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The Crystal Structure of $OsSi_2$

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The crystal structure of $OsSi_2$ has been determined and refined by the single crystal X-ray technique. The unit cell is orthorhombic with the following dimensions: $a=10.1496$ Å, $b=8.1168$ Å, and $c=8.2230$ Å. There are sixteen formula units in the unit cell and the atoms occupy the following positions of the space group *Cmca*: 16 osmium atoms in two different sets of eightfold positions, 8(*d*) and 8(*f*), and 32 silicon atoms in two sets of the sixteenfold position 16(*g*).

The structure of $OsSi_2$ represents a new structure type, which can be derived from the fluorite type structure. $OsSi_2$ is probably isotypic with β-$FeSi_2$.

The binary system Os–Si has been investigated a number of times.[1] Most of the earlier investigators report the existence of a compound with unknown structure at a composition of about 67 at.-% Si. A reinvestigation of the Os–Si system has now been made at this institute, when it was found possible to obtain single crystals of this compound and determine the crystal structure. This paper gives an account of the structure determination of the compound, whose composition has now been established as $OsSi_2$. In addition, some phase analytical observations in the Os–Si system are presented.

EXPERIMENTAL

Preparation. Alloys were prepared by arc-melting osmium metal powder (Heraeus, claimed purity 99.9 %) and silicon powder (Pechiney, claimed purity 99.9 %). The subsequent heat-treatments were carried out in evacuated silica capsules.

Powder diffraction examination. X-Ray powder photographs were recorded in a Guinier-Hägg type focusing camera with $CuK\alpha_1$ radiation. Silicon ($a=5.4305$ Å) was used as an internal calibration standard.

Single crystal examination. The single crystal fragment of $OsSi_2$ was obtained from an arc-melted alloy of the nominal composition $OsSi_{2.22}$. In the powder diffraction pattern of the sample weak lines belonging to Os_2Si_3 were observed. The intensity data were recorded in an equi-inclination Weissenberg camera with Zr-filtered Mo*K* radiation. The multiple film technique was used with thin iron foils interleaved with the films. The crystal was rotated about the *a* and *c* axes and the reflections of the *hk*0, *hk*1, *hk*2, and 0*kl* layers were recorded. The intensities were estimated visually by comparison with a calibrated intensity scale. No absorption and extinction corrections could be applied to the intensity data on account of the irregular shape of the crystal.

Calculations. The unit cell dimensions of the compounds were refined with a least squares program. In the structure factor calculations the atomic scattering factors for osmium and silicon were obtained from Ref. 2, together with the real and imaginary dispersion corrections. The least squares refinement was carried out employing a weighting scheme according to Cruickshank *et al.*,[3] $w=1/(a+|F_o|+c|F_o|^2)$, where the constants a and c were given the values 165 and 0.0032, respectively. All calculations were carried out on a CDC 3600 computer with programs listed in Table 2 of Ref. 4.

PHASE-ANALYTICAL INVESTIGATION OF THE Os–Si SYSTEM

The information in the literature about the number of intermediate phases in the Os–Si system is ambiguous (for further references see Ref. 1). A phase-analytical investigation made on arc-melted samples by the present author shows the existence of three intermediate phases: OsSi(FeSi type), Os_2Si_3(Ru_2Si_3 type), and $OsSi_2$. The investigation also shows that the solubility of silicon in osmium, as estimated from the change of the lattice parameters of osmium, is negligible. On the other hand the unit cell dimensions of OsSi(FeSi type) are different in the two two-phase regions on each side of the OsSi phase. This indicates a certain extension of the homogeneity range. The unit cell dimensions of Os_2Si_3 are in good agreement with those reported earlier.[1] To investigate whether there are two phases [5] with the composition $OsSi_2$, a sample with the composition $OsSi_{2.22}$ (containing traces of Os_2Si_3 in addition to $OsSi_2$) was analyzed after heat-treatments at three different temperatures: 1200, 1000, and 600°C. No transformation of $OsSi_2$ to the $OsGe_2$ type occurred. The results of the phase-analysis are given in Table 1.

Table 1. Unit cell dimensions of arc-melted osmium silicides. Standard deviations are given in parenthesis and refer to the last decimal place of respective values.

