Debye-Scherrer diffraction patterns of powder samples with three cubic Bravais lattices

Physics | Modern Physics | Production & use of X-rays

Difficulty level	Group size	Preparation time	Execution time
hard	2	45+ minutes	45+ minutes

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General information

Application

Setup

Most applications of X rays are based on their ability to pass through matter. Since this ability is dependent on the density of the matter, imaging of the interior of objects and even peaple becomes possible. This has wide usage in fields such as medicine or security.

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Other information (1/2)

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Prior knowledge

The prior knowledge required for this experiment is found in the Theory section.

Main principle

Polycrystalline powder samples, which crystallize in the three cubic Bravais types, simple, face-centered and body-centered, are irradiated with the radiation from a X-ray tube with a copper anode. A swivelling Geiger-Mueller counter tube detects the radiation that is constructively reflected from the various lattice planes of the crystallites. The Bragg diagrams are automatically recorded. Their evaluation gives the assignment of the Bragg lines to the individual lattice planes, their spacings as well as the lattice constants of the samples, and so also the corresponding Bravais lattice type.

Other information (2/2)

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Learning objective

The goal of this experiment is to get to investigate Debeye-Scherrer patterns for Bragg-Brentano-geometry.

Tasks

1. Record the intensity of the Cu-X-rays back scattered by the four cubic crystal powder samples with various Bravais lattice types as a function of the scattering angle.
2. Calculate the lattice plane spacings appropriate to the angular positions of the individual Bragg lines.
3. Assign the Bragg reflections to the respective lattice planes. Determine the lattice constants of the samples and their Bravais lattice types.
4. Determine the number of atoms in the unit cell.

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Theory (1/5)

When X-rays of wavelength λ strike a mass of lattice planes of a crystal of spacing d at a glancing angle of θ, then the reflected rays will only be subject to constructive interference when Bragg's condition is fulfilled, i.e.:

$2\mathrm{d}\sin(\theta) = \mathrm{n}\lambda$ (n = 1, 2, 3, ...)   (1)

Bragg's condition implies that all of the waves scattered at the atom are in phase and so amplify each other, whereas partial waves that are scattered in directions not fulfilling Bragg's conditions are of opposite phase and so extinguish each other. A more realistic way of looking at this must, however take the actual phase relationships of all of the partial waves scattered by the atom in a certain direction into consideration. When there are N atoms in a unit cell, then the total amplitude of the X-rays scattered by the cell is described by the structure factor F, which is calculated by summing up the atomic scattering factors f of the individual N atoms, taking their phases into account.

Theory (2/5)

In general, the following is valid for F:

$\mathrm{F_{hkl}} = \sum_1^{\mathrm{N}} \mathrm{f_n} \cdot e^{2\pi i(\mathrm{hu_n+kv_n+lw_n})}$ (2)

where h, k, l = Miller indices of the reflecting lattice planes and $\mathrm{u_n}$, $\mathrm{v_n}$, $\mathrm{w_n}$ are the coordinates of the atoms in fractions of the particular edge lengths of the unit cell. As F is in general a complex number, the total scattered intensity is described by $|\mathrm{F_{hkl}}|^2$.

A cubic simple unit cell contains only one atom with the coordinates 000. According to equation (2), therefore, the structure factor F for this lattice type is given by:

$\mathrm{F} = \mathrm{f} \cdot e^{2\pi i(0)} = \mathrm{f};\ |\mathrm{F}|^2 = \mathrm{f}^2$ (3)

This means that F^2 is independent of h, k and l and all Bragg reflections can therefore occur.

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Theory (3/5)

The unit cell of a cubic face-centered lattice has 4 atoms at 000, ½ ½ 0, ½ 0 ½ and 0 ½ ½. The unit cell of a cubic body-centered lattice has in comparison only 2 atoms at 000 and ½ ½ ½. When the lattice only consists of one sort of atom, then the following conditions are valid for the structure factor:

fcc Lattice

$|\mathrm{F}|^2 = 16\mathrm{f}^2$, with hkl only even or only odd; $|\mathrm{F}|^2 = 0$ with hkl mixed.

bcc Lattice

$|\mathrm{F}|^2 = 4\mathrm{f}^2$, with (h+k+l) even; $|\mathrm{F}|^2 = 0$ with (h+k+l) odd (4)

Theory (4/5)

The situation is somewhat different when a lattice is made up of different sorts of atoms.

