

THE STRUCTURE OF SYNTHETIC, METAMICT, AND RECRYSTALLIZED FERGUSONITE

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WITH 3 TEXT FIGURES

The Metamict Minerals.

It is a wellknown fact that some minerals are met with in nature in the metamict condition. These minerals have originally been crystalline but they have been transformed into a glass like, isotropic mass with a conchoidale fracture, though the original external forms of the crystals have remained unchanged.

The term "metamict" has been introduced by W. C. BRØGGER¹. The amorphous substances had by BREITHAUPT, according to their genesis, been divided into the two groups: porodine and hyaline substances. BRØGGER has pointed out that there also exists a third group: the metamict substances. Characteristic metamict minerals (a lot of which only have been found in the metamict condition) are: orthite, gadolinite, samarskite, euxenite, polycrase, pyrochlore, polymignite, æschynite, ytrotantalite, etc. BRØGGER seeks the reason of this transformation in the small degree of stability of the complicated crystal molecules, which commonly are met with in such minerals.

As a matter of fact, this transformation is especially observed in minerals which contain weak bases combined with

¹ Article "Amorph" in Salomonsen's Conversationslexicon (Encyclopedia). Copenhagen 1893.

Ref.: Zeitschr. f. Krist., 25, 427 (1896).

weak acids. The physical explanation of the transformation is given by V. M. GOLDSCHMIDT¹ who assumes that the original space lattice of the crystal has been built of ions; but owing to the weak chemical joints, a subsequent rearrangement of the peripheric electrones has taken place.² In this way, for example in fergusonite $Y \cdots (NbO_4)'''$ is transformed into $Y_2O_3 \cdot Nb_2O_5$.

Characteristic of the metamict minerals is the isotropism, as well as the lack of Röntgen interferences. By ignition of such a mineral it will frequently recrystallize, and the anisotropism, as well as the röntgen interferences, will appear. Simultaneously with the recrystallisation an incandescence will take place, and the specific gravity will increase.

The Metamict Fergusonite.

Fergusonite as mineral is almost only met with in the metamict condition. The only known occurrence of crystalline fergusonite is that of Hundholmen, Norway³.

The fergusonite chosen for these investigations was from Høgtveit, Setesdalen. — Ignited at about 400° C the mineral showed incandescence. Before ignition it showed the following properties:

Colour velvet black with a glass like lustre. In section brown, isotropic. Index of refraction high⁴. No röntgen interferences. After ignition the colour was black with a greenish tinge; in section brown, and anisotropic. A röntgen photograph

¹ Über die Umwandlung krystallisierter Minerale in den metamikten Zustand. (Isotropisierung); Anhang zu "Geochemische Verteilungsgesetze der Elemente" III; Vid.-Selsk. Skr. I, 1924, No. 5.

² Different opinions concerning this transformation have been maintained. Thus A. HAMBERG, J. SCHETELIG, and especially O. MÜGGE thought of a transformation owing to a content of some radioactive substances. (Cfr. O. MÜGGE, Centralbl. f. Min. 1922, 721, 753). But as GOLDSCHMIDT has shown, the transformation is not especially observed in radioactive minerals.

³ TH. VOGT, Centralbl. f. Min., 1911, 373. Neues Jahrb., 9, (1914).

⁴ According to E. S. LARSEN, "Micr. Determ. of Nonopaque Min.". (Bull. U. S. G. S., 679 (1921)) the refractive index of isotropic fergusonite lies at about 2,15. After ignition, however, the index *decreases* to about 2,07.

made according to the powder method, showed interference lines, which were broad and hazy, thus obviously showing a Scherrer effect. By grounding the mineral before ignition, however, a different result was obtained, for after the ignition, the mineral remained in fact perceptibly isotropic; and though the mineral was heated to 800—900° C no birefringence would appear. A powder diagram showed, however, a röntgen pattern which was quite identical with that from the birefringent fergusonite.

