

Chemistry of Metals and Alloys

Table S1

Interatomic distances, coordination numbers and coordination polyhedra for the atoms in the structure of the $\text{HfAu}_{0.61}\text{Al}_{1.39}$ intermetallic compound

Atoms	d (Å)	CN	CP
Hf1 - - 6M2 - 3M3 - 3M1 - 1Hf1 - 3Hf2	3.071(1) 3.079(3) 3.108(1) 3.145(3) 3.236(1)	16	Frank-Kasper
Hf2 - - 3M2 - 3M1 - 6M3 - 1Hf2 - 3Hf1	3.068(2) 3.083(1) 3.095(5) 3.234(3) 3.236(1)	16	Frank-Kasper
M1 - - 3M3 - 3M2 - 3Hf2 - 3Hf1	2.621(6) 2.667(4) 3.083(1) 3.108(1)	12	Icosahedron
M2 - - 4M2 - 2M1 - 4Hf1 - 2Hf2	2.638(1) 2.667(4) 3.071(1) 3.068(1)	12	Icosahedron
M3 - - 2M3 - 2M1 - 2M3 - 2Hf1 - 4Hf2	2.539(7) 2.621(6) 2.737(7) 3.079(3) 3.095(5)	12	Icosahedron

Table S2
 Interatomic distances, coordination numbers and coordination polyhedra for the atoms in the structure of the $\text{HfAu}_{0.84}\text{Al}_{1.16}$ intermetallic compound

Atoms	d (Å)	CN	CP
Hf - - 3M2 - 6M2 - 3M1 - 1Hf - 3Hf	3.065(4) 3.073(5) 3.112(1) 3.111(1) 3.265(1)	16	Frank-Kasper
M1 - - 6M2 - 6Hf	2.660(4) 3.112(1)	12	Icosahedron
M2 - - 2M2 - 2M1 - 2M2 - 2Hf - 4Hf	2.528(7) 2.660(4) 2.771(7) 3.065(4) 3.073(5)	12	Icosahedron

Table S3

Interatomic distances, coordination numbers and coordination polyhedra for the atoms in the structure of the $\text{HfAu}_{1.18}\text{Al}_{0.82}$ intermetallic compound

Atoms	d (Å)	CN	CP
Hf - - 4M2 - 1M1 - 2M3 - 4M3 - 4Hf	2.871(1) 2.885(3) 3.042(7) 3.234(2) 3.492(3)	15	Equatorially fifth-capped pentagonal prism
M1 - - 6M3 - 3Hf	2.613(4) 2.885(3)	9	Equatorially tri-capped trigonal prism
M2 - - 3M3 - 6Hf	2.626(6) 2.871(1)	9	Equatorially tri-capped trigonal prism
M3 - - 2M1 - 2M2 - 2M3 - 2Hf - 4Hf	2.613(4) 2.626(6) 2.820(12) 3.042(7) 3.234(2)	12	12-vertex polyhedron

Table S4
Interatomic distances, coordination numbers and coordination polyhedra for the atoms in the structure of the $\text{Hf}_{1.31}\text{Pt}_4\text{Al}_{10.13}$ intermetallic compound

Atoms	d (Å)	CN	CP
Hf - - 6Al3 - 6Al2 - 2Al1 - 6Pt	2.917(5) 3.012(5) 3.230(6) 3.334(1)	20 (17)*	Deformed hexagonal prism with additional atoms
Pt - - 3Al3 - 3Al2 - 1Al1 - 3Al1 - 3Hf	2.392(6) 2.502(2) 2.583(7) 2.634(2) 3.334(1)	13 (10)	Trigonal prism with additional atoms
Al1 - - 1Pt - 3Pt - 3Al2 - 3Al1 - 1Hf	2.583(7) 2.634(2) 2.861(5) 2.934(5) 3.230(6)	11 (11)	11-vertex polyhedron
Al2 - - 3Pt - 6Al3 - 3Al1 - 3Hf	2.502(2) 2.788(7) 2.861(5) 3.012(5)	15 (10)	Trigonal prism with additional atoms
Al3 - - 2Pt - 4Al2 - 2Al3 - 2Hf	2.392(6) 2.788(7) 2.896(18) 2.917(5)	10 (10)	Trigonal prism with additional atoms

* - coordination numbers of the ordered structure.