When, for example, an fcc lattice consists of the atoms A and B, whereby the A atoms lie at 000, ½ ½ 0, ½ 0 ½ and 0 ½ ½ , and the B atoms at ½ ½ ½ , 0 0 ½ , 0 ½ 0 and ½ 0 0, then the following additional condition is given for the structure factor F:

fcc Lattice with atoms A and B:

$|\mathrm{F}|^2 = 16(\mathrm{f_A} + \mathrm{f_B})^2$, with (h+k+l) even; $|\mathrm{F}|^2 = 16(\mathrm{f_A} - \mathrm{f_B})^2$ with (h+k+l) odd (5)

In such fcc lattices, when the atomic scattering factors f of the two atoms are almost equal ($\mathrm{f_A} \approx \mathrm{f_B}$), then 111 reflections will only be very weak, if they occur at all.

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Theory (5/5)

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For the cubic crystal system, the spacing d of the individual lattice planes with the indices (hkl) is obtained from the quadratic form:

$\frac{1}{d_{hkl}} = \frac{1}{a}(h^2 + k^2 + l^2)$ (a = lattice constant) (6)

From this and equation (1), with n = 1, the quadratic Bragg equation is obtained:

$\sin^2(\theta) = \frac{\lambda^2}{4a^2}(h^2 + k^2 + l^2)$ (7)

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Equipment

Position	Material	Item No.	Quantity
1	XR 4.0 expert unit, 35 kV	09057-99	1
2	XR 4.0 X-ray goniometer	09057-10	1
3	XR4 X-ray Plug-in Cu tube	09057-51	1
4	XR 4.0 X-ray structural analysis upgrade set	09145-88	1
5	Ammonium chloride 250 g	30024-25	1
6	Potassium chloride 250 g	30098-25	1
7	Potassium bromide, 100 g	30258-10	1
8	Molybdenum, Powder, 99,7%, 100 g	31767-10	1
9	Vaseline 100 g	30238-10	1

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Setup and Procedure

Setup

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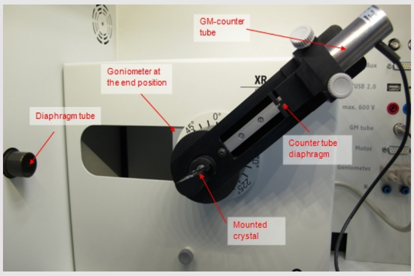
Connect the goniometer and the Geiger-Müller counter tube to their respective sockets in the experiment chamber (see the red markings in Fig. 1). The goniometer block with the analyser crystal should be located at the end position on the right-hand side. Fasten the Geiger-Müller counter tube with its holder to the back stop of the guide rails. Do not forget to install the diaphragm in front of the counter tube (see Fig. 2). Insert a diaphragm tube with a diameter of 2 mm into the beam outlet of the tube plug-in unit.

For calibration: Make sure, that the correct crystal is entered in the goniometer parameters. Then, select “Menu”, “Goniometer”, “Autocalibration”. The device now determines the optimal positions of the crystal and the goniometer to each other and then the positions of the peaks.

← Fig. 1: Connectors in the experiment chamber

↓ Fig. 2: Set-up of the goniometer



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Procedure (1/4)

- Connect the X-ray unit via the USB cable to the USB port of your computer (the correct port of the X-ray unit is marked in Figure 3).
- Start the “measure” program. A virtual X-ray unit will be displayed on the screen.
- You can control the X-ray unit by clicking the various features on and under the virtual X-ray unit. Alternatively, you can also change the parameters at the real X-ray unit. The program will automatically adopt the settings.

