1.5.5.2.5 Hydrogen absorption

The absorption of hydrogen by the alloy Cu_2ZrAl leads to a structural transformation from the $L2_1$ Heusler-type phase to the quaternary G hydride phase $Cu_{16}Zr_6Al_7H_x$ (O_h^5 (Fm3m); Z = 116 + 4 x atoms).

Table 11. X-ray diffraction analysis of the G hydride phase $Cu_{16}Zr_6Al_7H_x$ (space group Fm3m; type D8a; z = 116) [90M2]. R_p and R_{wp} are the reliability factors of the refinement. Cf. Table 12.

	Basic data set	Rietveld-profile-analysed samples, refined data			
Composition	$Cu_{16}Zr_6Al_7H_{8.3}$	$Cu_{16}Zr_6Al_7H_{3.0}$		$Cu_{16}Zr_6Al_7H_{8.2}$	
Lattice constant [pm]	1207.1	1195.2(1)		1205.8(1)	
Volume [10^{-6} pm^3]	1758.85	1707.4		1753.2	
	x	x	B [10^{-4} pm^2]	x	B [10^{-4} pm^2]
Cu(1) on 32f$_1$ (x,x,x)	0.173(3)	0.1723(6)	0.038(5)	0.1741(6)	0.034(5)
Cu(2) on 32f$_2$ (x,x,x)	0.376(3)	0.3796(5)	0.009(4)	0.3791(6)	0.007(3)
Zr on 24e (x,0,0)	0.205(3)	0.2015(8)	0.009(2)	0.2020(8)	0.010(2)
Al(1) on 24d	0,¼,¼	0,¼,¼	0.011(9)	0,¼,¼	0.009(8)
Al(2) on 4b	½,½,½	½,½,½	0.026(8)	½,½,½	0.016(9)
H(1) on 4a	0, 0, 0	0, 0, 0		0, 0, 0	
H(2) on 32f$_3$ (x,x,x)		0.0901 [a])		0.0912 [a])	
R_p		0.076		0.054	
R_{wp}		0.100		0.070	

[a]) Calculated.

Table 12. Coordination, hole (void), radii r_h and position parameters for interstitial sites [90M2].

Site	Symmetry	Coordination			r_h	x	y	z
		Zr	Cu	Al	[pm]			
$Cu_{16}Zr_6Al_7H_{3.0}$ (space group, Fm3m; a = 1195.2 pm)								
4a	m3m	6	0	0	80.8	0	0	0
32f$_3$	3m	3	1	0	42.3	0.0901	0.0901	0.0901
$Cu_{16}Zr_6Al_7H_{8.2}$ (space group, Fm3m; a = 1205.8 pm)								
4a	m3m	6	0	0	83.6	0	0	0
24e	4mm	1	4	1	28.2	0.358	0	0
32f$_3$	3m	3	1	0	45.1	0.0912	0.0912	0.0912
48h	mm2	2	2	1	30.3	0	0.1484	0.1484
48i	r	2	2	2	17.8	0.5	0.1209	0.1209
96j$_1$		1	2	1	24.3	0	0.043	0.358
96j$_2$		1	2	1	24.3	0	0.110	0.326
96k		2	1	1	20.2	0.147	0.147	0.042
192l		1	2	1	16.5	0.254	0.127	0.080

Table 13. Volume expansion on hydrogen absorption in the G phase $Cu_{16}Zr_6Al_7H_x$ [90M2].

x	*a* [pm]	ΔV [10^{-6} pm^3]	ΔV [10^{-6} pm^3 (H atom)$^{-1}$]
0	1192.5		
3.0	1195.2	11.69	0.97
8.24	1205.8	45.47	2.17
$0 \rightarrow 8.24$		57.16	1.73

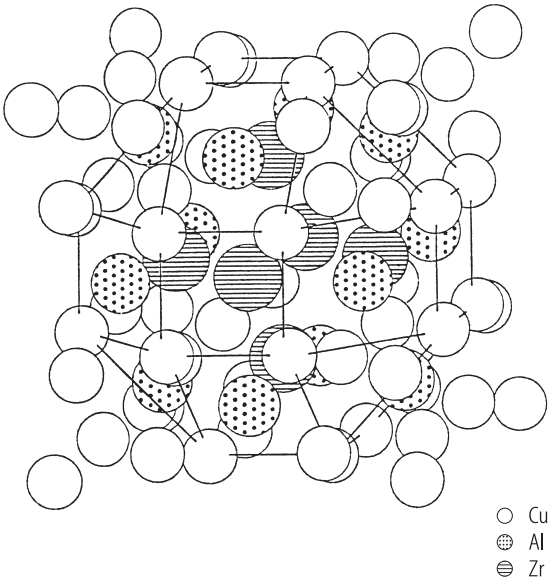

Fig. 49. Cu_{24} cubo-octahedron with its centre in the origin of the G phase $Cu_{16}Zr_6Al_7$ and within this arrangement a Zr_6 octahedron is situated [90M2].