Nominal composition	Observed phases	Lattice parameters (in Å units)
$OsSi_{0.82}$	Os	$a=$ 2.7316 (5), $c=$4.3185 (11).
	OsSi	$a=$ 4.7284 (4)
$OsSi_{1.33}$	OsSi	$a=$ 4.7205 (5)
	Os_2Si_3	$a=$11.1603 (18), $c=$8.9638 (15)
$OsSi_{2.22}$	Os_2Si_3	[a]
	$OsSi_2$	$a=$10.1495 (15), $b=$8.1168 (11), $b=$ 8.2230 (11)
$OsSi_{3.35}$	$OsSi_2$	$a=$10.1530 (10), $b=$8.1190 (8), $c=$ 8.2272 (9)
	Si	[a]

[a] Traces of the compound were found in the powder diffraction pattern of the sample. The very few lines did not allow an accurate determination of the unit cell dimensions.

DETERMINATION OF THE CRYSTAL STRUCTURE

The orthorhombic symmetry was evident from the Weissenberg photographs recorded with the *a* and *c* axes as rotation axes. Systematic extinctions showed that the unit cell is centered and together with additional extinction conditions two space groups were possible, *Cmca* and *C2ca* (=*Aba2* according to the standard setting in *International Tables for X-Ray Cryst.*, Vol. I).

The Patterson projections $P(UV)$ and $P(VW)$ were calculated and from them the arrangement of the metal atoms could be deduced. The positions corresponded to two eightfold positions, 8(*d*) and 8(*f*), of the space group *Cmca*. From difference syntheses and spatial considerations it was possible to determine the positions of the silicon atoms. They were found to occupy two sets of the general position 16(*g*). Altogether the unit cell contains 48 atoms, 16 osmium atoms and 32 silicon atoms, giving the composition $OsSi_2$.

The atomic parameters were refined using a full matrix least squares program. The first refinements were carried out separately for the two zero layers *hk*0 and 0*kl*. Finally the four layers, *hk*0, *hk*1, *hk*2, and 0*kl* were refined simultaneously. The intensities of some fifteen 0*kl* reflections were measured twice, depending on the rotation of the crystal about two axes. Since no absorption corrections could be applied to the intensity data, these reflections were included twice in the final refinement. The final atomic parameters and their standard deviations are given in Table 2. The parameters varied during the refinement were nine positional parameters, four isotropic temperature factors and four scale factors. The *R* value given in the table is based on the 270 observed reflections only.*

Observed and calculated structure factors are given in Table 3 and interatomic distances less than 4.2 Å are listed in Table 4.

Table 2. Final structure data for $OsSi_2$. Standard deviations are given in parenthesis and refer to the last decimal place of respective values.
Space group: *Cmca* (No. 64), $Z=16$. $a=10.1496$ (15) Å, $b=8.1168$ (11) Å, $c=8.2230$ (11) Å. $U=677.43$ Å^3.

Atom	Position	Position parameters			Isotropic temp. fact.
		x	*y*	*z*	*B*
Os_I	8(*d*)	.2142 (3)			.21 (2)
Os_{II}	8(*f*)		.1881 (3)	.1812 (4)	.15 (3)
Si_I	16(*g*)	.3699 (16)	.2208 (13)	.0597 (18)	.34 (14)
Si_{II}	16(*g*)	.1280 (18)	.0534 (13)	.7252 (18)	.54 (16)

Final *R* value=0.083.

* A refinement based on the space group *C2ca* gave no significant deviations of the atomic positions from those obtained with the higher symmetry of the space group *Cmca*.

DESCRIPTION AND DISCUSSION OF THE $OsSi_2$ CRYSTAL STRUCTURE

The crystal structure of $OsSi_2$ represents a new structure type. A projection of the structure on (100) is shown in Fig. 1. It is evident from the figure that the silicon atoms are arranged in four layers perpendicular to the *a* axis. Only very small differences occur between the *x* coordinates of the atoms within each layer. For the sake of simplicity, the silicon layers at $x \sim \pm 0.129$ can be designated the A layers and those at $x \sim \pm 0.371$ the B layers. Expressed in the symbols A and B the sequence of the silicon layers is A A B B A A B B . . . in the direction of the *a* axis. The distance between two adjacent layers is 2.5 – 2.6 Å. Each silicon atom, Si_I and Si_{II}, has five rather close silicon neighbours, three of them situated in the same layer and the other two in surrounding layers. The five silicon neighbours to both Si_I and Si_{II} occupy five of the six corners of a somewhat irregular octahedron. In addition, the two silicon atoms are coordinated by four metal atoms. These atoms form irregular tetrahedra about the silicon atoms.