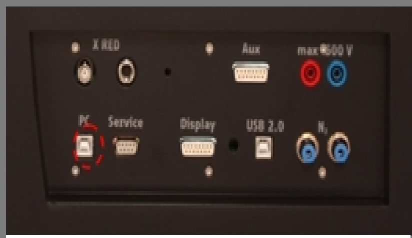

Fig. 3: Connection of the computer

Procedure (2/4)

Fig. 4: Part of the user interface of the software

- Click the experiment chamber (see the red marking in Fig. 4) to change the parameters for the experiment.
- If you click the X-ray tube (see the red marking in Figure 4), you can change the voltage and current of the X-ray tube. Select the settings as shown in Figure 5.

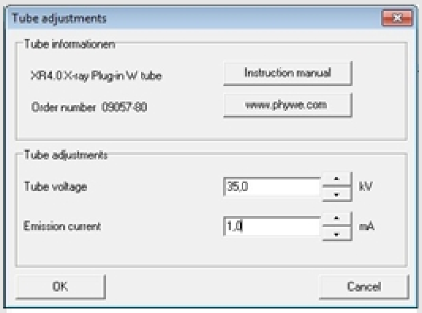

Fig 5: Voltage and current settings

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Procedure (3/4)

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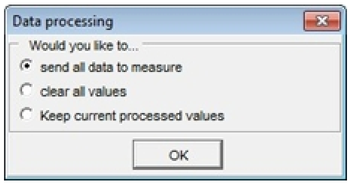
- Start the measurement by clicking the red circle: 

- After the measurement, the following window appears:



- Select the first item and confirm by clicking OK. The measured values will now be transferred directly to the "measure" software.
- At the end of this manual, you will find a brief introduction to the evaluation of the resulting spectra.

Procedure (4/4)

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Sample preparation:

The sample must be so finely powdered that no grains can be felt when a little of it is rubbed between finger and thumb. A relatively high sample concentration can be obtained by mixing the powder with a little vaseline. To do this, transfer a small amount of the sample onto a sheet of paper and use a spatula to knead it to a firm paste. To achieve the highest concentration of material as possible, use very little vaseline (a spatula tip of it). Fill the relatively solid sample paste into the specimen for powder samples and smooth it flush. Use the universal crystal holder to hold the specimen.

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Evaluation

Examination of fcc lattices (1/10)

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Potassium bromide

Fig. 6 shows the Debye-Scherrer spectrum of potassium bromide (KBr).

As no filter is used for the monochromatization of the X-rays, when individual lines are evaluated consideration must be given to the fact that the very intense lines that result from K_α-radiation are accompanied by secondary lines that result from the weaker K_β radiation. These pairs of lines can be identified by means of equation (1). It is namely approximately true with $\lambda(\mathrm{K}_\alpha) = 154.18\,\mathrm{pm}$and $\lambda(\mathrm{K}_\beta) = 139.22\,\mathrm{pm}$:

$$\frac{\lambda(\mathrm{K}_\alpha)}{\lambda(\mathrm{K}_\beta)} = \frac{\sin(\theta_\alpha)}{\sin(\theta_{beta})} \approx 1.1 \qquad (8)$$

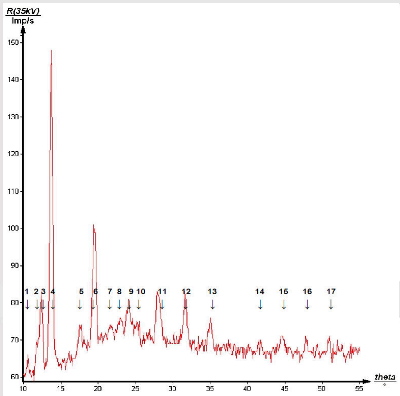

Fig. 6: Bragg $\mathrm{Cu}-\mathrm{K}_\alpha$ and $\mathrm{Cu}-\mathrm{K}_\beta$ lines of KBr.

