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Description of Alloys by Means of Polyhedra Packing: Binary Alloys of Niobium (and Tantalum) with Group III B and IV B Elements

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Niobium and Tantalum are found to exhibit a range of coordination numbers (CN) from 10 to 17 in their alloys with group III B and IV B elements. The III B and IV B elements in these binary alloys have CN ranging from 6 to 14. The polyhedra around Nb, Ta, III b, and IV b elements have been characterized and a description of the polyhedra in terms of certain symbols is suggested. The structures of the binary alloys considered have been described in terms of polyhedra packing. *Most of the structures examined up until now could be built up with one or two polyhedra,* only in a few cases more than 2 polyhedra are required.

[Keywords: Coordination Polyhedra; Nb-III B (IV B) Alloys; Polyhedra-Packing Model; Ta-III B (IV B) Alloys)]

Beschreibung von Legierungen mittels des Polyederpackungsmodells. Binäre Legierungen von Niob (und Tantal) mit III B- und IV B-Elementen

Niob und Tantal haben in den Legierungen mit III B- und IV B-Elementen Koordinationszahlen von 10 bis 17, die III B- und IV B-Elemente solche von 6 bis 14. In dieser Arbeit werden die Koordinationspolyeder um Nb, Ta und um die III B- und IV B-Elemente beschrieben, wobei eine neue Symbolik verwendet wird. Die Beschreibung erfolgt mit dem Polyederpackungs-Modell. Es zeigt sich, daß die meisten Strukturen mit einer oder zwei Polyedersorten aufgebaut werden können.

Introduction

A fruitful approach to understand the crystal chemical features of alloy structures is to consider the coordination spheres around particular atoms. *Frank* and *Kasper*[1,2] considered the coordination geometries around an atom as made up of only triangular faces and examined the topological and geometrical properties of the triangulated shells with

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CN 12, 14, 15, and 16. The coordination characteristics of structural types with high coordination numbers have been studied by *Kripyakevich*[3]. He has also deduced the characteristics of the polyhedra with CN 12 to 17, 20, 22, and 24.

A glance through the literature on the crystal structures of alloys shows that very few papers (*Brown*[4, 5]; *Girgis, Petter,* and *Pupp*[6]) deal with the coordination polyhedra as building blocks of the structure. Such a description of structures, even though not supported by any specific theory of the structures, arises from observations of their pecularities and the most general inferences that can be drawn from them (*Black*[7]). *An approach to characterize the polyhedra in various known binary alloys and to use them to build up the structures* has been introduced by *Bhandary* and *Girgis*[8]. Their aim was to present a simple description of the complex alloy structures and to classify the different known structure types. The aim of this study is to verify the general applicability of this model for binary intermetallic compounds. We examined for this purpose the alloys of Nb (Ta) with group III B and IV B elements.

Coordination Polyhedra

In order to define a coordination polyhedron it is essential to limit the coordination sphere of an atom. During the last half century many attempts have been made to suggest methods for limiting the coordination sphere of atoms in alloys (*Brunner* and *Laves*[9]). The coordination sphere as defined by the maximum gap concept (*Brunner* and *Schwarzenbach*[10]) seems to be a realistic factor (*Brunner*[11]). *Bhandary* and *Girgis*[12] studied the coordination behavior of V in its binary alloys with III B and IV B elements using the maximum gap concept to limit the coordination sphere of V and the B-elements. In this study too, we used the maximum gap concept to limit the coordination sphere.

To define a coordination polyhedron, we first limit the coordination sphere. *Brunner*[11] proposed the "$1/d$ method". The normalized $1/d_n$, where d_n is the interatomic distance between the central atom and the n^{th} neighbour, versus the number of atoms are represented in a histogram. The widest range in which no atoms are present is called the "max. gap". The number of neighbours before the "max. gap" is taken to be the coordination number (CN). The atoms (neighbours) constitute the coordination polyhedron for the corresponding (central) atom.

Niobium and Tantalum exhibit a range of coordination numbers from 10 to 17 in these alloys; the B-elements CN range from 6 to 14. The geometries of these coordinations (coordination polyhedra) have been characterized and are listed in Tables 1 and 2 and are shown in Fig. 1.

Table 1. *Description of polyhedra from the transition-elements (Nb, Ta)*

	CN	Polyhedron	Sym.	Ideal.	No. of faces* △	No. of faces* □	Arrangement of vertices**	Found in
I	10	10-verticon of $ZrSi_2$-type	mm2		6	5	$3^4:2^3+2^4:3^4$	$TaAl_2$
II	11	11-verticon of ß-Ti_6Sn_5-type	m		18		$2^5:1^4:1^6:2^5:2^4+2^5:1^6$	Nb_6Sn_5
III	11	11-verticon of Ti_5Ga_4-type	mm2		6	6	$1^3:3^4:3^4:3^4:1^3$	Nb_5Ga_4, $Nb_{10}Ge_7$
IV	12	Cubooctahedron (tetr.dist.)	4/mmm	m3m	8	6	$4^4:4^4:4^4$	Nb_5Ga_{13}, $TaGa_3$
V	12	Cubooctahedron	m3m	m3m	8	6	$4^4:4^4:4^4$	Nb_3Si, Ta_3Si, Ta_3Ge
VI	12	Kasper (distorted)	$\bar{1}$	$\bar{5}\bar{3}$ (2/m)	20		$2^5:2^5:4^5:2^5:2^5$	Nb_6Sn_5
VII	12	12-verticon of Ni_3Sn-type	mm2	$\vec{6}$m2	8	6	$3^4:6^4:3^4$	Ta_3Si
VIII	12	12-verticon of ß-Ti_6Sn_5-type	mm2		16	2	$3^5:2^4:1^6+1^4:2^4:3^5$	Nb_6Sn_5
IX	13	13-verticon of Ni_3P-type	1		22		$2^5:1^6+1^5+1^4:2^5+1^6:3^5:2^5$	Ta_3Ge
X	14	Kasper (distorted)	mm2	$\bar{1}\bar{2}\cdot$2m	24		$3^5:3^5:2^6:3^5:3^5$	x
XI	14	14-verticon of $CrSi_2$-type	222		20	2	$2^4+2^5:2^6+4^5:2^4+2^5$	$NbSi_2$, $NbGe_2$, $TaSi_2$
XII	14	Tetrakishexahedron (t.d.)	4/mmm	$\bar{4}$3m	24		$1^4:4^6:4^4:4^6:1^4$	o, Nb_3Ga_2, Nb_5Si_3, Ta_3Ga_2
XIII	14	14-verticon of Ni_3P-type	1		24		$3^5:2^6+1^5:2^4+1^6:2^4:3^5$	Ta_3Ge
XIV	15	Kasper (distorted)	mm2	$\bar{6}$m2	26		$2^5:4^5:2^6:2^5:4^5:1^6$	Nb_6Sn_5
XV	15	15-verticon of Al_2Cu-type	mm2		22	2	$2^5+1^6:2^4:4^5+1^6:2^4:2^5+1^6$	Ta_2Si
XVI	16	16-verticon of Cr_5B_3-type	m		24	2	$2^5+1^6:2^4:4^5+1^6:3^6+2^4+1^3$	Nb_5Si_3, Ta_5Ga_3, Ta_5Si_3
XVII	16	Kasper	$\bar{4}$3m	$\bar{4}$3m	28		$2^5:2^6:4^5:4^5:2^6:2^5$	$Ta_{17}Al_{12}$
XVIII	17	17-verticon of U_3Si_2-type	mm2		26	2	$1^5:1^4+4^5:4^5+1^6:1^4+4^5:1^6$	Nb_3Ga_2, Ta_3Ga_2