Table 3. Observed and calculated structure factors of $OsSi_2$.

h	k	l	$\lvert F_o\rvert$	$\lvert F_c\rvert$	h	k	l	$\lvert F_o\rvert$	$\lvert F_c\rvert$	h	k	l	$\lvert F_o\rvert$	$\lvert F_c\rvert$	h	k	l	$\lvert F_o\rvert$	$\lvert F_c\rvert$	h	k	l	$\lvert F_o\rvert$	$\lvert F_c\rvert$
0	0	2	132.6	152.1	0	4	0	469.2	504.9	0	6	4	295.3	276.2	0	10	3	118.4	99.1	0	12	16	121.6	121.0
0	0	4	465.5	514.4	0	4	1	478.1	582.8	0	6	5	135.0	114.3	0	10	4	191.4	185.1	0	14	2	300.4	317.5
0	0	6	582.0	590.6	0	4	2	378.0	484.8	0	6	6	596.1	554.1	0	10	5	187.3	165.5	0	14	4	230.6	217.6
0	0	10	345.6	329.9	0	4	3	156.0	147.3	0	6	7	326.8	285.8	0	10	6	447.5	423.3	0	14	5	134.3	124.3
0	0	12	335.2	326.9	0	4	4	402.5	429.4	0	6	8	150.1	115.8	0	10	7	132.4	143.1	0	14	8	258.5	263.2
0	0	16	298.1	335.9	0	4	5	83.2	71.2	0	6	9	201.0	165.2	0	10	9	127.0	101.9	0	14	14	212.8	232.0
0	0	18	194.1	181.2	0	4	6	322.0	297.0	0	6	10	372.0	334.8	0	10	10	273.8	252.0	0	16	0	304.4	341.9
0	2	0	112.3	129.1	0	4	7	354.5	322.8	0	6	12	337.9	294.7	0	10	12	265.7	250.3	0	16	4	136.7	149.0
0	2	1	243.7	257.7	0	4	8	299.3	246.7	0	6	15	146.2	164.0	0	10	16	238.1	249.3	0	16	6	301.7	314.0
0	2	2	436.3	517.6	0	4	9	241.1	213.0	0	6	16	260.4	253.6	0	12	0	181.9	163.9	0	16	10	225.0	214.2
0	2	4	497.9	571.5	0	4	10	263.6	225.5	0	8	1	100.7	81.5	0	12	1	240.6	243.1	0	16	12	198.4	194.1
0	2	5	184.2	173.6	0	4	12	227.9	218.4	0	8	2	638.7	614.9	0	12	2	253.2	247.0	0	18	2	213.2	224.7
0	2	6	198.5	162.4	0	4	14	223.8	213.2	0	8	4	316.9	297.5	0	12	3	176.3	136.0	0	18	4	205.6	177.7
0	2	7	323.8	294.2	0	4	15	170.2	183.1	0	8	5	114.0	94.6	0	12	4	206.7	202.1	0	18	8	204.0	218.7
0	2	8	710.3	654.3	0	4	16	179.1	188.7	0	8	8	496.7	476.6	0	12	5	148.8	140.8	0	20	0	124.2	133.9
0	2	9	191.9	171.7	0	4	18	174.6	165.7	0	8	10	141.8	132.4	0	12	6	243.3	236.7	0	20	1	123.8	128.3
0	2	10	280.0	255.3	0	4	20	122.0	126.5	0	8	12	132.0	111.4	0	12	7	200.2	182.5	0	20	4	126.9	131.0
0	2	12	192.7	156.8	0	4	21	138.4	122.2	0	8	14	329.6	341.3	0	12	8	234.6	221.4	0	20	6	118.2	130.0
0	2	14	334.1	346.8	0	6	0	516.6	561.7	0	8	20	194.8	217.6	0	12	9	143.9	134.2	0	20	7	112.0	121.6
0	2	15	181.1	157.6	0	6	1	204.4	194.0	0	10	0	432.5	440.5	0	12	10	192.6	193.2	0	20	8	120.3	122.4
0	2	18	144.0	152.1	0	6	2	221.3	214.2	0	10	1	169.1	136.9	0	12	12	157.1	166.8	0	20	10	107.0	120.5
0	2	20	171.8	183.8	0	6	3	125.1	100.9	0	10	2	274.0	215.9	0	12	13	133.6	143.2	0	22	0	165.9	203.3
																				0	22	1	98.8	70.9