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Examination of fcc lattices (2/10)

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These values correspond to the quotients of the sinq values (Fig. 6) of the pairs of lines 2-1, 4-3, 6-5 and 9-7, showing that the lines 1, 3, 5 and 7 originate from the CuK_β radiation.

The correctness of this conclusion can be shown by a control measurement (see Fig. 7) using the diaphragm tube with nickel foil to reduce the intensity of the K_β radiation. The reflexes in Fig. 6 that were previously assigned to the K_β lines are no longer to be seen. As the intensity of the K_β-radiation is also somewhat weakened by the Ni foil, the detection of reflexes of weak intensity at larger glancing angles is made difficult when this is used.

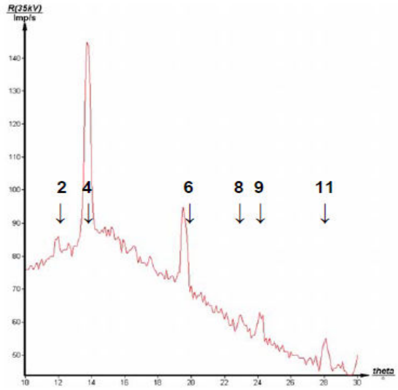

Fig. 7: Bragg-diagram of KBr only with $\mathrm{Cu}-\mathrm{K}_\alpha$ beam (a nickel filter was used here)

Examination of fcc lattices (3/10)

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The following method for evaluating the spectrum is given as an example, and is representative for that for the spectra of other samples. First determine the $\sin(\theta)$ and $\sin^2(\theta)$ values for each individual reflex from the angle of diffraction θ of the particular line. From equation (7), the ratios of the observed $\sin^2(\theta)$ values must be representable by the ratios of the sums of the squares of the three integer numbers(h, k, l).

The ratios of the $\sin^2(\theta)$ values of the individual lines (n) to the $\sin^2(\theta)$ value of the first line (2) are calculated as in column J of Table 1. The numbering in column E relates to the reflex lines indicated in Fig. 6. In column A, all of the possible hkl numbers are listed. Columns B, C and D show the individual ratios of the sums of squares of these numbers.

When an attempt is made to allot the indices 100 or 110 to the first reflexes, then no agreement with the ratios of the $\sin^2(\theta)$ values is found. When the index 111 is assigned to the first line, however, then all of the other lines can be assigned hkl index triplets with a certain accuracy.

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Examination of fcc lattices (4/10)

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A	B	C	D	E	F	G	H	I	J	K	L
hkl	$h^2+k^2+l^2$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{011}}$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{111}}$	Reflex no.	Intensity	ϑ/°	$\sin\vartheta$	$\sin^2\vartheta$	$\frac{\sin^2\vartheta(n)}{\sin^2\vartheta(2)}$	d / pm	a / pm
100	1										
110	2	1									
111	3	1,5	**1**	2	w	11,80	0,20449	0,04182	**1,00**	377,0	652,9
200	4	2	**1,33**	4	vs	13,72	0,23718	0,05625	**1,34**	325,0	650,1
210	5	2,5	1,67								
211	6	3	2								
220	8	4	**2,67**	6	vs	19,46	0,33315	0,11099	**2,65**	231,4	654,5
221/300	9	4,5	3								
310	10	5	3,33								
311	11	5,5	**3,67**	8	w	22,95	0,38993	0,15204	**3,64**	197,7	655,7
222	12	6	**4**	9	s	24,08	0,40801	0,16647	**3,98**	188,9	654,5
320	13	6,5	4,33								
321	14	7	4,67								
400	16	8	**5,33**	11	s	27,97	0,46901	0,21997	**5,26**	164,4	657,5
410/322	17	8,5	5,67								
441/330	18	9	6								
331	19	9,5	6,22								
420	20	10	**6,67**	12	s	31,69	0,52532	0,27596	**6,60**	146,8	656,3
421	21	10,5	7								
332	22	11	7,33								
422	24	12	**8**	13	s	35,03	0,57401	0,32948	**7,88**	134,3	657,9
500/430	25	12,5	8,33								
510/431	26	13	8,67								
511/333	27	13,5	9								
520/432	29	14,5	9,67								
521	30	15	10								
440	32	16	**10,67**	14	vw	41,61	0,66406	0,44097	**10,54**	116,1	656,7
522/441	33	16,5	11								
530/433	34	17	11,33								
531	35	17,5	**11,67**	15	w	44,56	0,70166	0,49232	**11,77**	109,9	650,0
600/442	36	18	12								
610	37	18,5	12,33								
611/532	38	19	12,67								
620	40	20	**13,33**	16	w	47,86	0,74151	0,54983	**13,15**	104,0	657,5
621/540/443	41	20,5	13,67								
541	42	21	14								
533	43	21,5	14,33								
622	44	22	**14,67**	17	w	50,91	0,77656	0,60242	**14,40**	99,3	658,5