* △ Triangular ; □ Quadrangular

** Bhandary, Girgis [8]

x Ta_2Al, Nb_2Al, Ta_3Al, Nb_5Ga_4, $Nb_{10}Ge_7$, Nb_3Si, Ta_3Ge, Ta_3Si

o Ta_5Ga, Ta_5Si_3, Ta_5Ge_3

Table 2. *Description of polyhedra from B-elements*

	CN	Polyhedron	Sym.	Ideal.	No. of faces* △	□	Arrangement of vertices**	Found in
XIX	6	Bicapped rhombohedron	3m		8		$3^4:3^4$	Nb_2AlC,Nb_2SnC,Ta_2AlC
XX	7	7-verticon of β-Ti_6Sn_5-type	m		8	1	$2^4:2^3:1^6:2^4$	Nb_6Sn_5
XXl	8	8-verticon of $ZrSi_2$-type	mm2		4	4	$2^4+1^3:2^3:2^4+1^3$	$TaAl_2$
XXII	8	8-verticon of β-Ti_6Sn_5-type	mm2		10	1	$3^4:2^5:3^4$	$TaAl_2$, Nb_6Sn_5
XXIII	8	8-verticon of β-Ti_6Sn_5-type	mm2		12		$1^3:2^4:1^4+1^6:2^5:1^3$	Nb_6Sn_5
XXIV	9	9-verticon of Cr_5B_3-type	mm2		14		$3^5:3^4:3^5$	x
XXV	10	Bicapped square antiprism	422	$\bar{8}$2m	16		$1^4:4^5:4^5:1^4$	o
IV	12	Cubooctahedron (tetr.dist.)	mmm	m3m	8	6	$4^4:4^4:4^4$	$TaGa_3$
VI	12	Kasper (distorted)	m	$\bar{5}\bar{3}$(2/m)	20		$2^5:2^5:4^5:2^5:2^5$	Ta_2Al,Nb_2Al, Ta_3Al
VII	12	12-verticon of Ni_3Sn-type	$\bar{6}$m2		8	6	$3^4:6^4:3^4$	+
XXVI	13	13-verticon of Ti_5Ga_4-type	mm2		14	4	$2^4:2^5+1^4:3^4:2^5+1^4:2^4$	Nb_5Ga_4,$Nb_{10}Ge_7$
XXVII	13	13-verticon of α-Mn-type	m		20	1	$1^6:2^4:2^5:2^5:2^5:2^5:1^5:1^5$	$Ta_{17}Al_{12}$
Xl	14	14-verticon of U_3Si_2-type	2		20	2	$2^4+2^5:2^6+4^5:2^4+2^5$	$NbSi_2$,$NbGe_2$, $TaSi_2$,$TaGe_2$
XII	14	14-verticon of Ti_5Ga_4-type	$\bar{3}$m		24	0	$1^6:3^4+3^6:3^4+3^6:1^6$	Nb_5Ga_4,$Nb_{10}Ge_7$
XIV	15	Kasper (distorted)	mm2	$\bar{6}$m2	26	0	$1^6:4^5:2^5:4^5:2^6:2^5$	Nb_6Sn_5

* Triangular ; Quadrangular

** Bhandary,Girgis [8]

x Nb_3Ga_2,Nb_5Si_3,Ta_3Ga_2,Ta_5Ga_3,Ta_5Si_3,Ta_5Ge_3,Ta_3Ge,Nb_3Si,Ta_3Ge

o Nb_5Si_3,Ta_2Si,Ta_5Ga_3,Ta_5Si_3,Ta_5Ge_3

\+ Ta_3Si,Nb_2AlC,Nb_2SnC,Ta_2AlC

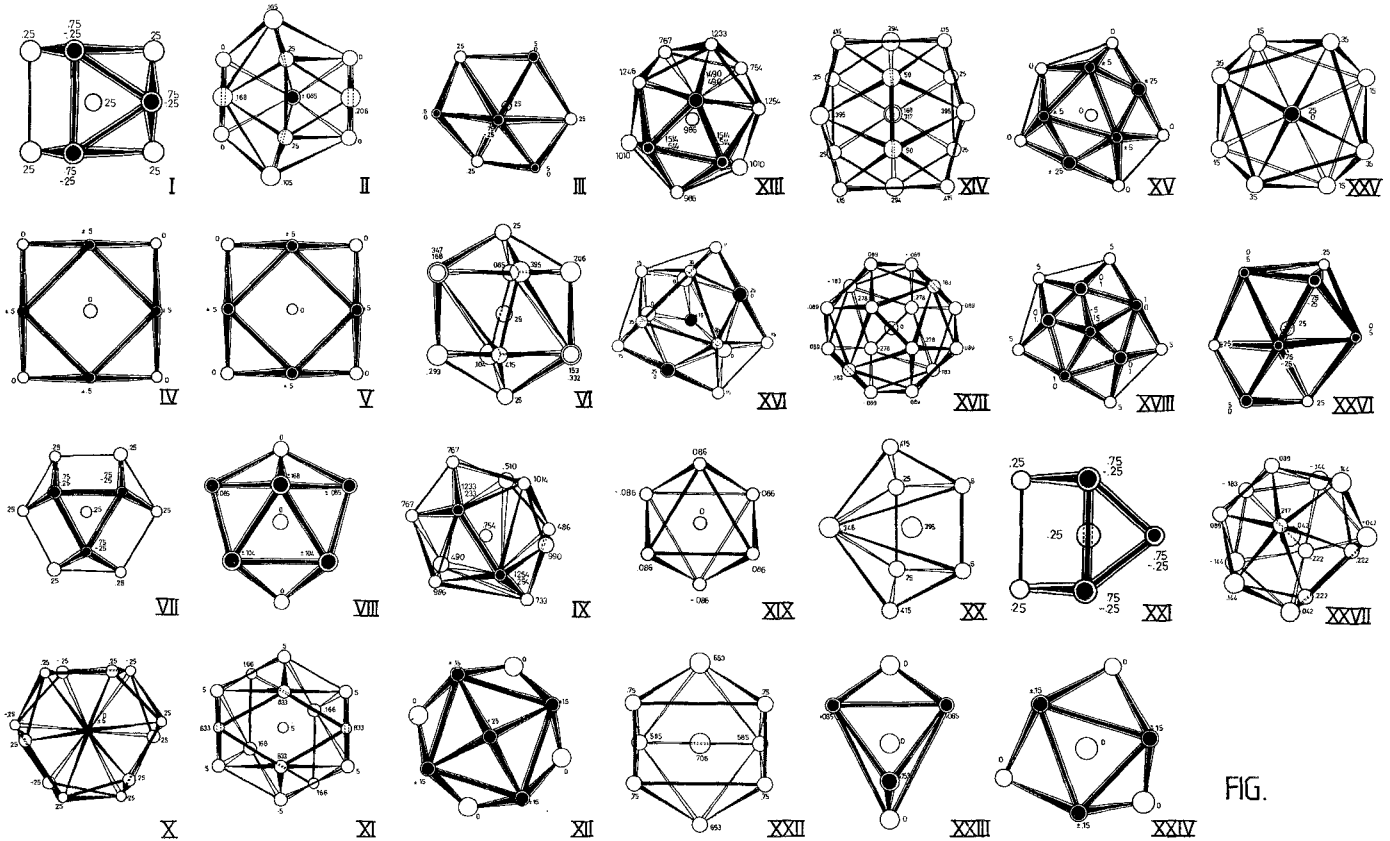


FIG.