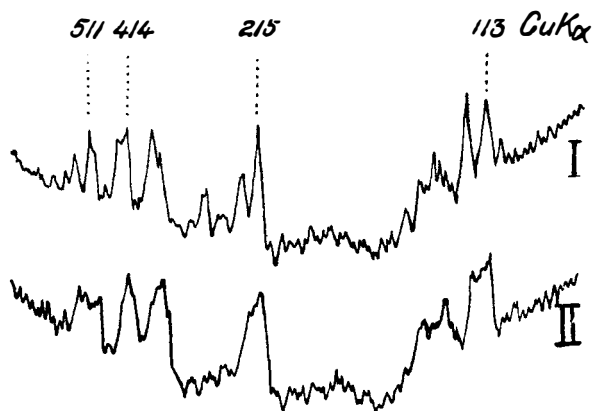


Fig. 1.

I. Regigram of fused fergusonite. II. Regigram of ignited fergusonite.

(The regigrams were made with a photometer from the firm P. J. Kipp & Zonen, Delft, Holland).

Then the fergusonite was fused in an acetylene-oxygen torch and a powder diagram was made. The interference lines were the same as on the other films, but the lines were very distinct without any Scherrer effect (see fig. 1).

From the width of the lines on the films of ignited fergusonite it is possible to calculate the average size, D , of the crystals by using SCHERRER'S formula¹:

$$B = 2 \sqrt{\frac{\ln 2}{\pi}} \cdot \frac{\lambda}{D} \cdot \frac{1}{\cos \varphi}$$

where B is the "half intensity width" of the line, λ is the wave length of the X-rays, and φ the angle of diffraction.

¹ P. SCHERRER, Gött. Nachr., 1918 p. 98.

On the films of fergusonite, for a diffraction angle about 45° , B is about 0,3 mm. (0,01 radians) and hence the average size of the crystalline particles, D , is about $200 \cdot 10^{-8}$ cm. A consequence of this fact is a new explanation of the birefringence of ignited fergusonite; for the crystals formed at the ignition are then so minute, that it is impossible to observe their own birefringence. On that account the ground and ignited fergusonite shows perceptibly isotropic grains, but when giving the röntgen pattern of a tetragonal mineral, this means that the grains must consist of anisotropic, crystalline particles. There appears however a *statistical isotropism*, as a consequence of the haphazard orientation of the particles. The greater grains are anisotropic in owing their birefringence to *strain*, caused by the recrystallisation. This inference is confirmed by the fact that it has been impossible to produce a Laue pattern from an ignited splinter of fergusonite. But the most conclusive proof is perhaps, that a needle like splinter of fergusonite without being ground, nevertheless gave an excellent powder diagram, and moreover the reflection lines were broad and hazy and quite identical with those on the other fergusonite films. The haphazard orientation of the crystalline particles thus has been confirmed, for if they were arranged in a regular manner, it is obvious, that at least a variation of the relative intensities of the reflection lines had to appear¹.

Composition and Synthesis of Fergusonite.

As shown from several analyses fergusonite consists mainly of yttrium niobate, $Y\text{NbO}_4$. But isomorphous with niobium there enters tantalum. Besides, there always occur some monoxydes, which, as BRØGGER (loc. cit.) has shown have the formula $R_3(\text{NbO}_4)_2$, which leads him to claim the formula $Y_2\text{Nb}_2\text{O}_8$ for the main component. Further fergusonite has a relatively great

¹ It is worth noticing, that W. C. BRØGGER, who has investigated several ignited fergusonites literally says: "Eine Restitution der ursprünglichen, tetragonalen Molekularstruktur, läßt sich aber nicht nachweisen". (Vid. Selsk. Skr. I, 1906, No. 5).

