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An extension of the precise method of Kunzl and Köppel for determining the constants of a crystal grating.

F. Bouchal and V. Dolejšek, Praha.

(Recieved August 28, 1934.)

Just as Kunzl and Köppel have derived and experimentally verified a new precise method for determining the constants of a crystal grating from the Pavelka's equation, we have applied the equation of Valouch and deduced from it a new precise method serving the same purpose. Thereby the scope of the Kunzl and Köppel's method has been greatly enlarged. Another advantage of the new method is that the same fictive values of the grating constant are derived, as it is done using directly the Bragg's law, but with greater accuracy.

Some time ago, Kunzl and Köppel¹) have worked out a new method for the precise determination of the constants of crystal grating which in some cases yields better results than other precise methods. The principle of it — firstly used by Pavelka²) and Valouch³) — consists in measuring the difference between two glancing angles instead of measuring the glancing angle itself, as it is usually done. Let us denote by $\varphi_{m,\mu}$ the glancing angle corresponding to the spectral line of the wave length λ_{μ} in the m^{th} order and by $\varphi_{n,\nu}$ the glancing angle belonging to the line of the wave length λ_{ν} in the n^{th} order. Then we have according to the simple Bragg's law

$$m\lambda_{\mu}=2d\sin\,\varphi_{m,\mu},\quad n\lambda_{\nu}=2d\sin\,\varphi_{n,\nu},$$

and from it the following equation for the grating constant d may be deduced

$$\sin \varphi_{n,\nu} = \frac{n\lambda_{\nu}}{2d} = \frac{\sin \varkappa}{\sqrt{a^2 - 2a\cos \varkappa + 1}},$$
 (1)

V. Kunzl and J. Köppel: C. R. 196 (1933), 787; 196 (1933) 940; Casopis 63 (1934), 109; Journ. de Phys. 5 (1934), 145.
 A. Pavelka: Bull. de l'Acad. de Sc. de Bohême 28 (1927), 442.
 M. A. Valouch: Bull. de l'Acad. de So. de Bohême 28 (1927), 31.

$$a=rac{m\lambda_{\mu}}{n\lambda_{
u}} \quad ext{and} \quad arkappa=arphi_{m,\mu}-arphi_{n,
u}.$$

Pavelka has measured the angle \varkappa in two different orders but using the same spectral line $(m + n, \lambda_{\mu} = \lambda_{\nu})$, while Valouch's measurements were performed in the same order but with different lines $(\dot{m}=n, \lambda_{\mu}+\lambda_{\nu}).$

Owing to the fact that the Bragg's equation does not hold exactly and the values of the grating constant d derived from it vary with the spectral order, both these methods yield only approximate values of d. Pavelka's method gives the values depending not only on m and n but also on λ and Kunzl and Köppel⁴) have deduced an equation enabling us to calculate from approximate values of d obtained by the Pavelka's method the true values of a grating constant. They have determined by this method the constant of the rhomboidal surface of a quartz crystal (1011) measuring the angles z in a way similar to the Siegbahn's precise method for determining glancing angles. In this connection we wish to point out that with the Kunzl and Köppel's method it is possible to determine directly the true constant of a crystal grating, without a knowledge of the index of refraction of the X-rays and without the aid of the theory of Lorentz.

Values of d obtained by the Valouch's method $(m = n, \lambda_{\mu} + \lambda_{\nu})$ depend only on n and are identical with the fictive grating constants d_n derived from the Bragg's law

$$n\lambda = 2d_n \sin \varphi$$
.

As we have shown elsewhere, 5) they can be calculated directly from the measurements of the angle \varkappa by means of the equation

$$d_n = \frac{1}{4}n \left[\left(\frac{\lambda_{\nu} - \lambda_{\mu}}{\sin \frac{1}{2} \varkappa} \right)^2 + \left(\frac{\lambda_{\nu} + \lambda_{\mu}}{\cos \frac{1}{2} \varkappa} \right)^2 \right]^{\frac{1}{2}}. \tag{2}$$

The true grating constant d_{∞} is given by the known relation

$$d_n = d_\infty \left(1 - \frac{4d^2_\infty \delta}{n^2 \lambda^2}\right).$$

The equation (2) affords us a new possibility of precise determination of constants of crystal grating. The precision of this new method may be seen from measurements made by us on the rhomboidal surface of a quartz crystal. The results of these measurements are given in Tables 1 and 2; Table 1 contains the measurements

V. Kunzl and J. Köppel: Časopis 68 (1934), 109; Journ. d. Phys. 5 (1934), 145.
 F. Bouchal and V. Dolejšek: C. R. 199 (1934), 1054.