Fig. 1. Polyhedra arranged according to the number of vertices for the transition-elements and for the B-elements

The symmetry given is that found for the figure obtained from the structural parameters reported. In some cases the idealized symmetry has been indicated. Each polyhedron has been described in terms of certain symbols according to the arrangement of vertices; hence, $1^6:4^4+2^5:2^4+3^5:1^5$ means that starting from a six-fold vertex at the top there is a plane of four four-fold and two five-fold vertices followed by another plane of two four-fold and three five-fold vertices and a five-fold vertex at the bottom. The starting point of the description is located either on a symmetry axis or a symmetry plane. An n-fold vertex is taken to mean a point where n edges meet (for the sake of convenience we have not considered the symmetry of the vertex).

Description of Alloy Structures by Means of Polyhedra Packing

The phases found in the Nb(Ta)-III B(IV B)-binary systems, *Pearson* symbols and structure types are given in Table 3. *The structure of one representative of each structure type is described in terms of polyhedra packing which is valid for the rest of the representatives also.* Wherever the structure has already been determined the positional parameters have been used to calculate the necessary details of the structure and in case of characterization of the alloy in terms of structure type the parameters from that type are taken. It will be seen in the following sections that the structures could be explained using one or at most a few polyhedra.

Nb-Al *System*

$NbAl_3$, Nb_2Al, and Nb_3Al phases have been found in this system.

Nb_2Al (σ-FeCr *Type*)[13]

Nb_2Al crystallizes in the tetragonal space group $P4_2/mnm$ and has 30 atoms in the unit cell. The Al_2 (8 i) atom is twelve coordinated, building a "distorted icosahedron" having a mm2 symmetry.

The structure can be described by packing Al_2 ($z = 0$) polyhedra which build a zig-zag chain along the b-axis (Fig. 2) sharing a corner and an edge alternatively with each other. A similar chain of Al_2 ($z = 1/2$) polyhedra is also present. These 2 chains share atoms with each other as shown in Fig. 2. Along the c-axis the Al_2 polyhedra share the upper edges with each other.

Nb-Ga *System*

$NbGa_3$, Nb_5Ga_{13}, Nb_5Ga_4, Nb_3Ga_2, Nb_5Ga_3, and Nb_3Ga phases are present in this system.

Table 3. *Phases present in the Nb(Ta)-III B(IV B)-binary systems*

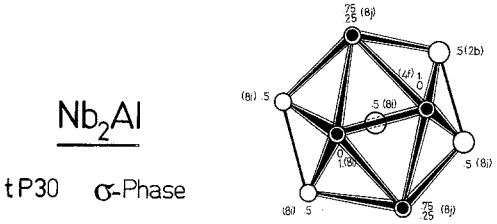
T:B \ System	Nb-Al	Nb-Ga	Nb-Si	Nb-Ge	Nb-Sn	Ta-Al	Ta-Ga	Ta-Si	Ta- Ge
3:1	Nb_3Al cP8 Cr_3Si	Nb_3Ga cP8 Cr_3Si	Nb_3Si cP8 AuCu$_3$- tP32 Ti_3P	Nb_3Ge cP8 Cr_3Si	Nb_3Sn cP8 Cr_3Si	Ta_3Al tP30 σ-phase		$Ta_3(Ta_{.28}Si_{.72})$ hP8 Ni_3Sn Ta_3Si tP32 Ti_3P	Ta_3Ge tI32 Ni_3P tP32 Ti_3P
2:1	Nb_2Al tP30 σ-Phase					Ta_2Al tP30 σ-phase		Ta_2Si tI12 Al_2Cu	
5:3		Nb_5Ga_3 tI32 W_5Si_3 $Nb_5Ga_3(C_x)$ hP16 Mn_5Si_3	Nb_5Si_3 tI32 Cr_5B_3 tI32 W_5Si_3 $Nb_5Si_3(C_x)$ hP16 Mn_5Si_3	Nb_5Ge_3 tI32 W_5Si_3 $Nb_5Ge_3(C_x)$ hP16 Mn_5Si_3			Ta_5Ga_3 tI32 W_5Si_3 tI32 Cr_5B_3 $Ta_5Ga_3(C_x)$ hP16 Mn_5Si_3	Ta_5Si_3 tI32 W_5Si_3 tI32 Cr_5B_3 $Ta_5Si_3(C_x)$ hP16 Mn_5Si_3	Ta_5Ge_3 tI32 W_5Si_3 tI32 Cr_5B_3 $Ta_5Ge_3(C_x)$ hP16 Mn_5Si_3
3:2		Nb_3Ga_2 tP10 U_3Si_2					Ta_3Ga_2 tP10 U_3Si_2		
10:7				$Nb_{10}Ge_7$ hP17 "Ti_5Ga"*					
17:12						$Ta_{17}Al_{12}$ cI58 α-Mn			
5:4		Nb_5Ga_4 hP18 Ti_5Ga_4							
6:5					Nb_6Sn_5 oI44 β-Ti_6Sn_5				
1:2			$NbSi_2$ hP9 $CrSi_2$	$NbGe_2$ hP9 $CrSi_2$	$NbSn_2$ oF48 Mg_2Cu			$TaSi_2$ hP9 $CrSi_2$	$TaGe_2$ hP9 $CrSi_2$
5:13		Nb_5Ga_{13} oA36 Nb_5Ga_{13}							
1:3	$NbAl_3$ tI8 $TiAl_3$	$NbGa_3$ tI8 $TiAl_3$				$TaAl_3$ tI8 $TiAl_3$	$TaGa_3$ tI8 $TiAl_3$		

* as Ti_5Ga_4 type but the 2b equivalent position is half occupied.

Further the following compounds of the Cr_3Si structure type in the Nb-In, Nb-Pb and Ta-Sn systems are known: Nb_3In, Nb_3Pb, Ta_3Sn.

Nb_5Ga_{13} (Nb_5Ga_{13} *Type*)[14]

Nb_5Ga_{13} crystallizes in the orthorhombic space group Ammm and has 36 atoms per unit cell. The structures building polyhedra are Nb_1 (2 b), Nb_2 (4 j), and Nb_3 (4 i). The 3 polyhedra are similar; Nb_1 and Nb_2 are tetragonally distorted cubooctahedra (CN 12) with the symmetry 4/mmm, while Nb_3 has a symmetry 4 mm (Fig. 3).



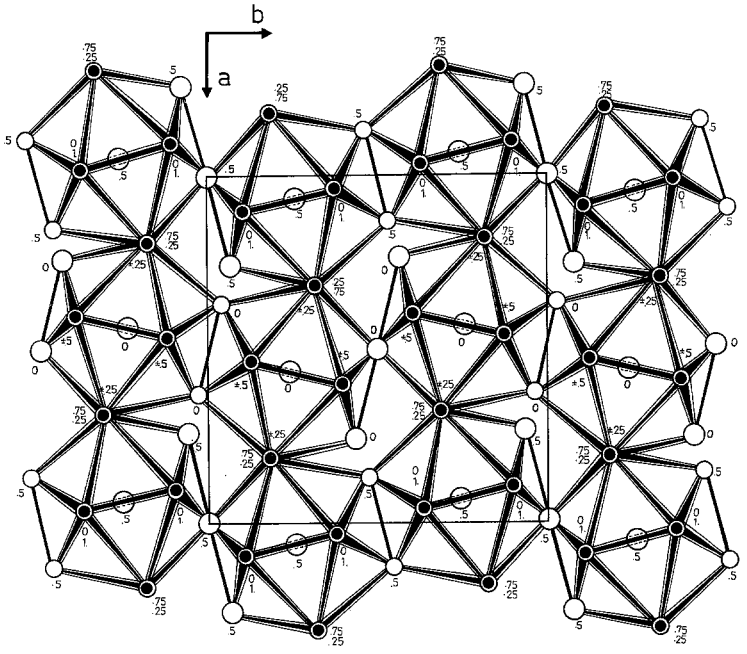


Fig. 2. Structure of Nb_2Al (tP 30 σ-FeCr type)

The Nb_3 polyhedra share quadrangular faces with each other along the *a*- and *b*-axes. The same is valid for the Nb_1 and Nb_2 polyhedra. The sequence of polyhedra along the *c*-axis is Nb_3—Nb_2—Nb_1—Nb_2. These polyhedra share edges with each other along the *c*-direction.