water content. But water is not to be regarded as a true constituent, for it has probably been absorbed by the mineral simultaneously with the metamict transformation, as BRØGGER especially has maintained. In accordance with this it turned out, that fergusonite crystallizes out of a dry melt. The synthesis was made according to a method described by V. M. GOLDSCHMIDT¹: A ground mixture of Y_2O_3 and Nb_2O_5 in equimolecular proportions was pressed to a pastil in a hydraulic press and then fused in an acetylene oxygen torch. In that way there were obtained large drops consisting of crystals of $YNbO_4$. A powder diagram showed that the crystal structure of this compound was practically identical with that of natural fergusonite. In the same manner the synthesis of $YTaO_4$ was made. This compound also gave a röntgen pattern almost identical with natural fergusonite.

The Crystal Structure of Scheelite.

Crystallographic data show that fergusonite crystallizes with the symmetry of the tetragonal bipyramidal class.

The best known mineral assigned to this class is scheelite, on account of which a crystal analysis of this mineral was commenced, in order to seek structural relations between scheelite and fergusonite.

Scheelite has been investigated by DICKINSON² with the spectroscopic method. He has shown that in the unit tetragonal cell, containing eight molecules, the *Ca*- and *W*-atoms were situated so as to form a somewhat distorted diamond lattice. The dimensions given were: $a = 7,42 \text{ \AA}$, $c_0 = 11,4 \text{ \AA}$.

Quite recently VEGARD³ has published a paper dealing with the structure of some tetragonal crystals including scheelite. Using the powder method he gets results which are in close agreement with those of DICKINSON: The dimensions of the unit cell containing eight molecules, are given as $a_0 = 7,44 \text{ \AA}$; $c_0 = 11,35 \text{ \AA}$; $c a = 1,527$.

¹ Vid.-Akad. Skr. I, 1925, No. 5, p. 7.

² R. G. DICKINSON, Journ. Am. Chem. Soc., 42 (1920).

³ L. VEGARD, Vid.-Akad. Skr. I, 1925, No. 11.

The Ca - and W -atoms were found to form a distorted diamond lattice, and further VEGARD has stated that the 32 oxygen atoms are situated in the general positions of the space group concerned, which are said to be C_{4h}^6 ; and the three parameters, (x, y, z) , of the oxygen atoms have been determined.

As will be seen, this structure of scheelite is similar to that which the present author has found, but there is one difference, however, which is to be emphasized in the sequel.

As seen in table 1, the present analysis leads to the following dimensions for the tetragonal cell containing eight molecules: $a_0 = 7,44 \text{ \AA}$; $c_0 = 11,41 \text{ \AA}$; $c/a = 1,533$.

It is, however, worth noticing that only the planes with all even or all odd indices appear. Consequently the fundamental lattice of scheelite is a face centered tetragonal lattice. According to the lattice theory, there exist only two unit tetragonal space lattices: the simple lattice, I'_t , and the bodycentered lattice, I''_t .

By rotating the X - and Y -axis of scheelite through 45° about the Z -axis, another cell, containing four molecules, is obtained. This cell is to be regarded as the correct or "true" unit cell, for it is the smallest prism, which by simple repetition along the coordinate axes, will build up the entire crystal.

The dimensions of the unit cell are:¹

$$a_0 = 5,26 \text{ \AA}; c_0 = 11,41 \text{ \AA}; c/a = 2,17.$$

New indices, different from those in ordinary crystallographic use, are then required for the planes. Simultaneously the axial ratio changes from 1,53 to 2,17.

The new indices ascribed to the planes are either all even or one even and two odd, which indicates that the fundamental lattice of the space group is the body centered tetragonal lattice, I''_t .

According to crystallographic data scheelite has to be assigned to one of the space groups C_{4h}^m . In this class there occur four space groups derived from the simple tetragonal space lattice, and two from the body centered space lattice.

¹ The specific gravity computed from these figures is $G = 5,98$.