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Plate	√ mm	ε.	α.	×	<i>∆</i> ×″	× ₁₈	κ_{18} middle
80	0,68323	13' 02.2"	2° 49′ 30,0″	1° 18′ 13,5″	0,1"	1° 18′ 13,6″	
11	0,62698	11, 57,8"	2° 24′ 14,6″	1° 18′ 06,2″	.0,1″	1° 18′ 06,3″ ·	
13	0,65273	12' 27.2"	2° 24′ 54,4″	1° 18′ 10,8″	0,2″	1° 18′ 11,0″	·
14	0,64888	12, 22,9"	2° 24′ 07,1″	1° 18′ 15,0″	0,2″	1° 18′ 15,2″	
15	1,09765	20' 55.7"	2° 15′ 24,3″	1° 18′ 10,0″	0,2"	1° 18′ 10,2″	
19	1,12812	21, 31,3"	2° 14′ 40,0″	1° 18′ 05,7″	.0,1"	1° 18′ 05,8″	e.
21	2,81391	53' 40,7"	1° 42′ 34,0″	1° 18′ 07,5″	0,1″	1° 18′ 07,6″	
22	0,29452	5' 37,8"	2° 42′ 06,0″	1° 18′ 14,1″	0,5″	1° 18′ 14,3″	* Section 19 Section 1
23	0.70308	13' 24.9"	2° 49′ 55.0″	1° 18′ 15,0″	0,1″	1° 18′ 15,1″	$1^{\circ} 18' 11,0''$
24	0.78524	14' 58.9"	2° 51′ 27.9″	1° 18′ 14,5″	0,1"	1° 18′ 14,6″	⊢ 0,9
26	0,41440	7' 54,4"	2° 28′ 28,0″	1° 18′ 11,2″	0,2″	1° 18′ 11,4″	
29	0,38693	7, 23,0"	$2^{\circ} 28' 51,4''$. 1° 18′ 07,2″	0,3″	1° 18′ 07,5″	
30	0,55272	10' 32,7"	2° 46′ 52,9″	1° 18′ 10,1″	0,2″	1° 18′ 10,3″	
31	0,54455	10' 23,4"	2° 46' 45,2"	1° 18′ 10,9″	0,2″	1° 18′ 11,1″	

Table 2.

				Table z.			
Plate	J mm	3	×	×	7 κ"	×18	κ ₁₈ middle
62	0.53976	10′ 17″	28,	49,	0.3″	49'	
63	0,61460	11' 44"	27'	49,	0,3″	49′	
64	0.5463	10' 25"	28,	49,	0,3″	49'	27
65	0,7098	13, 32"	25'	49'	0,3″	49′	
	0,75796	14' 28"	25'	49,	0.3″	49'	
67	0,49797	9, 30"	29'	49,	0,3″	49,	*:
. 89	0,7357	14' 02"	25'	49,	0,3″	49'	
69	0,5222	9, 28,	5° 29' 40,0"	2° 49′ 49,0″	0,3″	49′	
70	0.7820	14' 55"	5° 24′ 35.2″	2° 49′ 45.1″	0.3″	2° 49′ 45.4″	2° 49′ 45,9″
	0.49727	9, 29,	5° 30′ 07.0″	2° 49′ 48,0″	0.2″	49′	0,1.∺
72	0.72096	, C 13' 43"	25,	49	0,3″	49′	
	0.5253	10' 02"	29	49	0,3″	49′	=
14	0.77096	14' 43"	24	49,	0,3″	49′	
	0.5177	9' 53"	29'	49,	0.3″	49′	

n the first order, Table 2 those in the second order. In the first columns the numbers of the plates are given, in the second we have noted the differences Δ between both lines measured on the plates in millimeters, in the third the corresponding values ε in degrees, in the fourth the values α of the angles measured on the scale of the spectrometer, the relation between ε , α and ε being given by the equation

$$\varkappa = \frac{1}{2}(\alpha + \varepsilon).$$

The values of \varkappa thus obtained and corrected to temperature of 18°C are given in the following columns. The last column contains the middle value of \varkappa_{18} . For these measurements the following waves have been chosen:

Cu K
$$\alpha_1$$
 $\lambda = 1537,395$ X. U. Cu K β_1 $\lambda = 1389,3$ X. U.

Values of the constants of quartz crystal grating calculated from these results by means of equation (2) are in good agreement with those found by Kunzl and Köppel as it is shown below:

Bouchal-Dolejšek	Kunzl-Köppel
$d_1 = 3336,11 \text{ X. U.}$	$d_1 = 3336,09 \text{ X. U.}$
$d_2 = 3336,46 \text{ X. U.}$	$d_2 = 3336,49 \text{ X. U.}$
$d_{\infty} = 3336,62 \text{ X. U.}$	$d_{\infty} = 3336,63 \; \mathrm{X. \; U.}$

There are some special advantages in the measurement of crystal grating according to our new method. The errors due to the displacement of the crystal caused by lack of adjustment or by temperature changes, or due to the displacement of the centre of gravity of spectral lines are eliminated to a much greater extent than in the method of measuring directly the glancing angles. They are eliminated even more than in the Kunzl and Köppel's method.