Nb_5Ga_4 (Ti_5Ga_4 *Type*)[14]

Nb_5Ga_4 crystallizes in the hexagonal space group $P\,6_3/mcm$ with 18 atoms per unit cell and belongs to the Ti_5Ga_4 type.

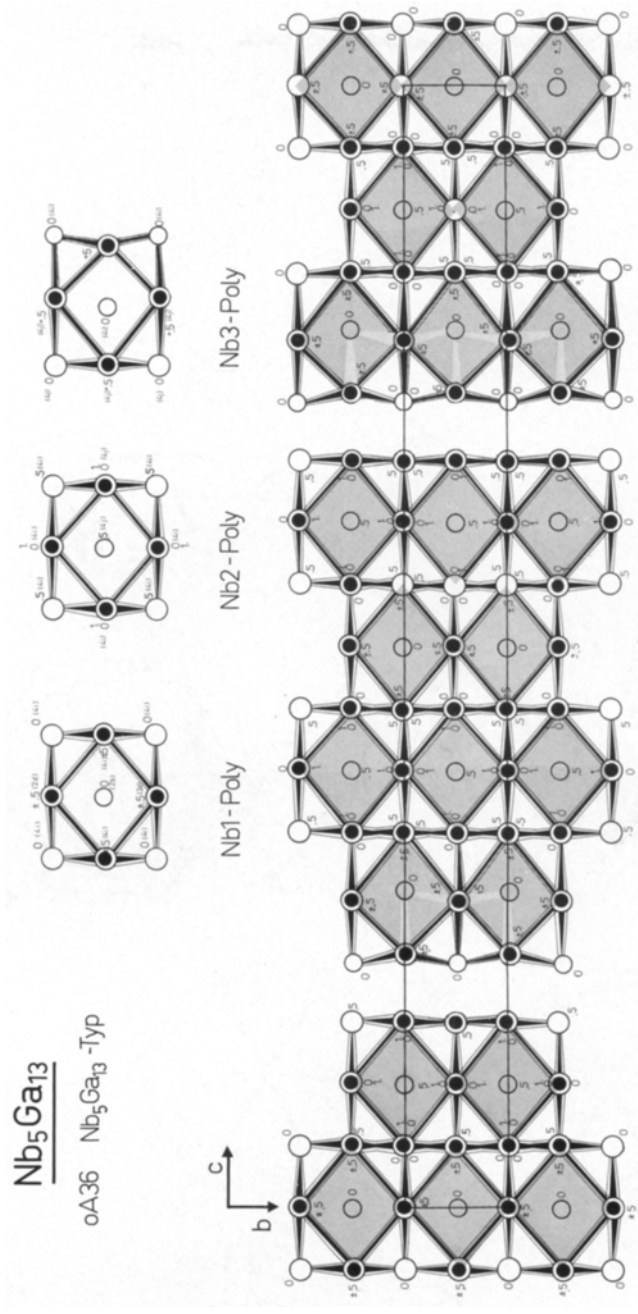


Fig. 3. Structure of Nb_5Ga_{13} (oA 36 Nb_5Ga_{13} type)

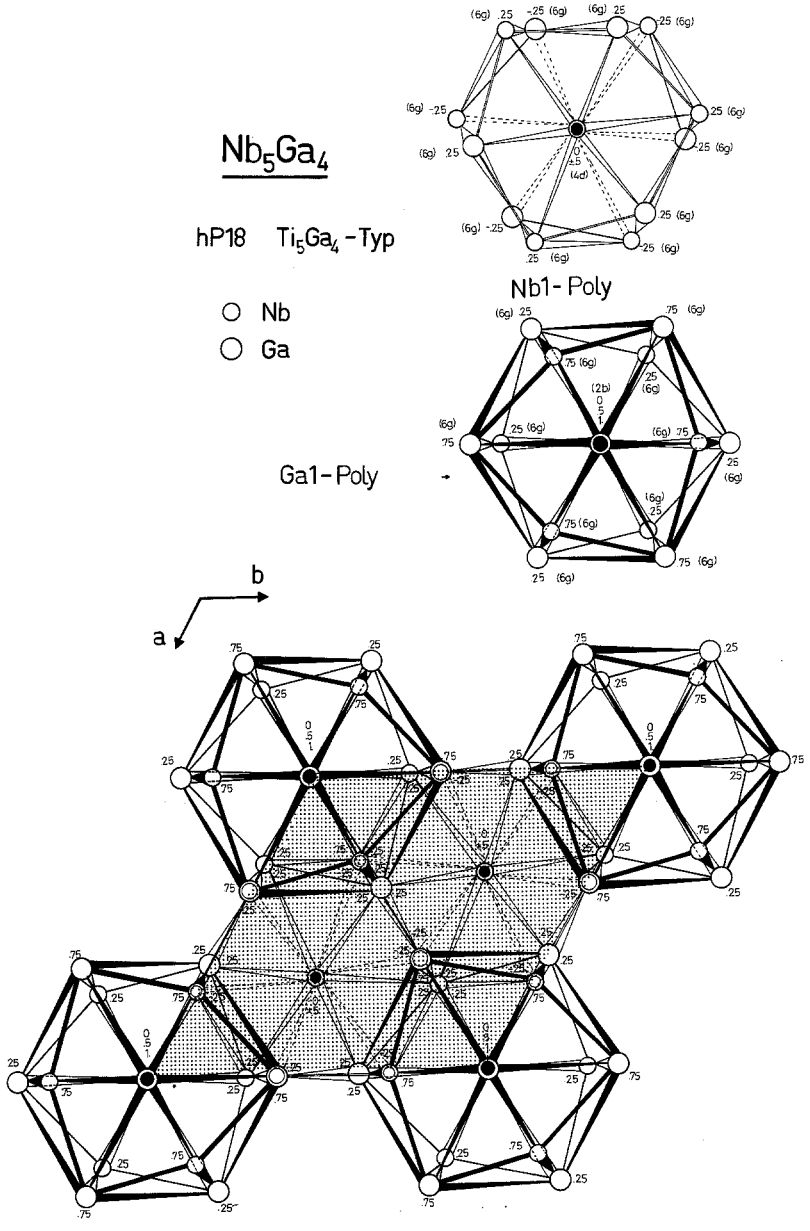


Fig. 4. Structure of Nb_5Ga_4 (hP 18 Ti_5Ga_4 type)

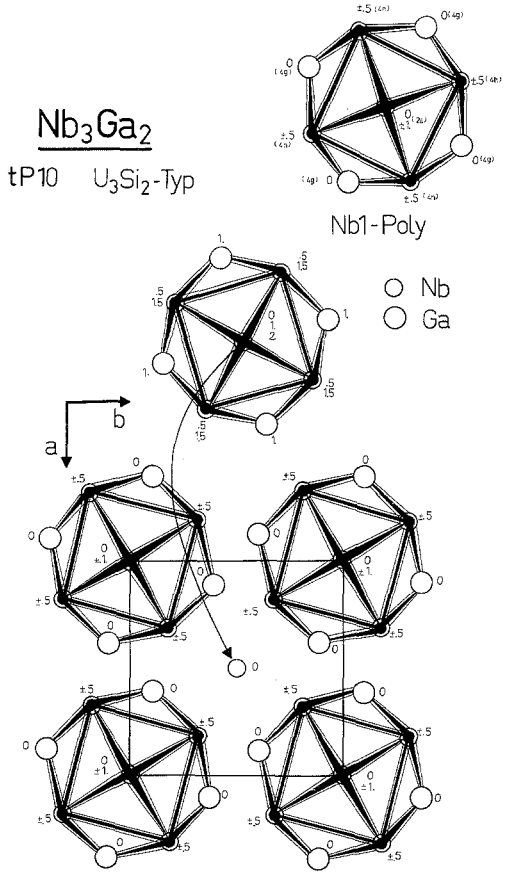


Fig. 5. Structure of Nb_3Ga_2 (tP 10 U_3Si_2 type)

The structure can be described in terms of packing Nb_1 and Ga_1 polyhedra. The polyhedron around Nb_1 (4 d) is a 12-, 14-, 15-, or 16-Kasper polyhedron with the 32 symmetry. Ga_1 (2 b) is surrounded by a 14-*Kasper* polyhedron of $\bar{3}$ m symmetry.