These two are then to be taken into consideration. They are C_{4h}^5 and C_{4h}^6 . The space group C_{4h}^6 is, contrary to C_{4h}^5 in agreement with the observed intensities. (Provided that the four *Ca*-atoms as well as the four *W*-atoms are equivalent). According to the tables of WYCKOFF¹ the only possible positions of the metal atoms in the space group C_{4h}^6 are:

$$W: 0 \frac{3}{4} \frac{1}{8}, 0 \frac{1}{4} \frac{7}{8}, \frac{1}{2} \frac{1}{8} \frac{5}{8}, \frac{1}{2} \frac{3}{8} \frac{3}{8}. \quad Ca: 0 \frac{3}{4} \frac{3}{8}, 0 \frac{1}{4} \frac{3}{8}, \frac{1}{2} \frac{1}{8} \frac{1}{8}, \frac{1}{2} \frac{7}{8} \frac{7}{8}.$$

In order to get a better image of the structure the origin may be changed to the point $(0 \frac{1}{4} \frac{7}{8})$. This new origin is used in fig. 2.

It is worth noticing that scheelite, according to F. ZAMBONINI² is isomorphous and forms mixed crystals with the tungstates and molybdates of the rare earth metals, in spite of the different atomic composition. He has also shown that the molecular volume of $Me_2(WO_4)_3$. (*Me* stands for a rare earth metal), is close on three times as great as the molecular volume of $CaWO_4$.

Further ZAMBONINI and LEVI³, and ZAMBONINI and CAROBBI⁴ have carried out X-ray investigations on the molybdates of the rare earths, of the earth alkali metals, and of lead. But the results arrived at are quite different from those of VEGARD and of the present investigation.

The said authors have found, that the unit cell of the molybdates of the earth alkali metals, and the unit cell of the molybdates of the rare earths have similar dimensions, con-

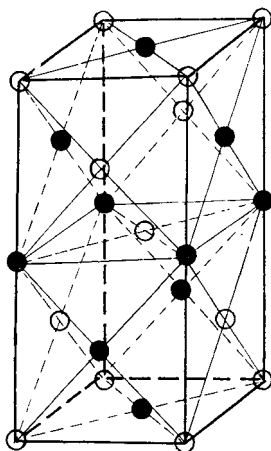


Fig. 2.
Unit cell of scheelite.
(White = *W*-atoms;
black = *Ca*-atoms).

- ¹ R. W. G. WYCKOFF, The Analytical Expression of the Results of the Theory of Space-Groups; Carnegie Inst. Publ., 318, Washington 1922.
- ² F. ZAMBONINI, Rivista ital. di min. 54, 55, 1918. Zeitschr. f. Krist., 58, 226, (1923).
- ³ F. ZAMBONINI e A. G. LEVI, Rendiconti R. Accad. dei Lincei [6], 2, 303, 377 (1925).
- ⁴ F. ZAMBONINI e G. CAROBBI, Rendiconti R. Accad. dei Lincei [6], 2, 462, (1925).

Table 1. Scheelite.

Camera diameter = 57,65 mm. Copper Radiation. $K\alpha = 1,539 \text{ \AA}$.