Table 1: Evaluation of the K_α -Debye-Scherrer lines of KBr.

Examination of fcc lattices (5/10)

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Only even or odd numbers are now given, no mixed indices hkl triplets. According to this, KBr forms an fcc lattice. The corresponding lattice plane spacings d, calculated using equation (1), are given in column K. Values for the lattice constant a determined from equation (6) are given in column L. Taking both the K_α lines and the K_β lines into consideration, the mean value of the lattice constant a is found to be:

$\mathrm{a} = (655.1 \pm 2.9)\,\mathrm{pm}; \Delta(\mathrm{a})/\mathrm{a} < 0.5\%$ (literature value a = 658.0 pm)

On dividing the total mass M of a unit cell by its volume V, the density ρ is given, so that:

$$\rho = \frac{\mathrm{M}}{\mathrm{V}} = \mathrm{n} \cdot \mathrm{m} \cdot \frac{1}{\mathrm{a}^3} \text{ with } \mathrm{m} = \frac{\mathrm{m_A}}{\mathrm{N}} \rightarrow \mathrm{n} = \frac{\rho \cdot \mathrm{N} \cdot \mathrm{a}^3}{\mathrm{m_A}} \qquad (9)$$

where n = the number of atoms or molecules in the unit cell; m = atomic/molecular mass; $\mathrm{m_A}$ = atomic/molecular weight; N = $6.022 \cdot 10^{23}$ = Avogadro's number.

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Examination of fcc lattices (6/10)

A	B	C	D	E	F	G	H	I	J	K	L
hkl	$h^2+k^2+l^2$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{011}}$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{111}}$	Ref-lex no.	In-ten-sity	$\vartheta/°$	$\sin\vartheta$	$\sin^2\vartheta$	$\frac{\sin^2\vartheta(n)}{\sin^2\vartheta(2)}$	d/ pm	a/ pm
100	1										
110	2	1									
111	3	1,5	1	1	s	10,61	0,18412	0,03390	**1,00**	378,1	652,9
200	4	2	1,33	3	vs	12,38	0,21439	0,04596	**1,36**	324,7	650,1
210	5	2,5	1,67								
211	6	3	2								
220	8	4	2,67	5	s	17,61	0,30254	0,09153	**2,70**	230,1	654,5
221/300	9	4,5	3								
310	10	5	3,33								
311	11	5,5	3,67								
222	12	6	4	7	w	21,73	0,37023	0,13707	**4,04**	188,0	651,3

Table 2: Evaluation of the K_β-Debye-Scherrer lines of KBr.

On entering the appropriate values for KBr, $\rho = 2.75\,g/cm^3$ and $m_A = 119.01\,g$ in equation (9), it follows that $n = 3.91 \approx 4$, i.e. the unit cell contains 4 atoms.

The K_β lines 1, 3, 5 and 7 that occur in Fig. 6 are evaluated in Table 2.

Examination of fcc lattices (7/10)

Potassium chloride

The Debye-Scherrer pattern for potassium chloride (KCl) is shown in Fig. 8, and the evaluation of this with respect to the K_α-radiation is given in Table 3.