The Nb_1 ($z = 0$) polyhedron is surrounded by 3 Nb_1 polyhedra sharing a triangular face with each other; (in Fig. 4 just one of them is shown). The Ga_1 ($z = 1/2$) polyhedra also share a triangular face with each of the Nb_1 polyhedra.

The Nb_1 (as well as Ga_1) polyhedra share among each other apices along the c-directions. The shaded area in the figure shows the unit cell.

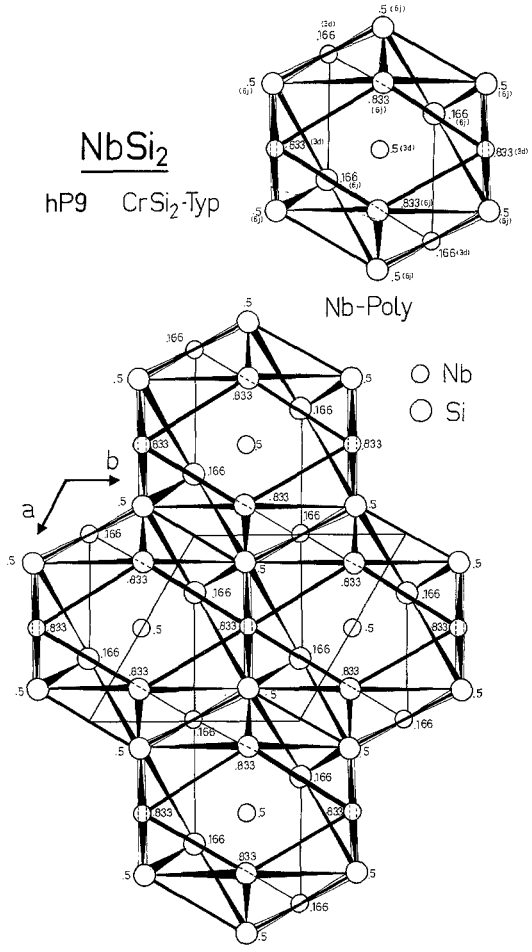


Fig. 6. Structure of $NbSi_2$ (hP 9 $CrSi_2$ type)

Nb_3Ga_2 (U_3Si_2 *Type*)[13]

Nb_3Ga_2 belongs to the U_3Si_2 type and crystallizes in the tetragonal space group P 4/mbm with 10 atoms per cell. The structure can be built up by Nb_1 polyhedra (tetrakishexahedra with 4/mmm symmetry; idealized: $\bar{4}3$ m).

At the centre of the unit cell there is a tetrakishexahedron which is surrounded by 4 other tetrakishexahedra, four corners of the central polyhedron being shared by a corner of one of the surrounding

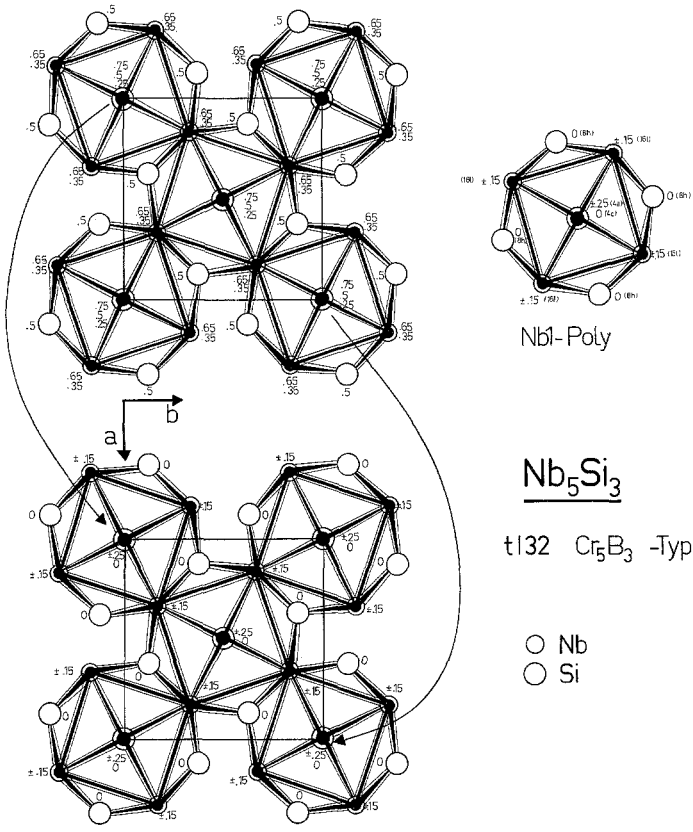


Fig. 7. Structure of Nb_5Si_3 (tI 32 Cr_5B_3 type)

polyhedra. The latter are 180° rotated along the [010] direction with respect to the central polyhedron (Fig. 5).

The polyhedra at the corners as well as in the centre of the cell form parallel chains along the *c*-axis sharing apices.

Nb-Si *System*

$NbSi_2$, Nb_5Si_3 and Nb_3Si phases are known in this system.

$NbSi_2$ ($CrSi_2$ *Type*)[13]

$NbSi_2$ crystallizes in the hexagonal space group $P6_222$ with the $CrSi_2$ type. The Nb atom has CN 14. The polyhedron around Nb has 20 triangular and 2 quadrangular faces with 222 symmetry.