Intensities	Indices		q	$\sin^2 q = \Sigma h^2 \cdot x + l^2 \cdot z$
	According to crystallogr. use	According to the true unit cell		
S	113	103	14,37	$1 \cdot 0,02150 + 9 \cdot 0,00456$ $16 \cdot 0,00453$
W	004	004	15,62	
W	220	200	16,97	$4 \cdot 0,02130$
W	204	114	20,02	$2 \cdot 0,02140 + 16 \cdot 0,00465$
		β 204	20,96	
W	115	105	21,51	$1 \cdot 0,02150 + 25 \cdot 0,00452$
		β 220	21,96	
W	313	213	22,61	$5 \cdot 0,02150 + 9 \cdot 0,00452$
S	224	204	23,46	
M	400	220	24,41	$4 \cdot 0,02140 + 16 \cdot 0,00456$
		β 303	25,75	
W		β 312		
W	331	301	26,50	$9 \cdot 0,02162 + 1 \cdot 0,00455$
S	206	116	27,05	
S	315	215	28,05	$2 \cdot 0,02140 + 36 \cdot 0,00455$
		215	28,05	
S	333	303	28,85	$5 \cdot 0,02140 + 25 \cdot 0,00456$
	422	312		
	404	224	29,60	$9 \cdot 0,02134 + 9 \cdot 0,00455$
M	117	107		
W	511	321	32,10	$10 \cdot 0,02146 + 4 \cdot 0,00455$
W	008	008	32,61	
W	335	305	33,68	$8 \cdot 0,02140 + 16 \cdot 0,00455$
W	513	323	34,48	
W	317	217	35,12	$13 \cdot 0,02136 + 1 \cdot 0,00455$
W	440	400	35,71	
	426	316	37,88	$16 \cdot 0,02140 + 49 \cdot 0,00456$
S	228	208		
	515	325	38,60	$10 \cdot 0,02140 + 36 \cdot 0,00453$
M	119	109		
	533	413	39,36	$4 \cdot 0,02148 + 64 \cdot 0,00455$
W	602	332		
	444	404	40,10	$13 \cdot 0,02120 + 25 \cdot 0,00455$
W	337	307		
W	620	420	40,80	$17 \cdot 0,02124 + 9 \cdot 0,00455$
W	408	228	42,69	
	319	219	43,58	$18 \cdot 0,02132 + 4 \cdot 0,00455$
M	535	415		
	624	424	45,02	$16 \cdot 0,02136 + 16 \cdot 0,00455$
S	2010	1110		

$$\sin^2 q = \Sigma h^2 \cdot 0,02137 + l^2 \cdot 0,00455.$$

$$a_0 = 5,264 \text{ \AA}, \quad c_0 = 11,41 \text{ \AA}, \quad ca = 2,167.$$

taining respectively one and one third molecule. But by this it is obvious, that the indices ascribed to the reflection planes are not correct. This case of isomorphism is on the contrary beyond doubt a case of polymere isomorphism, as newly described by V. M. GOLDSCHMIDT¹ in the case rutile-tapiolithe.

The Crystal Structure of Fergusonite.

In the tables 2, 3 and 4, the results of the calculations of the powder diagrams of natural, fused fergusonite; artificial yttrium niobate; and artificial yttrium tantalate are recorded.

Table 2. Fused Fergusonite.

Camera diameter = 168,75 mm. Cupper Radiation: $K\alpha = 1,539 \text{ \AA}$.

Inten- sities	Indices	η		$\sin^2 \eta = \Sigma h^2 \cdot x + l^2 z$
		obs.	calc	
10	113	14,31	14,31	$2 \cdot 0,00990 + 9 \cdot 0,00460$
10	122	15,11	15,11	$5 \cdot 0,00986 + 4 \cdot 0,00465$
2	220	16,31	16,33	$8 \cdot 0,00985$
1	104	16,89	16,89	$1 \cdot 0,00985 + 16 \cdot 0,00466$
1	301	17,74	17,73	$9 \cdot 0,00991 + 1 \cdot 0,00466$
1	105	20,91	20,89	$1 \cdot 0,00990 + 25 \cdot 0,00470$
10	{ 401	23,92	{ 23,80	$5 \cdot 0,00985 + 25 \cdot 0,00461$
	{ 304		{ 23,97	
	{ 215			
6	{ 411	24,48	24,52	$17 \cdot 0,00982 + 1 \cdot 0,00465$
	{ 314			
2	331	25,33	25,27	$18 \cdot 0,00991 + 1 \cdot 0,00465$
2	225	26,00	26,14	$8 \cdot 0,00980 + 25 \cdot 0,00455$
6	333	27,91	27,91	$18 \cdot 0,00986 + 9 \cdot 0,00461$
2	007	28,41	28,44	$49 \cdot 0,00462$
5	414	29,43	29,46	$17 \cdot 0,00985 + 16 \cdot 0,00464$
4	{ 226	29,63	{ 29,64	$8 \cdot 0,00989 + 36 \cdot 0,00460$
	{ 500		{ 29,71	
	{ 430			
1	511	30,72	30,79	$26 \cdot 0,00982 + 1 \cdot 0,00460$
1	424	31,47	31,41	$20 \cdot 0,00994 + 16 \cdot 0,00462$
1	440	34,21	34,20	$32 \cdot 0,00988$

