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Keywords:	Heusler compounds, intermetallic phases, crystal structure, X-ray diffraction		



Crystal Structure of New Heusler Compounds

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Received

Dedicated to Professor Dr. Gerd Meyer on the Occasion of his 60th birthday

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Abstract. Heusler compounds are promising materials in many fields of contemporary research. The spectrum of their possible applications ranges from magnetic and magneto-mechanical materials over semiconductors and thermoelectrics to superconductors. An important feature of the Heusler compounds is the possibility of controlling the valence electron concentration by partial substitution of elements. On the other hand, the properties also depend on the degree of ordering of the the crystal structure. In general, Heusler compounds crystallize in the Cu₂MnAl-type structure but in many cases certain types of disorder are observed. In this paper a detailed description of the different types of disordered structures is given. Additionally, the synthesis of new Heusler compounds is reported. The prepared compounds contain ternary Cr-, Rh-, Ru-, Ni-, Pd-, and Pt-based Heusler systems as well as quaternary Co₂-based compounds and compounds of the general formula XX'YZ. The crystal structure was determined by XRD measurements and the structural ordering of the compounds is discussed.

Keywords: Heusler compounds, intermetallic phases, crystal structure, X-ray diffraction

Introduction

Heusler compounds are ternary intermetallics with a 2:1:1 stoichiometry [1].

They first attracted interest of the magnetism community when *Heusler et al.* [2] had shown that the compound Cu_2MnAl becomes ferromagnetic, even though none of its constituents is ferromagnetic by itself. However, it took three decades before their

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structure was explained to be that of an ordered compound with a face centred cubic structure [3, 4].

Interest in Heusler compounds persists since it has been established that the properties of these intermetallic compounds can be altered by changing the degree and kind of chemical order as well as by substituting one element by another. Co-based compounds were synthesized and investigated in the 1970s [5]. They attracted a great deal of interest due to their high Curie temperatures [6, 7] and being predicted to be half metallic ferromagnets [8, 9]. Many of the Co₂-based compounds are now used in magnetic tunnel junctions [10, 11]. Today Heusler compounds have various applications, for example they are investigated due to their properties as half-metallic ferromagnets in the field of spintronics, thermoelectrics and superconductors [12-15].

Experimental Section

Polycrystalline ingots of the compounds were prepared by arc melting of stoichiometric amounts of high purity elements in an argon atmosphere to avoid oxygen contamination at a pressure of 10^{-4} mbar. Additionally, a Ti sponge was used to bind remaining oxygen. The samples were melted three times. They were turned over after each melting process to yield a homogeneous sample. The weight loss after the whole melting procedure was less than 1 %. The polycrystalline ingots were annealed in an evacuated quartz tube for one to three weeks.

The crystallographic structure was investigated by X-ray powder diffraction using excitation by Mo K_{α} radiation ($\lambda = 0.7093165$ nm; Bruker, AXS D8) in reflection geometry or Cu K_{α} radiation ($\lambda = 1.540598$ nm; Bruker, D5000) in transmission geometry in a θ - θ scanning mode. The experimental diffraction patterns were refined using the FULLPROF program [16].

Results and Discussion

Crystal Structure

The properties of Heusler compounds depend significantly upon the degree and type of chemical order. In general, X_2YZ Heusler compounds crystallize in the cubic Cu₂MnAl structure (space group no. 225: F m3m, L2₁). The X and Y atoms are transition metals and Z is a main group element. In some cases Y is replaced by a rare earth element or an earth alkali metal. The cubic Cu₂MnAl structure consists of four interpenetrating *fcc* sub-lattices, two of which are equally occupied by X. These two X-site *fcc* sub-lattices combine to form a simple cubic lattice. The Y and Z atoms occupy alternating the centers of the simple cubic lattice. This results in a CsCl-like superstructure. The X atoms are placed on the Wyckoff position 8c (1/4, 1/4, 1/4). The Y and Z atoms are located on 4a (0, 0, 0) and 4b (1/2, 1/2, 1/2) positions, respectively. The 4a and 4b positions have O_h symmetry whereas the 8c position has T_d symmetry. The crystal structure is displayed in Fig. 1. The illustration is shifted by (1/4, 1/4, 1/4) with respect to the standard illustration of the F m3m cell to show the CsCl-like superstructure.