0	2	0	158.7	129.1	14	0	0	586.4	555.1	4	12	1	189.9	195.1	13	5	1	213.1	167.7	5	3	2	177.0	184.9
0	4	0	478.7	604.9	14	4	0	303.0	264.0	5	1	1	489.2	507.2	14	4	1	240.0	242.4	5	5	2	114.9	97.4
0	6	0	608.4	561.7	14	6	0	411.8	370.7	5	3	1	182.5	187.3	16	4	1	252.8	246.1	5	7	2	223.6	204.6
0	10	0	455.3	440.5	14	10	0	324.2	327.5	5	5	1	520.0	530.3	17	3	1	201.0	205.8	5	9	2	228.5	206.1
0	16	0	345.7	341.9	14	16	0	267.1	270.3	5	7	1	210.3	183.8	19	1	1	212.7	206.4	6	0	2	353.0	361.0
0	22	0	145.2	203.3	16	2	0	415.4	368.0	5	9	1	253.7	244.2	19	5	1	271.5	250.2	6	6	2	236.0	225.5
2	2	0	747.3	838.5	16	8	0	405.8	385.7	5	11	1	263.8	281.2	21	3	1	223.0	225.9	6	8	2	174.7	135.8
2	4	0	353.1	407.2	18	0	0	292.2	295.0	6	2	1	257.4	260.3	21	7	1	162.1	176.0	7	1	2	242.1	220.2
2	8	0	579.3	619.3	18	6	0	277.9	253.9	6	4	1	356.3	363.9	0	2	2	407.8	517.6	7	5	2	137.7	106.1
2	12	0	241.9	219.0	18	10	0	221.4	219.4	6	6	1	225.0	219.7	0	4	2	425.5	484.8	7	7	2	240.3	237.7
2	14	0	331.1	324.7	24	0	0	255.9	260.9	6	10	1	131.7	156.4	0	6	2	220.9	214.2	7	9	2	199.3	186.5
4	0	0	509.5	501.1	26	2	0	200.9	194.3	6	12	1	185.2	208.1	0	8	2	563.5	614.9	8	0	2	389.9	344.5
4	4	0	158.6	148.8	0	2	1	236.5	257.7	7	1	1	343.0	363.8	0	10	2	191.1	215.9	8	6	2	218.8	201.9
4	6	0	595.2	571.9	0	4	1	515.2	582.8	7	3	1	491.7	483.3	0	12	2	234.2	247.0	8	8	2	194.4	177.1
4	10	0	427.9	411.0	0	6	1	192.8	194.0	7	5	1	275.2	266.0	0	14	2	283.3	317.5	9	1	2	264.6	218.1
4	12	0	184.5	193.2	0	12	1	234.4	243.1	7	7	1	314.9	286.2	1	5	2	108.5	124.1	9	7	2	222.3	209.5
4	16	0	261.4	299.0	1	5	1	188.8	196.3	7	9	1	332.8	349.6	1	7	2	283.6	272.9	9	9	2	176.2	175.9
6	0	0	369.9	377.9	1	11	1	190.9	198.5	7	13	1	291.7	302.5	1	9	2	234.0	210.2	10	2	2	420.8	376.7
6	2	0	384.1	402.4	2	2	1	321.7	331.1	8	2	1	221.9	186.3	2	2	2	212.5	205.1	10	8	2	317.4	310.0
6	6	0	164.4	149.4	2	4	1	399.1	400.1	8	4	1	437.4	424.0	2	4	2	332.4	398.6	11	1	2	307.6	258.8
6	8	0	371.2	371.3	2	6	1	249.2	252.6	8	6	1	155.1	161.5	2	6	2	512.4	503.8	11	3	2	170.6	145.3
8	0	0	549.4	508.7	2	10	1	207.1	176.3	9	1	1	412.7	352.7	2	10	2	358.7	379.9	12	0	2	458.8	430.0
8	2	0	421.7	362.6	2	12	1	195.6	219.6	9	5	1	404.8	369.5	2	12	2	197.2	202.4	12	4	2	267.0	263.3
8	8	0	369.3	391.6	3	1	1	192.8	199.4	9	7	1	245.0	235.8	3	1	2	389.7	415.2	12	10	2	325.4	323.4
10	0	0	576.4	493.7	3	3	1	498.6	513.2	9	11	1	279.2	301.9	3	3	2	212.3	221.7	13	1	2	259.4	204.3
10	6	0	402.4	387.6	3	7	1	382.7	349.3	10	2	1	269.0	213.8	3	5	2	105.4	99.2	14	2	2	388.1	335.7
10	10	0	309.5	312.3	3	9	1	188.9	180.1	10	6	1	182.6	190.1	3	7	2	211.4	209.1	14	4	2	300.3	244.2
12	2	0	537.1	450.2	3	13	1	184.4	201.0	11	1	1	153.7	117.8	3	9	2	213.8	215.8	14	8	2	368.3	352.1
12	4	0	331.2	301.4	4	2	1	345.3	365.9	11	3	1	360.0	327.9	4	2	2	583.0	684.4	16	0	2	309.7	354.1
12	8	0	388.3	407.2	4	4	1	215.7	235.4	11	7	1	249.9	254.8	4	4	2	214.3	210.2	16	6	2	307.5	269.9
12	14	0	248.4	281.6	4	6	1	291.7	295.8	12	2	1	252.9	216.0	4	8	2	329.0	320.1	18	2	2	235.6	234.7
12	18	0	226.5	242.2	4	10	1	225.5	205.9	12	4	1	175.0	176.5	5	1	2	331.6	355.1					