$$\sin^2 \eta = \Sigma h^2 \cdot 0,00987 + l^2 \cdot 0,00463.$$

$$a_0 = 7,744 \text{ \AA}, \quad c_0 = 11,305 \text{ \AA}, \quad ca = 1,460.$$

¹ Geochemische Verteilungsgesetze der Elemente VI, Vid.-Akad. Skr. I, 1926, No. 1.

Table 3. Artificial Yttrium Tantalate.

Camera diameter = 168,75 mm. Copper Radiation: $K\alpha = 1,539 \text{ \AA}$.

Inten- sities	Indices	φ	$\sin^2 \varphi = \Sigma h^2 \cdot x + l^2 \cdot z$
÷ 1	111	9,00	$2 \cdot 0,00996 + 1 \cdot 0,00455$
1	β 113	12,76	
1	β 122	13,65	
10	113	14,27	$2 \cdot 0,00988 + 9 \cdot 0,00455$
10	122	15,17	$5 \cdot 0,00990 + 4 \cdot 0,00475$
5	220	16,33	$8 \cdot 0,00988$
5	104	16,83	$1 \cdot 0,00990 + 16 \cdot 0,00450$
5	301	17,78	$9 \cdot 0,00986 + 1 \cdot 0,00455$
7	304	23,67	$9 \cdot 0,00986 + 16 \cdot 0,00450$
7	215	23,85	$5 \cdot 0,00988 + 25 \cdot 0,00456$
8	{ 411	24,46	$10 \cdot 0,00984 + 16 \cdot 0,00456$
	{ 314		
8	322	26,23	$18 \cdot 0,00986 + 4 \cdot 0,00460$
8	333	27,91	$18 \cdot 0,00987 + 9 \cdot 0,00460$
1	{ 007	28,46	$49 \cdot 0,00463$
	{ 404		
8	414	29,30	$17 \cdot 0,00986 + 16 \cdot 0,00450$
6	{ 500	29,76	$25 \cdot 0,00985$
	{ 430		
8	502	30,98	$25 \cdot 0,00988 + 4 \cdot 0,00450$
7	512	31,58	$26 \cdot 0,00986 + 4 \cdot 0,00450$
÷ 1	524	36,72	$29 \cdot 0,00985 + 16 \cdot 0,00450$
÷ 1	602	37,59	$36 \cdot 0,00984 + 4 \cdot 9,00450$

$$\sin^2 \varphi = \Sigma h^2 \cdot 0,00986 + l^2 \cdot 0,00455.$$

$$\mathbf{a}_0 = 7,749 \text{ \AA}, \quad \mathbf{c}_0 = 11,41, \quad \mathbf{c}_a = 1,472.$$

On purpose to get an accurate determination of the glancing angle, φ , from the different planes of fergusonite, a great camera with a diameter about 169 mm. was used.

The ground fergusonite was mixed with pure sodium chloride¹, and the differences between the sodium chloride lines and the fergusonite lines were used as basis for the calculation of φ .

Working in this way the usual sources of error are avoided.²

It is seen that these three substances have identical structures, but different from that of scheelite. The unit cell contains eight molecules. The dimensions were found be:

¹ According to the method of WYCKOFF, Zeitschr. f. Krist., 59, 55 (1923).

² Apparatus, procedure and calculation of the films, are described in a previous paper: Zeitschr. f. physik. Chemie 117, 378, (1925).