The quotients of the sine values of the pairs of lines 2-1, 4-3, 6-5 and 8-7 again give approximately 1.1, so that the lines 1, 3, 5 and 7 can again be assigned to the K_β radiation.

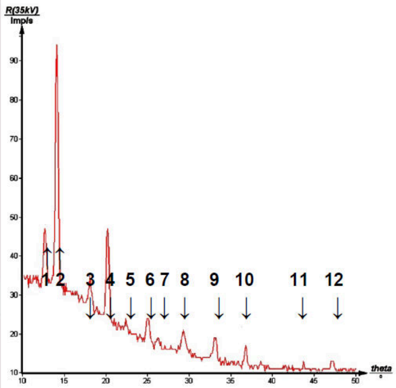

Fig. 8: Bragg $Cu - K_\alpha$ and $Cu - K_\beta$ lines of KCl.

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Examination of fcc lattices (8/10)

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A	*B*	*C*	*D*	*E*	*F*	*G*	*H*	*I*	*J*
h k l	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{002}}$	Reflex no.	Intensity	ϑ/°	sinϑ	sin$^2\vartheta$	$\frac{\sin^2\vartheta(n)}{\sin^2\vartheta(2)}$	*d*/pm	*a*/pm
200	**1**	2	vs	14, 13	0, 24412	0, 05960	**1**	315, 8	631,6
220	**2**	4	vs	20, 22	0, 34562	0, 11946	**2,00**	223, 0	630,9
222	**3**	6	s	25, 02	0, 42293	0, 17887	**3,00**	182, 3	631,4
400	**4**	8	s	29, 30	0, 48938	0, 23950	**4,02**	157, 5	630,1
420	**5**	9	s	33, 10	0, 54610	0, 29823	**5,00**	141, 2	631,5
422	**6**	10	s	36, 80	0, 59902	0, 35883	**6,02**	128, 7	630,5
440	**8**	11	vw	43, 72	0, 69113	0, 47767	**8,01**	111, 5	630,7
600/442	**9**	12	w	47, 16	0, 73326	0, 53766	**9,02**	105, 1	630,6

Table 3: Evaluation of the K_α -Debye-Scherrer lines of KCl.

Examination of fcc lattices (9/10)

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A	*B*	*C*	*D*	*E*	*F*	*G*	*H*	*I*	*J*
h k l	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{002}}$	Reflex no.	Intensity	ϑ/°	sinϑ	sin$^2\vartheta$	$\frac{\sin^2\vartheta(n)}{\sin^2\vartheta(2)}$	*d*/pm	*a*/pm
200	**1**	1	vs	12,71	0,22002	0,04841	**1**	316,4	632,8
220	**2**	3	s	18,12	0,31101	0,09673	**2,00**	223,8	633,1
222	**3**	5	vw	22,40	0,38107	0,14521	**3,00**	182,7	632,8
400	**4**	7	vw	26,25	0,44229	0,19562	**4,04**	157,4	629,6

Table 4: Evaluation of the K_β-Debye-Scherrer lines of KCl.

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Examination of fcc lattices (10/10)

Although KCl forms an fcc lattice, in contrast to KBr it gives exclusively even numbered hkl values and no, as expected for an fcc lattice, odd numbered hkl index triplets (see Tables 3 and 4). This is understandable when one considers that the atomic scattering factor f is correlated directly with the number of electrons of an atom, among others. As KCl, in contrast to KBr, contains atoms with almost the same scattering power (Z = 19 for K and 17 for Cl), it follows from equation (5) that reflexes with odd numbered hkl index triplets should not occur.

The mean value found for lattice constant a in the experiment is: $\mathrm{a} = (631.3 \pm 1.1)\,\mathrm{pm}; \Delta(\mathrm{a})/\mathrm{a} < 0.2\%$ (literature value: a = 629.3 pm).