The insignificance of the error due to a possible displacement of the reflecting surface can be seen from the following. We have purposely displaced the quartz crystal by 0,1 mm from the position in which it had been fixed during the mentioned measurements, though such a big displacement cannot occur in a precise work. The deviation δ of the angle \varkappa caused by the displacement x can be calculated by the equation

$$\delta = -\frac{4x}{r} \frac{(\lambda_{\nu} + \lambda_{\mu}) \sin^2 \frac{1}{2} \varkappa}{[(\lambda_{\nu} - \lambda_{\mu})^2 \cos^2 \frac{1}{2} \varkappa + (\lambda_{\nu} + \lambda_{\mu})^2 \sin^2 \frac{1}{2} \varkappa]^{\frac{1}{2}}}$$

where r denotes the radius of curvature of the spectrograph. The deviations δ from the values \varkappa contained in Tables 1 and 2 calculated for r=180,17 mm, x=0,1 mm are given in the sixth column of Table 3. The corresponding measured differences between the

Table 3.

Order	Lines	, 2	;x
II	$\begin{array}{c} \mathrm{Cu}\; (\mathrm{K}\alpha_1 -\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!$		' 11,0" ' 45,9"
×*	$\Delta \varkappa = \varkappa - \varkappa^x$	δ	$\Delta \varphi$
1° 18′ 10,	,3 " 0,7"	0,57"	112"
2° 49′ 43.	.6" 2,3"	2,47''	103"

angles \varkappa (the third column) and the angles \varkappa^* with a displaced crystal (the fourth column) are in the fifth column. The last column of Table 3 contains the corresponding deviations of the glancing angles φ . A comparison shows that deviations of the angles \varkappa due to the displacement of the crystal are decidedly insignificant, when compared with deviations of the glancing angles. In the same way it can be easily seen that deviations of the angles \varkappa due to temperature changes are considerably less than those of the angles φ under the same conditions.

Our method can also be applied for determining the accuracy of adjustment. Thus for instance Siegbahn and Dolejšek⁶) have obtained for the constant of the prism surface of quartz grating in the first order

$$d_1 = 4246,64 \text{ X. U.},$$

while Berquist⁷) using a new and very precise tubus spectrometer of Siegbahn has found

$$d_1 = 4244,92 \text{ X. U.}$$

There is an unexpected difference between these values and it can be shown that it is due only to the displacement error in the Siegbahn and Dolejšek's measurements. They have determined the glancing angles for the K lines of Cu, Fe and Cr and obtained the following values:

	λ	$φ_{18^{0}}$ C
Cu Ka ₁	1537,30	100 25' 39,7"
Fe $K\alpha_1$	1932,30	130 8' 56,1"
$\operatorname{Cr} \mathbf{K}\alpha_1$	2284,84	150 36' 29,7".

From them we can calculate the corresponding values of \varkappa in each case and with the help of equation (2) we get

$$d_1 = 4244,26 \text{ X. U.}$$

This is in a fair agreement with the Berquist's value for d_1 . There is however one more point to consider: The values of the wave

⁶⁾ M. Siegbahn and V. Dolejšek: Zeitschr. f. Phys. 10 (1922), 159.

⁷⁾ O. Berquist: Zeitschr. f. Phys. 66 (1930), 494.

lengths of Cu $K\alpha_1$ and Fe $K\alpha_1$ used by Berquist are a little different from those used by Siegbahn and Dolejšek. Taking it into consideration we obtain by equation (2)

$$d_1 = 4244,92 \text{ X. U.}$$

This agrees within the limits of error of observation with the above mentioned Berquist's value. The accuracy of Berquist's measurements can be similarly controlled by our equation (2).

When controlling the precision of some measurements with equation (2) we have to regard the following: In the case that the angles φ_{Cu} and φ_{Fe} have been measured each with a different adjustment or generally with different errors of crystal, the adjustment errors are not the same and cannot be eliminated. But even in this case, the difference between the results derived from equation (2) and those derived from the equation where the glancing angle is used shows that there exists an error in the measurements. This condition is essential for the possibility of determining the angle \varkappa from two measured glancing angles φ , instead of directly measuring the angle \varkappa . We know from the data given by Siegbahn that the tubus spectrometer should be independent on adjustment and that in the vacuum spectrometer the possible accuracy of the adjustment of a crystal is about 0,001 mm or more.

In the former case (Siegbahn-Dolejšek), where the adjustment was the same in all three cases (Cu, Fe, Cr), we can firstly determine the adjustment error x by comparing the results calculated by equation (2) with those derived from the Bragg's equation. As a result we have found x = 0.018 mm. Of the two results, one obtained be equation (2) and the other by the Bragg's equation, the former is nearly correct, in as much as in this case the adjustment error is practically eliminated, as shown in Table 3.

By comparing the mentioned results with those obtained by Berquist with the tubus spectrometer, we see that the validity of our assertion is verified. By comparing the Berquist's results after equation (2) with the results derived directly by the help of Bragg's equation, we obtain two results which differ. This shows undisputably that there exists an error in the measurements. If it appeared from adjustment, the adjustment error should be 0,004 mm. It cannot be verified if this error is due to an irregularity in the used crystal or to an error in the reading of the glancing angle or to same other errors. It is certain that the difference of both results — equation (2) and Bragg's equation — can only be caused by the fact that different errors having influence on the measurements manifest themselves differently in both equations.

Our results prove that there are many possibilities for the improvement of the scope of the Kunzl and Köppel's method.