Fergusonite: $a_0 = 7,74 \text{ \AA}$; $c_0 = 11,31 \text{ \AA}$; $c/a = 1,46$,
Yttrium Niobate: $a_0 = 7,76 \text{ \AA}$; $c_0 = 11,32 \text{ \AA}$; $c/a = 1,46$,
Volume = $681 \cdot 10^{-24} \text{ cm}^3$
Yttrium Tantalate: $a_0 = 7,75 \text{ \AA}$; $c_0 = 11,41 \text{ \AA}$; $c/a = 1,47$,
Volume = $685 \cdot 10^{-24} \text{ cm}^3$

The correctness of the identifications of the lines is seen from the close agreement between the calculated and observed values of the reflection angle, φ , and further from fig. 3, where all the possible reflection lines with a greater angle than the reflection of the plane (113) from a tetragonal crystal with the axial ratio 1,460 are recorded, and compared with the observed lines of fergusonite.

Table 4. Artificial Yttrium Niobate.

Camera diameter = 57,45 mm. Copper Radiation: $K\alpha = 1,539 \text{ \AA}$.

Intensities	Indices	φ	$\sin^2 \varphi = \Sigma h^2 \cdot x = l^2 \cdot z$
8	113	14,32	$2 \cdot 0,00988 + 9 \cdot 0,00459$
8	122	15,07	$5 \cdot 0,00988 + 4 \cdot 0,00463$
1	220	16,37	$8 \cdot 0,00993$
1	104	16,92	$1 \cdot 0,00988 + 16 \cdot 0,00468$
1	301	17,72	$9 \cdot 0,00978 + 1 \cdot 0,00467$
10	215	23,94	$5 \cdot 0,00988 + 15 \cdot 0,00460$
10	411	24,50	$17 \cdot 0,00984 + 1 \cdot 0,00466$
2	225	26,05	$8 \cdot 0,00986 + 25 \cdot 0,00456$
8	404	28,50	$16 \cdot 0,00968 + 16 \cdot 0,00450$
10	414	29,47	$17 \cdot 0,00988 + 16 \cdot 0,00463$
4	511	30,79	$26 \cdot 0,00986 + 1 \cdot 0,00465$
3	424	31,34	$20 \cdot 0,00986 + 16 \cdot 0,00458$
2	440	34,24	$32 \cdot 0,00990$
1	602	37,38	$36 \cdot 0,00970 + 4 \cdot 0,00460$

$$\sin^2 \varphi = \Sigma h^2 \cdot 0,00984 + l^2 \cdot 0,00462.$$

$$a_0 = 7,757 \text{ \AA}, \quad c_0 = 11,32, \quad c/a = 1,460.$$

According to BROOKE and MILLER fergusonite has the axial ratio, $c/a = 1,464$. The fergusonite from Høgtveit has, however, been measured by P. SCHEI¹ who finds the axial ratio, $c/a = 1,460$.

¹ Nyt Mag. for Naturvidenskaberne 43, 137, (1905). Ref.: Zeitschrift f. Krist., 43, 638 (1906).

The specific gravity of the fergusonite computed from the *X*-ray data is only approximative, for the actual chemical composition is unknown. The yttria used for the synthesis of $YNbO_4$ and $YTaO_4$ had a molecular weight about 288¹. Using this figure the calculation of the specific gravity of $YNbO_4$ leads to $G = 5,38$, and of $YTaO_4$ leads to $G = 7,03$.

The specific gravity of fergusonite is given by SCHEI as $G = 5,68$.

As seen from the tables all kinds of indices appear. The fundamental lattice of fergusonite is consequently the simple tetragonal lattice, I_1' . The possible space groups are then:

$$C_{4h}^1, C_{4h}^2, C_{4h}^3, C_{4h}^4$$

If all the eight yttrium and all the eight niobium (viz. tantalum) atoms have equivalent positions, they have to be situated in general positions, (x, y, z) , without regard to which of the four said space groups they are assigned to. The thirty-two oxygen atoms are to be divided into four groups of eight atoms each, all in the general positions.