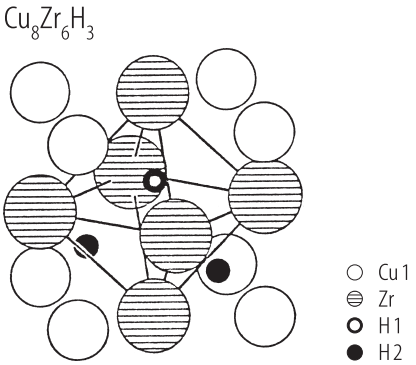

Fig. 50. $Cu_8Zr_6H_3$ subunit in the G hydride phase $Cu_{16}Zr_6Al_7H_x$ with its centre in the origin of the unit cell and the structural data for a composition with x = 3.0 [90M2]. Interatomic distances in pm:

H1-H2	186.4
H2-H2	215.3
H2-Cu1	170.3
H1-Zr	240.8
H2-Zr	202.3
Cu1-Zr	293.3
Cu1-Cu1	262.7
Al1-Cu1	244.2
Al1-Zr	304.4

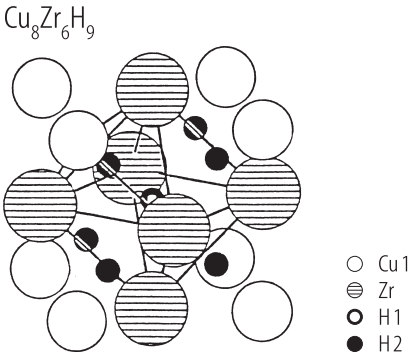

Fig. 51. $Cu_8Zr_6H_9$ subunit in the G hydride phase $Cu_{16}Zr_6Al_7H_x$ with its centre in the origin of the unit cell and the structural data for a composition with x = 8.2 [90M2]. Interatomic distances in pm:

H1-H2	190.5
H2-H2	220.0
H2-Cu1	173.1
H1-Zr	243.6
H2-Zr	205.0
Cu1-Zr	298.8
Cu1-Cu1	258.9
Al1-Cu1	246.6
Al1-Zr	307.0

1.5.5.2.6 Films/ribbons

The degree of atomic order can be influenced by preparing specimen in the form of ribbons or thin films. The crystallisation of amorphous Ni–Cu–Zr alloys has been investigated using X-ray and TEM techniques.

Table 14 indicates which elements are likely to form films with the Heusler structure.

Table 14. Formation of Heusler compounds for various compositions of X_2YZ. The plus sign refers to cases where alloying has led to the formation of the Heusler compound. The minus sign refers to cases where no Heusler compounds were found. A circle denotes systems for which Heusler phases are found experimentally over a broad temperature range and at normal pressure [87K3].

(**a**) Heusler compound Co_2YZ.

Y	Z								
	Al	Si	Ga	Ge	In	Sn	Sb	Tl	Pb
Li			+			+			
Be	+	⊕	+		+	+	+	+	+
Mg			+	⊕		+			
K		+	–	–	–	+	–	–	–
Sc		+	–	–	–	+	–	–	–
Ti	⊕	+	⊕	⊕	+	⊕	+	+	+
V	+	⊕	⊕	+	+	⊕	+	+	+
Cr	+	+	⊖			+			
Fe	⊕	⊖	–	–		+			
Ni			–	–	–	+	⊖	–	–
Y			+		–	+	–	–	–
Zr	⊕	+				⊕			
Nb	⊕	+				⊕			
Mo	+	+	+			+			
Ru	+	+	+			+			
Rh			+		–	+	–	–	–
Pd			+		–	+	–	–	–
Ag			+		–	+	–	–	–
Lu	+	+	+		+	+	+		
Hf	⊕	+	+	+	+	⊕	+		
Ta	⊕	+	⊕	+	+	+	+		
Au	+	+	+		+	+	+		