Table 4. Interatomic distances with standard deviations in $OsSi_2$ (in Ångström units). Distances less than 4.2 Å are listed.

Atom	Dist.	St.dev.	Atom	Dist.	St.dev.
Os_I — 2 Os_{II}	3.046	0.003	Os_{II} — 2 Os_I	3.046	0.003
— 2 Os_I	4.123	0.001	— 2 Os_I	4.128	0.003
— 2 Os_{II}	4.128	0.003	— 2 Os_I	4.197	0.003
— 2 Os_I	4.175	0.001			
— 2 Os_{II}	4.197	0.003	— 2 Si_{II}	2.474	0.014
			— 2 Si_I	2.492	0.015
— 2 Si_I	2.439	0.014	— 2 Si_{II}	2.495	0.013
— 2 Si_{II}	2.462	0.015	— 2 Si_I	2.521	0.015
— 2 Si_I	2.471	0.012	— 2 Si_I	3.894	0.017
— 2 Si_{II}	2.486	0.016	— 2 Si_{II}	4.116	0.015
— 2 Si_I	4.130	0.014	— 2 Si_I	4.138	0.012
— 2 Si_{II}	4.164	0.012			
— 2 Si_{II}	4.167	0.017	Si_{II} — Os_I	2.462	0.015
— 2 Si_I	4.194	0.015	— Os_{II}	2.474	0.014
			— Os_I	2.486	0.016
Si_I — Os_I	2.439	0.014	— Os_{II}	2.495	0.013
— Os_I	2.471	0.012	— Os_{II}	4.116	0.015
— Os_{II}	2.492	0.015	— Os_I	4.164	0.012
— Os_{II}	2.521	0.015	— Os_I	4.167	0.017
— Os_{II}	3.894	0.017			
— Os_I	4.130	0.014	— Si_{II}	2.509	0.035
— Os_{II}	4.138	0.012	— Si_I	2.548	0.018
— Os_I	4.194	0.015	— Si_{II}	2.599	0.036
			— Si_I	2.609	0.017
— Si_{II}	2.548	0.018	— Si_I	2.708	0.019
— Si_{II}	2.609	0.017	— Si_I	3.353	0.021
— Si_I	2.640	0.033	— Si_I	3.654	0.022
— Si_I	2.667	0.033	— Si_I	3.697	0.021
— Si_{II}	2.708	0.019	— Si_I	3.756	0.021
— Si_{II}	3.353	0.021	— Si_I	3.768	0.022
— Si_{II}	3.654	0.022	— Si_{II}	3.803	0.029
— Si_{II}	3.697	0.021	— Si_I	3.854	0.018
— Si_I	3.717	0.022	— Si_I	3.929	0.022
— Si_{II}	3.756	0.021	— 2 Si_{II}	4.079	0.003
— Si_{II}	3.768	0.022			
— Si_{II}	3.854	0.018			
— Si_{II}	3.929	0.022			
— Si_I	3.966	0.031			
— 2 Si_I	4.139	0.003			