The said opinion of BRØGGER, that the formula of fergusonite had to be multiplied, has proved correct. By claiming the formula $R_3(NbO_4)_2$ for the monoxides met with in fergusonite, twelve atoms of R have to replace eight yttrium atoms. This can be made by dividing the twelve atoms in one group of eight equivalent positions, and one group of four equivalent positions.

¹ The rare earths were separated from a thalénite by Miss H. HOUGEN.

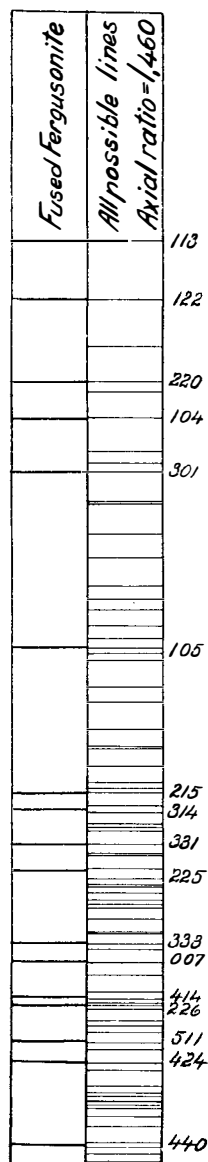


Fig. 3.

The reflection lines from fergusonite, compared with all possible reflection lines between the reflections (113) and (406).
Logarithmic scale.

As a matter of fact scheelite and fergusonite do not crystallize in the same space group.

Crystallographic data show that they are related in their external forms. From this *X*-ray analysis, however, it is shown that the unit cell of scheelite with axial ratio $c/a = 2,17$ containing four molecules, bears no resemblance to the unit cell of fergusonite with axial ratio $c/a = 1,46$, containing eight molecules. The structure of scheelite is further based on a body centered space lattice and the positions of the metal atoms are symmetrically without degrees of freedom. The structure of fergusonite, on the contrary, is based on a simple space lattice, the positions of the metal atoms are less symmetrical, all of them having three degrees of freedom.

Summary.

When metamict fergusonite is heated it recrystallizes into a conglomerate of haphazard orientated crystallites, the average size of which are about $200 \cdot 10^{-8}$ cm. As a consequence of this, the birefringence of ignited fergusonite depends upon strain caused by the recrystallisation.

Artificial fergusonite ($YNbO_4$) can be made by mixing equimolecular proportions of Y_2O_3 and Nb_2O_5 and fusing them in an acetylene-oxygen torch. In the same manner $YTao_4$ can be produced.

The structure of scheelite is based on the lattice I'_i ; space group C_{4h}^2 ; the unit cell containing four molecules, has the axial ratio $c/a = 2,17$. (In contrary to crystallographic use where c/a is taken as 1,53).

The dimensions of the unit prism are:

$$a_0 = 5,26 \text{ \AA}; c_0 = 11,41 \text{ \AA}.$$

Fergusonite; $YNbO_4$; and $YTao_4$ crystallize according to one of the following space groups:

$$C_{4h}^1, C_{4h}^2, C_{4h}^3, C_{4h}^4.$$

Their fundamental lattice are I'_i .

The dimensions of the unit tetragonal prisms, containing eight molecules are:

Fergusonite $a_0 = 7,74 \text{ \AA}$; $c_0 = 11,31 \text{ \AA}$; $c/a = 1,46$.

$YNbO_4$. . . $a_0 = 7,76 \text{ \AA}$; $c_0 = 11,32 \text{ \AA}$; $c/a = 1,46$.

$YTaN_4$. . . $a_0 = 7,75 \text{ \AA}$; $c_0 = 11,41 \text{ \AA}$; $c/a = 1,47$.

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