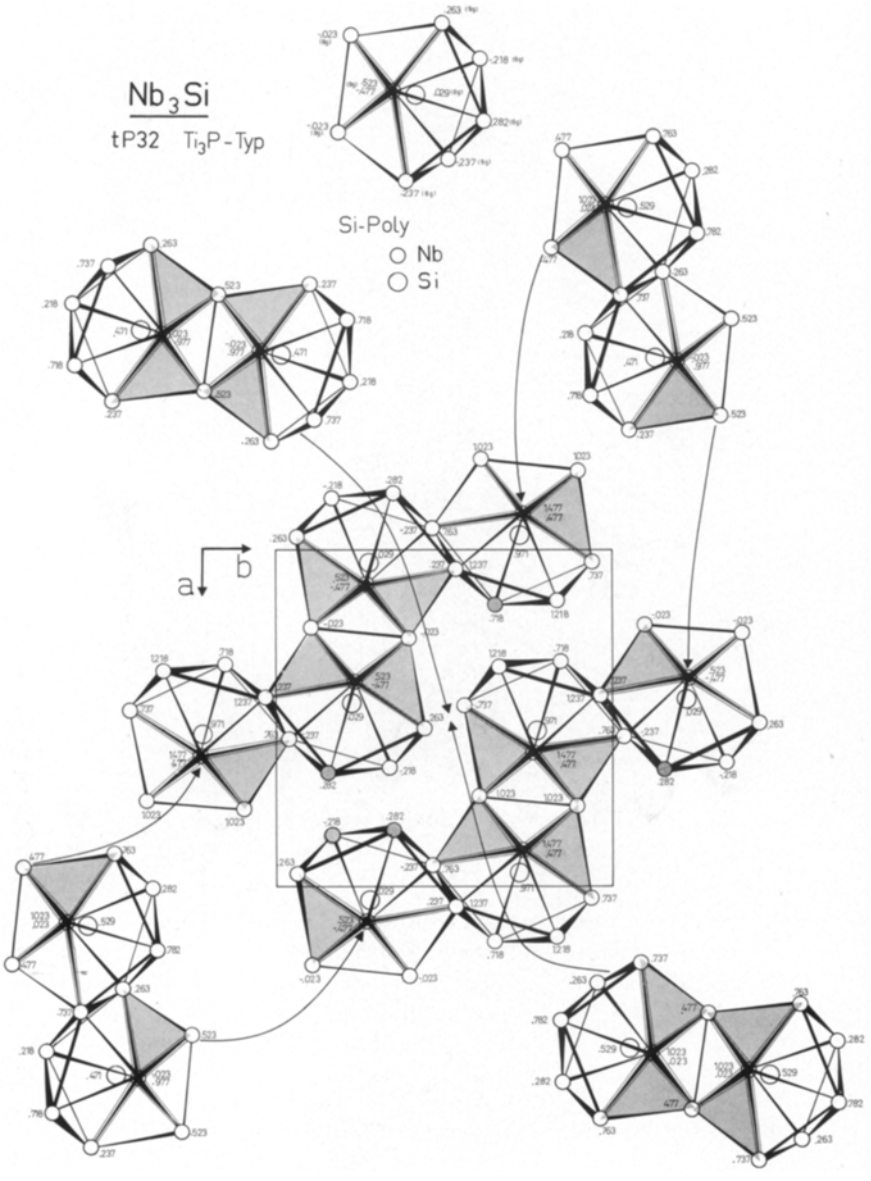


Fig. 8. Structure of Nb_3Si (tP 32 Ti_3P type)

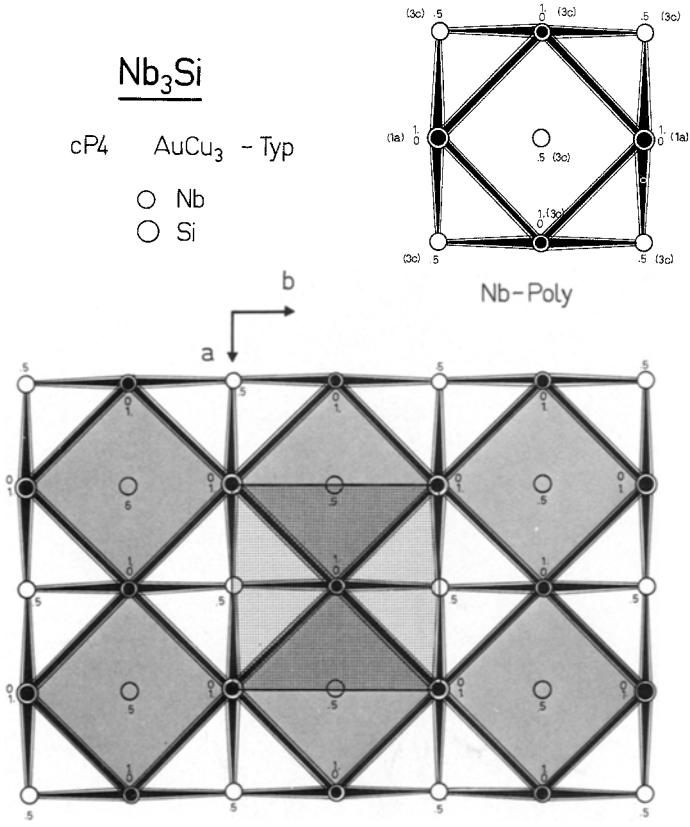


Fig. 9. Structure of Nb_3Si (cP 4 $AuCu_3$ type)

The structure can be described (Fig. 6) in terms of the packing of these Nb polyhedra. Each polyhedron is surrounded by six others sharing a common triangular face or an edge in the following sequence: a triangular face, a triangular face, an edge, a triangular face, a triangular face, and an edge.

Similar layers are located above and below this "polyhedra sheet" in the *c*-direction: the distance between the layers is 0.219 nm.

Nb_5Si_3 (Cr_5B_3 *Type*)[13]

Nb_5Si_3 crystallizes in the tetragonal space group I 4/mcm and belongs to the Cr_5B_3 type with 32 atoms/unit cell.

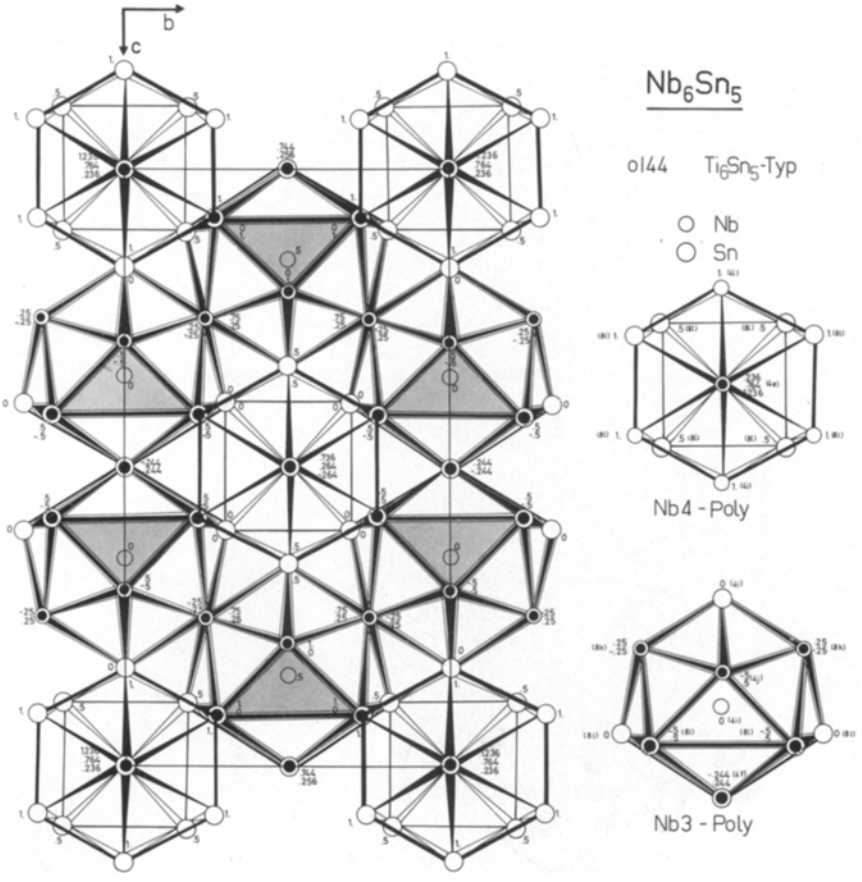


Fig. 10. Structure of Nb_6Sn_5 (oI 44 β-Ti_6Sn_5 type)

The structure can be built up of Nb_1 polyhedra (tetrakishexahedra with 4/mmm symmetry).

Each Nb_1 polyhedron is surrounded by 4 others at the same height, a triangular face being common to each. A similar "polyhedra layer" rotated by 180° along *c* lies above it, sharing apices, thus building Cr—Cr-chains along the *c*-axis (Fig. 7).

