig. 5a. The strokes at triangle vertexes indicate beam profile line. The arcs of spherical triangle have the following lengths: $\overset{\circ}{ab}=2\theta$, $\overset{\circ}{bc}=2\theta'$, $\overset{\circ}{ac}=\alpha$.

Let's find the angles of this triangle, $\varphi_a, \varphi_b, \varphi_c$, where φ_a is the angle at the triangle vertex ***a***. Note that the case of small angle φ_b is close to nondispersive (+,-)-setting, while large value of this angle corresponds to dispersive (+,+)-setting. Consider unit vectors t_{ab}, t_{ac}, tangent at vertex ***a*** to arcs (*ab*) and (*ac*), respectively, see Fig.5b.



Figures 5. (a) Spherical triangle on unit sphere; (b) tangent vectors at vertex ***a***.

It is easy to find that

$$\vec{t}_{ab}=\frac{\vec{b}-\vec{a}(\vec{a}\cdot\vec{b})}{\sqrt{1-(\vec{a}\cdot\vec{b})^2}}, \quad \vec{t}_{ac}=\frac{\vec{c}-\vec{a}(\vec{a}\cdot\vec{c})}{\sqrt{1-(\vec{a}\cdot\vec{c})^2}}$$

hence we are now about to obtain φ_a (and other angles – in a similar way):

$$\cos\varphi_a=(\vec{t}_{ab}\cdot\vec{t}_{ac})=\frac{(\vec{b}\cdot\vec{c})-(\vec{a}\cdot\vec{b})(\vec{a}\cdot\vec{c})}{\sqrt{1-(\vec{a}\cdot\vec{b})^2}\sqrt{1-(\vec{a}\cdot\vec{c})^2}}=\frac{\cos2\theta'-\cos2\theta\ \cos\alpha}{\sin\alpha\ \sin2\theta}\,. \tag{11}$$

The angle between the beam stroke and reflection arc (e.g. arc (*ab*) for the first reflection) does not change during reflection; in other words, the stroke is parallel translated along arc which is geodesic line on the unit sphere. The result of two translations along arcs (*ab*) and (*bc*) will some differ from the result of single parallel translation along (*ac*), and this difference is equal to the target angle ψ_l. This angle has simple relation to the angles of spherical triangle, Eq. (11), or to its area:

$$\psi_l=\varphi_a+\varphi_b+\varphi_c-\pi=S_{abc}$$

In the case of identical crystals (isosceles spherical triangle), one can obtain the next compact equation:

$$\sin(\psi_l/2)=\tan(\alpha/2)\frac{\sqrt{\sin^2 2\theta-\sin^2(\alpha/2)}}{1+\cos2\theta}.$$