Table S4

Interatomic distances, coordination numbers and coordination polyhedra for the atoms in the structure of the $\text{Hf}_6\text{Pt}_{1.42}\text{Al}_{5.58}$ (d_1) and $\text{Hf}_6\text{Pd}_{1.37}\text{Al}_{5.63}$ (d_2) intermetallic compounds

Atoms	d_1 (Å)	d_2 (Å)	CN	CP
Hf1 - - 1Hf1 - 6M2 - 1Hf2 - 3Hf3 - 3Hf3	2.638(8) 2.968(7) 3.079(8) 3.315(3) 3.348(3)	2.646(7) 2.981(8) 3.033(7) 3.329(3) 3.343(3)	14	Frank-Kasper
Hf2 - - 3M2 - 1Hf1 - 3M1 - 6M2 - 3Hf2	3.041(11) 3.079(8) 3.092(1) 3.172(8) 3.188(2)	3.047(13) 3.033(7) 3.101(1) 3.136(9) 3.212(2)	16	Frank-Kasper
Hf3 - - 3M2 - 3Hf3 - 3M2 - 3Hf1 - 3Hf1	3.035(11) 3.061(1) 3.091(11) 3.315(3) 3.348(3)	3.080(13) 3.063(1) 3.100(13) 3.329(3) 3.343(3)	15	Frank-Kasper
M1 - - 6M2 - 6Hf2	2.681(10) 3.092(1)	2.652(12) 3.101(1)	12	Icosahedron
M2 - - 2M2 - 2M2 - 1M1 - 2Hf1 - 1Hf3 - 1Hf2 - 1Hf3 - 2Hf2	2.623(8) 2.677(8) 2.681(10) 2.968(7) 3.035(11) 3.041(11) 3.091(11) 3.172(8)	2.632(9) 2.673(9) 2.652(12) 2.981(8) 3.080(13) 3.047(13) 3.100(13) 3.136(9)	12	Icosahedron

Table S5
Interatomic distances, coordination numbers and coordination polyhedra for the atoms in the structure of the $\text{Hf}_5\text{Ni}_4\text{Al}$ intermetallic compound

Atoms	d (Å)	CN	CP
Hf1 - - 4Ni - 4Hf2 - 2Hf1 - 4Hf3	2.745(6) 3.254(10) 3.259(1) 3.311(10)	14	Full-capped deformed cube
Hf2 - - 2Ni - 2Ni - 2Ni - 2Al - 2Hf1 - 2Hf3 - 1Hf2	2.626(17) 2.639(17) 2.725(15) 2.981(8) 3.254(10) 3.259(1) 3.390(15)	13	Tri-capped deformed pentagonal prism
Hf3 - - 2Ni - 2Ni - 2Ni - 2Al - 2Hf2 - 2Hf1 - 1Hf3	2.623(17) 2.625(18) 2.784(16) 2.940(8) 3.259(1) 3.311(10) 3.355(15)	13	Tri-capped deformed pentagonal prism
Ni - - 1Hf3 - 1Hf3 - 1Hf2 - 1Hf2 - 1Ni - 1Hf2 - 1Hf1 - 1Hf3 - 1Al	2.623(17) 2.625(18) 2.626(17) 2.639(17) 2.639(8) 2.725(15) 2.745(6) 2.784(16) 2.842(6)	9	Equatorially tri-capped deformed trigonal prism
Al - - 4Ni - 4Hf3 - 4Hf2 - 2Al	2.842(6) 2.940(8) 2.981(8) 3.259(1)	14	Full-capped deformed cube