Nb_3Si (Ti_3P *Type*)[15]

Nb_3Si is a representative of the Ti_3P type with 32 atoms/unit cell and crystallizes in the tetragonal space group $P4_2/n$. The 9 verticon

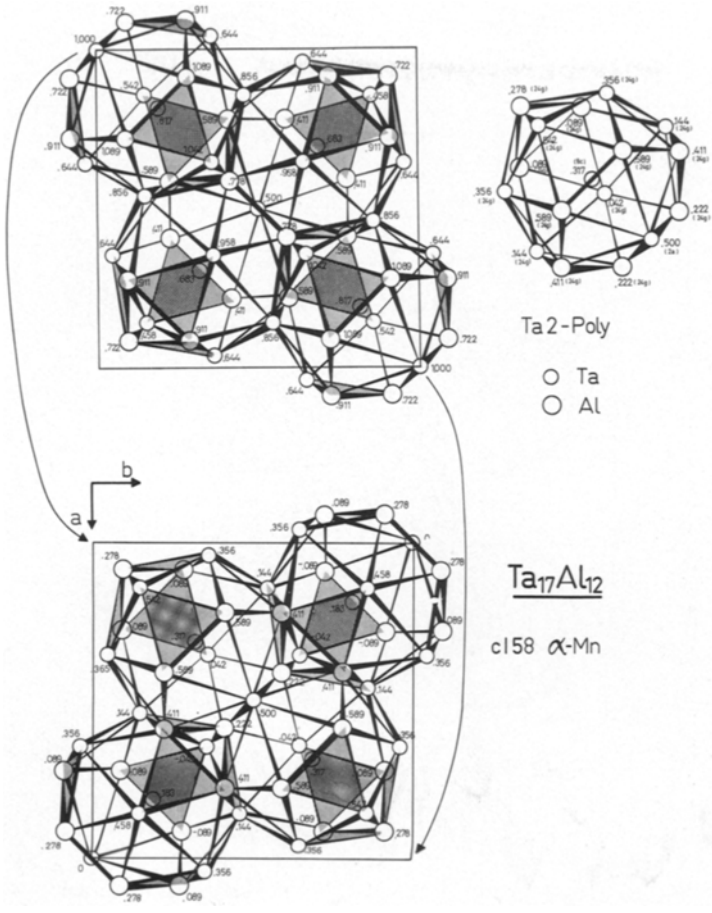


Fig. 11. Structure of $Ta_{17}Al_{12}$ (cI 58 α-Mn type)

polyhedron around Si has the symmetry 1. The Si polyhedra at almost the same height (around Si with $z = 0.029$ and 0.971) form a zig-zag chain, an edge being shared as shown in Fig. 8. Those polyhedra (around Si with $z = 0.471$ and 0.529 respectively) have a similar arrangement and share a triangular face (shaded in the figure) and an atom with each of the lower polyhedra.

Nb_3Si ($AuCu_3$ *Type*)[13]

Nb_3Si belongs to $AuCu_3$ type with 4 atoms/unit cell and crystallizes

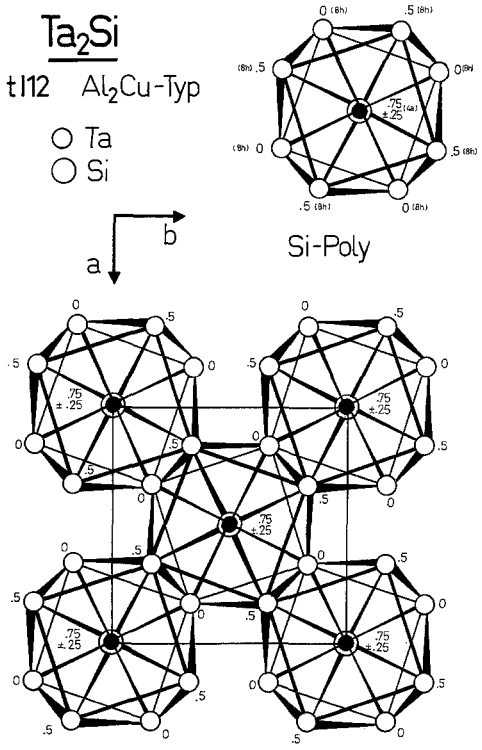


Fig. 12. Structure of Ta_2Si (tI 12 Al_2Cu type)

in the cubic space group Pm3m. The polyhedron around Nb is a cubooctahedron with m3m symmetry.

Each cubooctahedron shares one quadrangular face with its neighbour at the same height and another quadrangular face with the upper as well as with the lower cubooctahedra (Fig. 9).

Nb-Ge *System*

$NbGe_2$, $Nb_{10}Ge_7$, Nb_5Ge_3, and Nb_3Ge phases are found in this system.

$Nb_{10}Ge_7$ ("Ti_5Ga_4" *Type*)[16]

This compound possesses the arrangement of the representatives of the Ti_5Ga_4 type but in this case the 2 b equivalent position is half occupied.

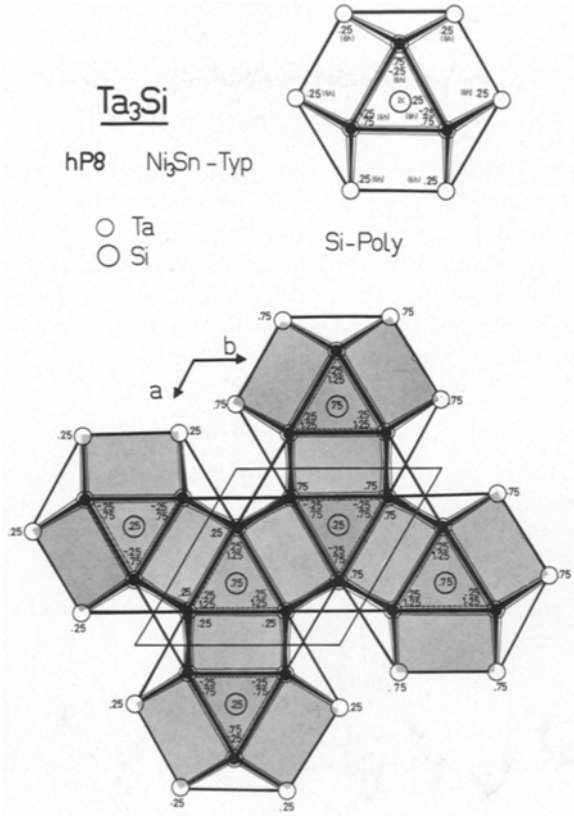


Fig. 13. Structure of $Ta_{3.28}Si_{0.72}$ (hP 8 Ni_3Sn type)

Nb-Sn *System*

$NbSn_2$, Nb_6Sn_5, and Nb_3Sn phases are present in this system.

Nb_6Sn_5 (β-Ti_6Sn_5 *Type*)[13]

Nb_6Sn_5 belongs to the β-Ti_6Sn_5 type. It crystallizes in the orthorhombic space group Immm with 44 atoms per unit cell.

The structure can be described on the basis of the packing of a 15 verticon *Kasper* polyhedron (Nb_3) with the symmetry mm 2 and a 12 verticon, one around Nb_4 of the β-Ti_6Sn_5 with the symmetry mm 2. The Nb_3 polyhedra form chains along the *a*-direction by sharing the shaded triangular faces (Fig. 10). The Nb_4 polyhedra also form chains (along the *a*-direction) by sharing apices. Each Nb_4 polyhedron is surrounded by six Nb_3 polyhedra, an atom being shared by each.

Ta-Al *System*

$TaAl_3$, $Ta_{17}Al_{12}$, Ta_2Al, and Ta_3Al phases are known in this system.