From the experimentally determined average value for a and the known values for KCl ($\rho = 1.984\,\mathrm{g/cm^3}$ and $\mathrm{m_A} = 74.56\,\mathrm{g}$), it follows from equation (9) that $\mathrm{n} = 4.04 \approx 4$, i.e. that the unit KCl cell contains 4 atoms.

Examination of bcc lattices (1/2)

Fig. 9 shows the spectrum of molybdenum (Mo)

The evaluation in Table 5 shows that agreement with the ratios of the $\sin^2(\theta)$-values can only be given when (h+k+l) is even, i.e. that molybdenum forms a bcc lattice.
The experiment gives an average value for lattice constant a of:
$\mathrm{a} = (314.22 \pm 0.58)\,\mathrm{pm}; \Delta(\mathrm{a})/\mathrm{a} < 0.2\%$ (literature value: a = 314.05 pm).

A bcc lattice should contain 2 atoms per unit cell.

From the experimentall determined average value for a and the known values for Mo ($\rho = 10.2\,\mathrm{g/cm^3}$ and $\mathrm{m_A} = 95.94\,\mathrm{g}$), it follows from equation (9) that $\mathrm{n} = 1.99 \approx 2$, i.e. that the unit Mo cell does actually contain 2 atoms.

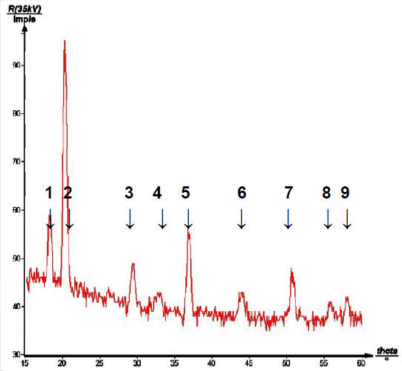

Fig. 9: Bragg $\mathrm{Cu - K_\alpha}$ and $\mathrm{Cu - K_\beta}$ lines of Mo.

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Examination of bcc lattices (2/2)

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A	B	C	D	E	F	G	H	I	J	K
hkl	$h^2+k^2+l^2$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{011}}$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{111}}$	Ref-lex no.	$\vartheta/°$	$\sin\vartheta$	$\sin^2\vartheta$	$\frac{\sin^2\vartheta(n)}{\sin^2\vartheta(2)}$	d/pm	a/pm
110 (β)	2			1	18,33	0,31449	0,09890		221,34	313,03
110	2	**1**		2	20,33	0,34743	0,12071	**1**	221,89	313,78
200	4	**2**	1	3	29,41	0,49106	0,24114	**1,99**	156,99	313,98
211 (β)	6			4	32,87	0,54273	0,29456		128,26	314,17
211	6	**3**	1,67	5	36,89	0,60029	0,36034	**2,99**	128,42	314,57
220	8	**4**	2	6	43,95	0,69403	0,48168	**3,99**	110,08	314,17
310	10	**5**	2,67	7	50,79	0,77483	0,60037	**4,97**	99,49	314,62
222	12	**6**	3,33	9	58,05	0,84851	0,71997	**5,96**	90,85	314,73
321 (β)	14			8	55,80	0,82708	0,68406		84,16	314,91

Table 5: Evaluation of the K_α and K_β-Debye-Scherrer lines of Mo.

Examination of cubic simple (pc)-lattices (1/4)

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Fig. 10 shows the Debye-Scherrer spectrum of ammonium chloride (NH_4Cl), the evaluation of which is given in Table 6.

Line 2 of the spectrum at $\theta = 14.83°$ is not taken into consideration, as the quotient of the $\sin(\theta)$ value of the pairs of lines 3 and 2 is namely sin(16.45°)/sin(15.83°) = 1.11. Line 2 must therefore be assigned to the K_β radiation (see equation (9)).