(Insert figure 1)

Fig. 1 shows the transition from the ordered to the most prominent disordered structures as will be explained in the following: If the *Y* and the *Z* atoms are evenly distributed, the 4a and 4b positions become equivalent. This leads to a CsCl-like structure, also known as B2-type disorder. The symmetry is reduced and the resulting space group is P m $\overline{3}$ m. The random distribution of the *X* and the *Y* or the *X* and the *Z* atoms results in the BiF₃type disorder (Space group no. 216: F m $\overline{3}$ m, DO₃). The NaTl-type structure is observed very rarely. In this structure type the *X*-atoms which occupy one *fcc* sub-lattice are mixed with the *Y* atoms whereas the *X*-atoms on the other sub-lattice are mixed with the *Z* atoms. This kind of disorder is also known as B32a disorder (Space group no. 227, F d $\overline{3}$ m). The *X*-atoms are placed at the Wyckoff position 8a (0, 0, 0), the *Y* and *Z* randomly distributed at position 8b (1/2, 1/2, 1/2). In contrast to these partial disorder phenomena all positions become equivalent in the tungsten-type structure with a bcc lattice and reduced symmetry I m $\overline{3}$ m (A2).

The cubic X₂YZ compounds are also found in the CuHg₂Ti-type structure as illustrated in Fig. 2 (note that the classification of the cubic X₂YZ compounds is sometimes not uniquely given in *Pearson's Handbook* [17]). In the CuHg₂Ti-type structure (space group no. 216: F $\overline{4}$ 3m, X) the X atoms do not build a simple cubic lattice but occupy the 4a and 4c Wyckoff positions at (0, 0, 0) and (1/4, 1/4, 1/4). The Y and Z atoms are located on 4b (1/2, 1/2, 1/2) and 4d (3/4, 3/4, 3/4) positions, respectively. All four positions have T_d symmetry. This structure is frequently observed if the nuclear charge

of the *Y* element is larger than the one of the *X* element from the same period (Z(Y)>Z(X)). The structure may also appear in compounds with transition metals from different periods. Space group no. 216 is also observed in quaternary noncentrosymmetric *XX'YZ* Heusler compounds. Every element occupies one of the *fcc* sublattices. The *X* atoms are located on the 4a sites whereas the *X'* atoms occupy the 4b positions. The *Y* and *Z* atoms are situated at the 4c and 4d positions, respectively. The prototype is LiMgPdSn (compare Fig. 2). The reviewing articles of Bacon and Plant [18] as well as *Neumann* and *Ziebeck* [19, 20] summarize different types of disorder in Heusler compounds.

(Insert figure 2)

Fig. 3 shows the group – subgroup relationship between all types of simple disorder that are possible in the Heusler structure. The numbers after t and k indicate the index of the reduction in symmetry. One should notice that there are 2 atoms per unit cell for the tungsten and the CsCl structure. For all other structure types there are 16 atoms per unit cell due the doubling of all cell axes.

(Insert figure 3)

Table 1 summarizes the different ordering variants of Heusler compounds. The site occupancy is correlated with the corresponding general formula. Different notations of

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the crystal structures according to the *ISCD*, the *Strukturberichte (SB)* and to *Pearson* as well as the space group are given.

(Insert table 1)