The two non-equivalent metal atoms of the structure, Os_I and Os_{II}, are both situated between the silicon layers described above. On closer inspection of the structure (see Fig. 1) it is clear, that the following sequence is obtained when the metal atoms are included:

$$A,Os_{II},A,Os_I,B,Os_{II},B,Os_I,A,Os_{II},A \ldots$$

The coordination polyhedra about the two non-equivalent metal atoms are composed of eight silicon atoms at the corners of deformed cubes. The polyhedra have almost the same shape for the two metal atoms, but different orientations in the structure. The average Os—Si distance is 2.48 Å, which

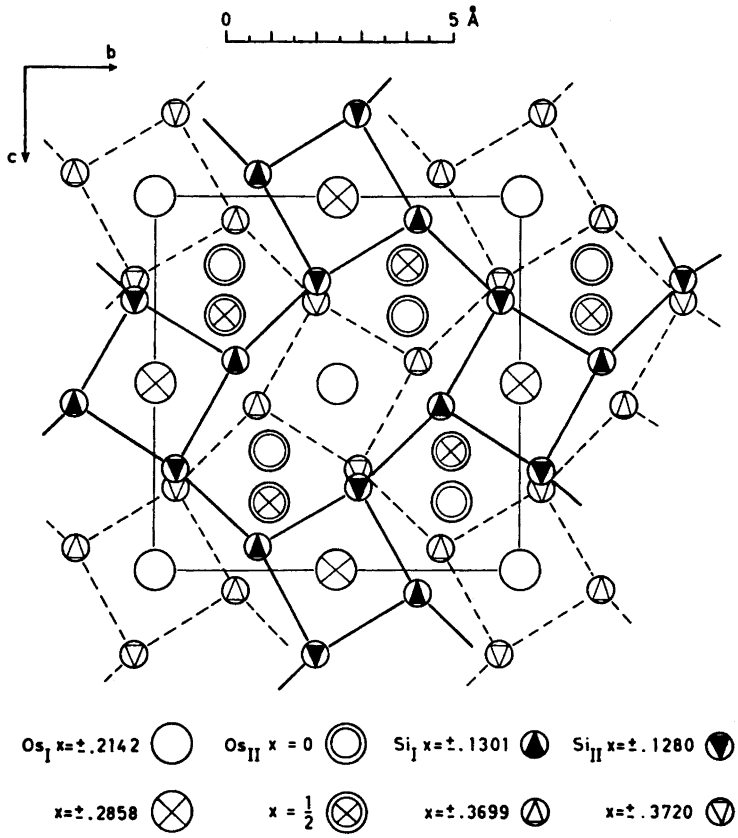

Fig. 1. Projection of $OsSi_2$ on (100).

is somewhat shorter than the sum of the Goldschmidt metal radius of osmium and the covalent tetrahedral radius of silicon.

Both osmium atoms have two osmium neighbours at a distance of 3.05 Å. This distance is, however, 14 % longer than the metal diameter in the pure element. Looking only at the arrangement of the metal atoms in the structure it is observed that they form isolated squares (angle 89°), where the sides of the squares are 3.05 Å. The planes of these squares are parallel to (011) and (01$\bar{1}$).

Only small changes of the atomic positions of $OsSi_2$ are needed in order to obtain an atomic arrangement corresponding to that of the fluorite structure type. Fig. 2 shows the relationship between the $OsSi_2$ unit cell as projected in Fig. 1 and the unit cell of the CaF_2 structure type. For the sake of simplicity only atoms necessary to show the relationship are shown in the figure. The dashed lines in Fig. 2 show the original unit cell of $OsSi_2$, and the full lines show the orientation of the CaF_2 structure type. It must be noted, that there

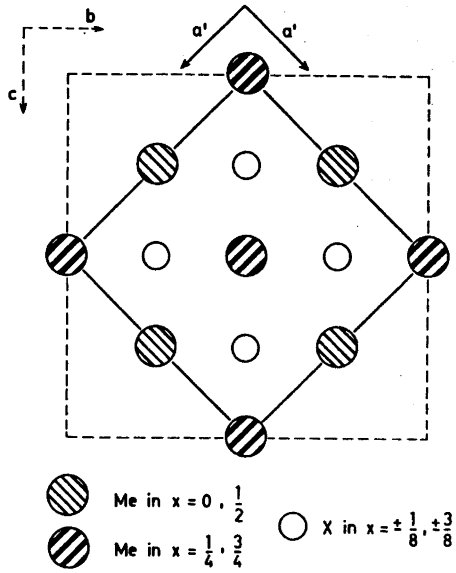

Fig. 2. Idealized version of $OsSi_2$, showing its relationship to the fluorite structure type.