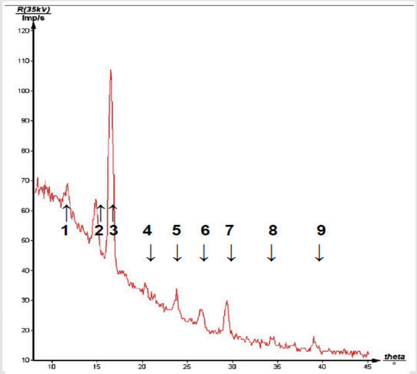

Fig. 10: Bragg $Cu - K_\alpha$ and $Cu - K_\beta$ lines of NH_4Cl.

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Examination of cubic simple (pc)-lattices (2/4)

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The quotient of the $\sin^2(\theta)$ values in column I is always approximately even-numbered, and could so be assigned both to the bold face numbers in column B as well as to column C, so that it is not yet possible to make an unambiguous assignment to the reflex planes.

If assignment to column B should be correct, then mixed index hkl triplets and even-numbered (h + k + l) values would occur. This means that NH_4Cl has neither an fcc lattice nor a bcc lattice, but has rather a cubic simple (pc) cell with a mean lattice constant a (see column K) of $\mathrm{a} = (384.5 \pm 1.7)\,\mathrm{pm}$

If assignment to column C should be correct, then only evennumbered (h + k + l) values would occur.

This would correspond to a bcc lattice with a mean lattice constant a (see column L) of $\mathrm{a}^* = (543.7 \pm 2.2)\,\mathrm{pm}$

Examination of cubic simple (pc)-lattices (3/4)

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A	*B*	*C*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	*L*
hkl	$h^2+k^2+l^2$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{011}}$	$\frac{h^2+k^2+l^2}{(h^2+k^2+l^2)_{111}}$	Ref-lex no.	ϑ/°	sinϑ	sin$^2\vartheta$	$\frac{\sin^2 \vartheta(n)}{\sin^2 \vartheta(2)}$	*d*/ pm	*a*/ pm	*a**/ pm
100	**1**			1	11,61	0,20125	0,04050	**1,00**	383,0	383,0	
110	**2**	**1**		3	16,45	0,28468	0,08105	**2,00**	270,8	383,0	541,6
111	**3**	1,5	1	4	20,34	0,34759	0,12082	**2,98**	221,8	384,1	543,3
200	**4**	**2**	1,33	5	23,79	0,40338	0,16272	**4,02**	191,1	382,2	541,6
210	**5**	2,5	1,67	6	26,51	0,44635	0,19923	**4,92**	172,7	386,2	
211	**6**	**3**	2	7	29,36	0,49030	0,24039	**5,93**	157,2	385,1	543,3
220	**8**	**4**	2,67	8	34,40	0,56497	0,31919	**7,88**	136,4	385,9	540,5
221/300	9	4,5	3								
310	**10**	**5**	3,33	9	39,06	0,63013	0,39707	**9,80**	122,3	386,8	546,1
311	11	5,5	3,67								
222	12	**6**	4								544,6
320	13	6,5	4,33								
321	14	7	4,67								
400	16	**8**	5,33								545,6
410/322	17	8,5	5,67								
441/330	18	9	6								
331	19	9,5	6,22								
420	20	**10**	6,67								546,9

Table 6: Evaluation of the K_α -Debye-Scherrer lines of NH_4Cl.

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Examination of cubic simple (pc)-lattices (4/4)

The following consideration helps to solve this dilemma.

The following values are given in Tables for NH_4Cl : $\rho = 1.527\,g/cm^3$ and $m_A = 53.49\,g$

Using these values and a = 384.5 pm in equation (9), $n = 0.977 \approx 1$, i.e. only one molecule is present in the cell. According to this, NH_4Cl crystallizes cubic, simple.

On repeating this same procedure, but with $a^* = (543.7 \pm 2.2)\,pm$, then n = 2.75 is obtained.

The number of 2¾ molecules in a unit cell can not be brought into accordance with a bcc lattice, as this contains only 2 atoms or molecules. From this it is clear that NH_4Cl forms a cubic simple lattice with the lattice constant $a = (384.5 \pm 1.7)\,pm; \Delta(a)/a \leq 0.5\%$ (Literature value: a = 386.0 pm)

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