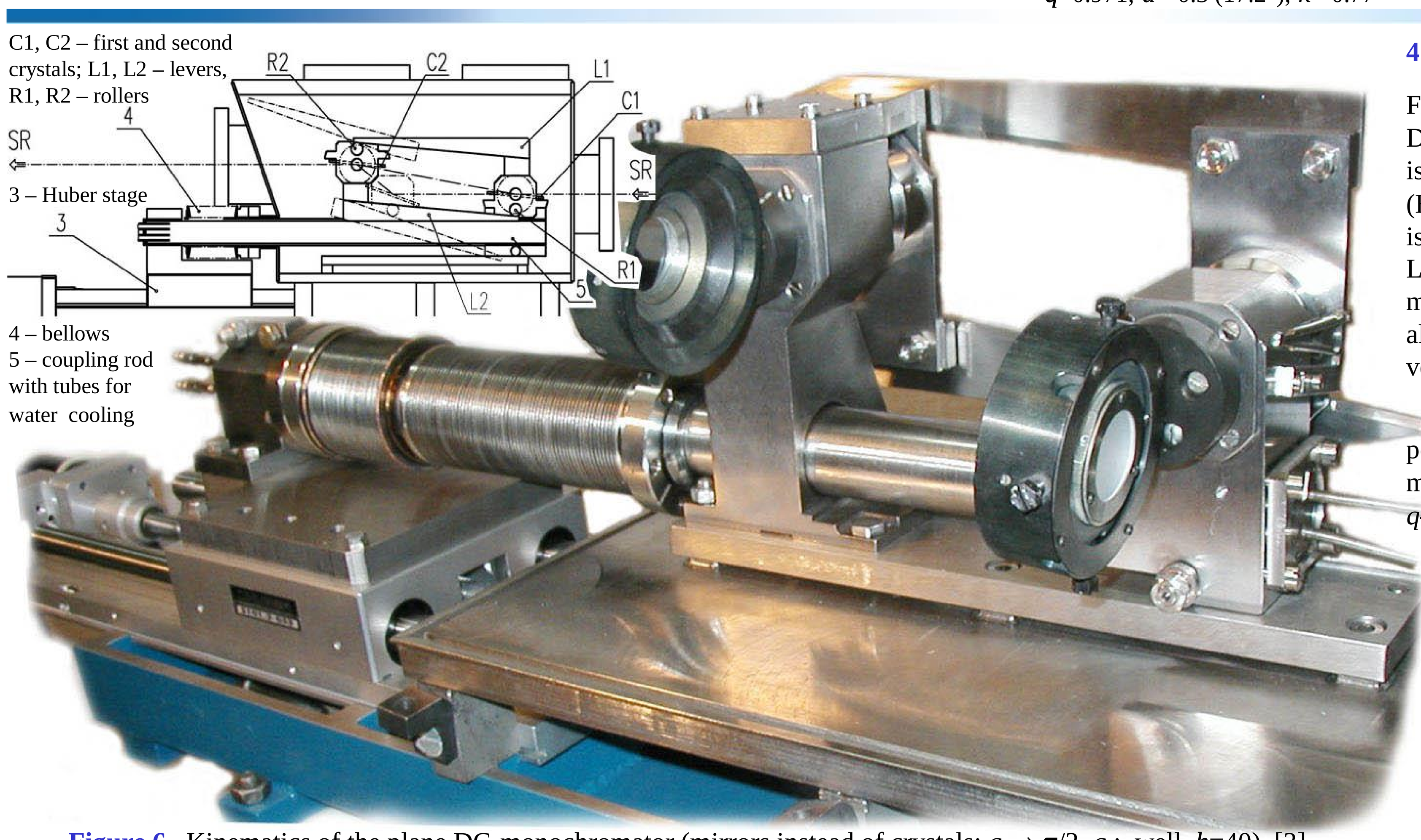


Figure 6. Kinematics of the plane DC-monochromator (mirrors instead of crystals; $\theta\to\pi/2-\theta$; well, $h=40$) [3].

4. Possible Design Approach

Figure 6 shows the kinematics of ultra-high vacuum DC-monochromator (with *practically* fixed exit) which is under construction now in Siberian SR centre [3]. (Here "practically" means that relative deviation $\Delta h/h$ is about $3\cdot10^{-4}$ for Bragg-angle range $5°<\theta<18.5°$. Less range gives less deviation.) The source of movement in this kinematics is linear positioner, and all the most crucial surfaces of parts of construction are very simple, plane or cylinder surface.

We believe that similar approach with two linear positioners could be applied to design of skew DC-mono. There is a dilemma which angle is the first: θ–angle or φ–angle, see Eq. (3) and Fig. 1. One choice is outlined in the Figure 7.

5. References

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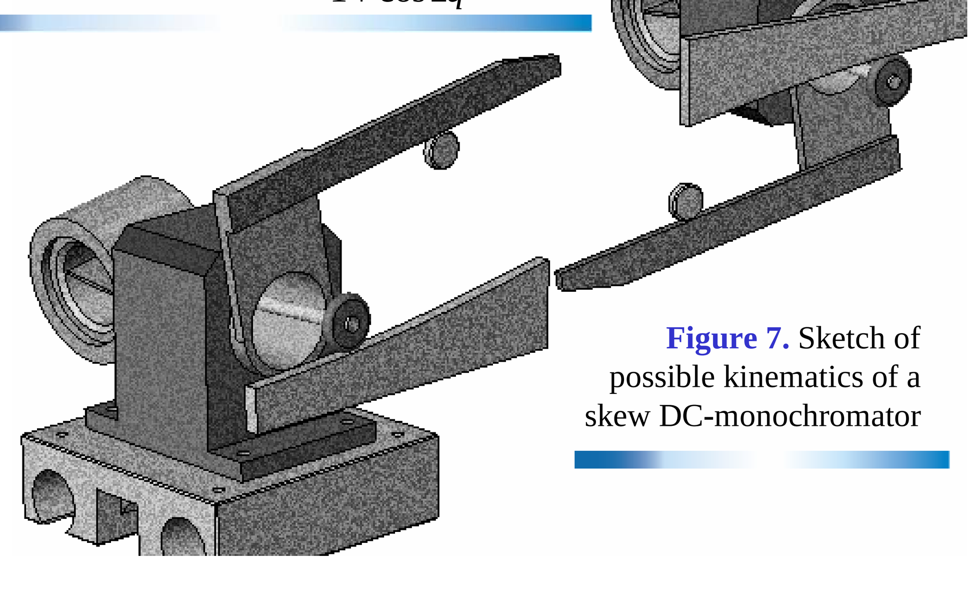

Figure 7. Sketch of possible kinematics of a skew DC-monochromator