are two CaF_2 type unit cells within the length of the *a* axis of $OsSi_2$ in Fig. 2. The distortion of the $OsSi_2$ structure from the CaF_2 structure type is reflected in the ratio between the length of the diagonal in the *bc* plane and the length of the *a* axis. The ratio, $d_{bc}/a = 1.14$, shows that the deviations from the CaF_2 type can be interpreted as an expansion in the *bc* plane and a contraction in the direction of the *a* axis. This is in good agreement with the fact that the number of short Si – Si distances parallel to the *bc* plane has been reduced by one as a result of the deformation of the silicon network. Moreover, the directions of the shortest Si – Si distances are parallel to the *a* axis.

Several authors have contributed to the structural systematization of the transition metal disilicides. Wallbaum [6] showed that the $TiSi_2$, $CrSi_2$, and $MoSi_2$ structure types can be generated by different stackings of a characteristic structural element, a close-packed layer of metal and silicon atoms. Other disilicide types have later been described as members of the structure family just mentioned. The shape of the silicon network and the positions of the metal atoms in that network have constituted the basis of a more general classification of the disilicides put forward by Nowotny.[7] The latter is the basis for a suitable classification of the crystal structure of $OsSi_2$. Considering the short Si – Si distances of the disilicides of the IIa – VIa groups of metals and the "isolated" silicon atoms in the fluorite type disilicides, $OsSi_2$ takes an intermediate position. While the number of close silicon atoms surrounding the metal atoms is the same in $OsSi_2$ as in the fluorite type disilicide, the metal-metal distances are considerably shorter, and of the same length as in the $TiSi_2$ structure family. The average Si – Si distance in $OsSi_2$ is also shorter than in the fluorite type of disilicides and a small tendency to the formation of silicon pairs arranged parallel to the *a* axis can be discerned. This effect gives a

certain connection between the $OsSi_2$ structure and the structure of α-$FeSi_2$. The relationship between the fluorite and the α-$FeSi_2$ structures has been made clear by Wittman *et al.*[8]

From comparisons between the structure of $OsSi_2$ and $OsGe_2$[9] it is evident that the metal atoms, which form isolated squares in $OsSi_2$, are arranged in isolated bands parallel to the *b* axis in $OsGe_2$. These bands are formed by repetitions of an almost square basic arrangement of metal atoms. The repeat distance along the band is the *b* axis (3.094 Å) and the width of the band is 2.98 Å. In this tendency to concentrate the metal atoms, the next step is the arrangement of the metal atoms in square-shaped isolated layers, as present in α-$FeSi_2$. There is also a marked formation of pairs of non-metal atoms in the $OsGe_2$ structure type. The structure of $OsGe_2$ can be described as a stacking of pseudo-hexagonal nets parallel to the *ab* plane. The nets are alternately composed of Os – Ge atoms and Ge atoms.

The low-temperature modification of $FeSi_2$, β-$FeSi_2$,[10] is probably isomorphous with $OsSi_2$. A comparison of the unit cell dimensions of the two compounds shows a striking similarity:

$OsSi_2$	β-$FeSi_2$
$a = 10.150$ Å	$a = 9.880$ Å
$b = 8.117$	$b = 7.798$
$c = 8.223$	$c = 7.839$

The number of formula units in the unit cell of β-$FeSi_2$, as determined from density measurements and the unit cell volume is the same as in $OsSi_2$, *i.e.* 16. From extinction conditions observed in the powder diffraction pattern the unit cell was found to be centered and four space groups were suggested (see Ref. 10). Wäppling *et al.*[11] proposed, on the basis of Mössbauer spectroscopic measurements, that *Cmmm* is the most probable of these. The Mössbauer spectra indicated only one set of crystallographic positions for the sixteen metal atoms in the unit cell of β-$FeSi_2$, and the only space group, among those suggested in Ref. 10, with a sixteen-fold position is *Cmmm*. Later Wandji *et al.*[12] made a single crystal X-ray investigation of the β-$FeSi_2$ phase and established the space group *Cmca*, which agrees with the one now established for $OsSi_2$. The suggested isomorphism between $OsSi_2$ and β-$FeSi_2$ has recently been confirmed by the published results of Wandji *et al.*[13]

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