$Ta_{17}Al_{12}$ (α-Mn *Type*)[17]

$Ta_{17}Al_{12}$ crystallizes in the cubic space group $I\bar{4}3m$ and belongs to the α-Mn type with 58 atoms per cell. This complicated structure can be described using only one polyhedron. The Ta_1 polyhedron is a distorted 16 *Kasper* polyhedron. These polyhedra share with the surrounding ones (alternately) an edge and a triangular face building a layer of polyhedra. A similar layer, rotated by 90° with respect to the lower one, lies over it, sharing the shaded triangular faces (Fig. 11).

Ta-Si *System*

$TaSi_2$, Ta_5Si_3, Ta_2Si, Ta_3Si, and $Ta_3(Ta_{0.28}Si_{0.72})$ phases have been reported in the literature.

Ta_2Si (Al_2Cu *Type*)[13]

Ta_2Si crystallizes in the tetragonal space group $I4/mcm$ and belongs to the Al_2Cu type with 12 atoms per unit cell. The Si is twelve coordinated building a bicapped square antiprism with the symmetry 422. The structure can be described in terms of packing these polyhedra. Polyhedra at the same height share edges with each other and apices with both the lower and the upper ones forming Ta—Ta chains (Fig. 12).

$Ta_3(Ta_{0.28}Si_{0.72})$ (Ni_3Sn *Type*)[13]

$Ta_{3.28}Si_{0.72}$ is a representative of the Ni_3Sn type and crystallizes in the hexagonal space group $P6_3mmc$ with 8 atoms per unit cell. The 12 verticon around Si is formed by 8 triangular and 6 quadrangular faces and has $\bar{6}m2$ symmetry (coordination polyhedra in hexagonal packing). The polyhedron around Si at $z = 0.25$ shares with 3 surrounding polyhedra (around Si at $z = 0.75$) a quadrangular face each. Along the c-axis it shares at triangular face with identical upper and lower polyhedra (Fig. 13).

Ta-Ge *System*

$TaGe_2$, Ta_5Ge_3, and Ta_3Ge phases are known in this system.

Ta_3Ge (Ni_3P *Type*)[18]

Ta_3Ge crystallizes in the tetragonal space group $I\bar{4}$ and belongs to the Ni_3P structure type with 32 atoms/unit cell.

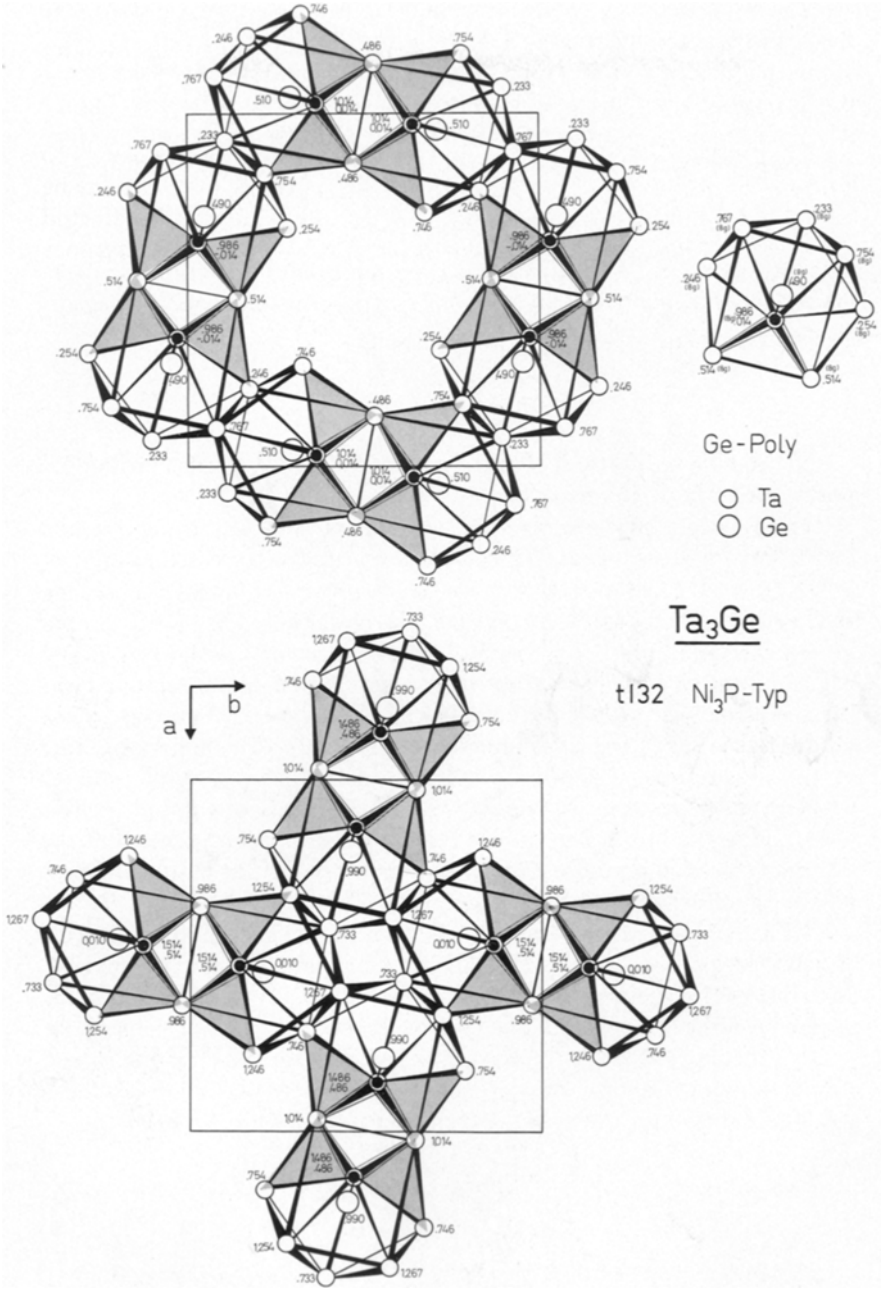


Fig. 14. Structure of Ta_3Ge (tI 32 Ni_3P type)

The 9 verticon polyhedron around Ge is formed by 14 triangular faces and has the symmetry 1.

Ge polyhedra at almost the same height (around Ge at $z = 0.990$ and 0.010 respectively) share an edge with each other as shown in Fig. 14. They share triangular faces (shaded in Fig. 14) with those around Ge at $z = 0.490$ and 0.510 respectively.

Nb-In, Nb-Pb, *and* Ta-Sn *Systems*

Only the Cr_3Si (A 15) phase has been reported in these systems. The crystal data are given in Table 3. For Cr_3Si description see *Bhandary* and *Girgis*[8].

Conclusion

Nb and Ta exhibit CN 10 to 17 and a wide variety of coordination polyhedra. The B-elements have CN 6 to 14.

The relation between the CN and the number of triangular and quadrangular faces forming the polyhedron can be expressed as follows:

$$\mathrm{CN} = (n \triangle + 2m \square + 4)/2$$

where n and m are the number of triangular and quadrangular faces (derived from the *Euler* formula). If we restrict the CN from 6 to 17 as found in this study and by *Bhandary* and *Girgis*[12] we come to a number of 142 theoretically possible polyhedra (only formed by $\triangle$ and $\square$ without consideration of symmetry). The 39 polyhedra found (in this work and in the literature) show a high number of $\triangle$. It seems that the intermetallic compounds form preferably polyhedra with the most possible number of triangular faces.

All structures (structure types) examined could be described in terms of packing of one or two polyhedra. This model delivers an easy description of structures even for quite complicated ones. *The polyhedra packing model can be used for all representatives of a certain structure type.*

Icosahedra, *Kasper* (14 verticon) polyhedra, tetrakishexahedra and cubooctahedra play an important role in the explanation of these structures although they belong to different structure types.

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