Theoretical X-ray diffraction patterns of Co₂MnSi which were simulated under the assumption of different crystal structures are displayed in Fig. 4. Table 2 provides a survey of the relative intensities of the reflexions for the XRD patterns displayed in Fig. 4. The Cu₂MnAl-type structure is identified by the occurrence of the *fcc*-typical (111) and (200) reflexions and their relation to the (220) reflexion. However, the intensity of the two *fcc*-typical reflexions is very low in many of the investigated compounds. If the Cu₂MnAl-type and the BiF₃-type structure are compared, a difference in the intensities of the (111) and (200) reflexions is evident. The Cu₂MnAl and the CuHg₂Ti structure are hardly distinguishable by X-ray diffraction. Much care has to be taken in the structural analysis, as both have general fcc-like symmetry. In the CsCl-type structure only the (111) reflexion vanishes whereas in the NaTl-type structure the (200) reflexion disappears. Both, the (111) and (200) reflexions vanish not only in the tungsten-type structure but also if all contained elements are from the same row of the periodic table due the nearly equal scattering factors. A small amount of disorder in an ordered compound or a low degree of order in a disordered structure may occur. This is not detectable by standard XRD. Thus, small amounts of partial disorder cannot be excluded without detailed analysis of further structural investigations, for example by neutron diffraction, Mössbauer spectroscopy, NMR or EXAFS, even if the XRD data indicate the Cu₂MnAl structure.

(Insert figure 4)

(Insert table 2)

Structural Characterization

We report on the crystal structure of newly synthesized Heusler compounds. Tables 3, 4, and 5 provide an overview of the different types of Heusler compounds and their crystal structure.

Table 3 summarizes the prepared ternary Heusler compounds. Fig. 5 shows the XRD results of Cr₂CoGa. The compound fulfils the criteria of Z(X) < Z(Y). Since the (200) reflexion is not present but the (311) reflexion is detectable, it is concluded that the compound exhibits the CuHg₂Ti structure. The (111) reflexion cannot be detected due to the fluorescence in that θ range. For comparison the calculated diffraction pattern for the Cu₂MnAl-type structure given as an inset in Fig. 5.

(Insert figure 5)

(Insert table 3)

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The Pd₂-based compounds with exception of Pd₂NbAl exhibit the Cu₂MnAl-type structure. The Pt₂-based compounds Pt₂ScSn and Pt₂ZrIn exhibit the Cu₂MnAl-type and the CsCl-type structure, respectively. Ru₂TiSi exhibits the Cu₂MnAl structure with a CsCl-type disorder of approximately 18%. The tungsten structure type is observed for the compound Ni₂MoGa (all atoms are randomly distributed).

The structural properties of quaternary Co₂-based Heusler compounds with different substitutions on the *Y* or *Z* side are given in Table 4. Fig. 6 displays the powder XRD pattern of Co₂Mn_{0.95}Sc_{0.05}Ga measured with Mo K_{α} radiation. The result of the refinement and the difference between refinement and measurement are included in the figure. The diffraction pattern exhibits only the (220) reflexion. This is caused by the low intensity of the (111) and (200) reflexions mentioned above. Typically all compounds containing solely elements from one row show only the cubic main reflexions by regular XRD measurements. The crystal structure of these compounds cannot be clearly determined by regular XRD measurements. For this reason the structure is denoted as "cubic" in the classification in Table 4. Co₂MnGa_{0.5}Si_{0.5} and Co₂MnAl_{0.5}Ge_{0.5} exhibit only the (200) reflexion. Thus the XRD data indicate a CsCl-type structure. Due to its weak intensity the (111) reflexion cannot be observed. The Cu₂MnAl-type structure may exist but cannot be confirmed by analysis using standard XRD methods. The remaining compounds mentioned in Table 4 exhibit the Cu₂MnAl-type structure.

(Insert figure 6)

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(Insert table 4)

Fig. 7 shows the refined powder XRD pattern of NiCuScAl. The data indicate the Cu_2MnAl -type structure according to the explanation above. This structure corresponds to the general formula $(Ni_{0.5}Cu_{0.5})_2ScAl$ with an equal distribution of Ni and Cu on the *X* sides. Since the relation of intensities is correct a significant amount of disorder in the compound can be excluded. However, it has to be mentioned that the data do not provide the information if the compound crystallizes in the LiMgPdSn structure which means that the Ni and Cu atoms are ordered on separate sublattices. This better ordered structure corresponds to the general formula NiCuScAl. Similar structural properties are observed for all other quaternary compounds listed in Table 5. These compounds are classified as crystallizing in the Cu₂MnAl-type structure although the LiMgPdSn-type structure might be present.

(Insert figure 7)

(Insert table 5)

Conclusion

Several new Heusler compounds have been synthesized and analysed by the means of X-ray diffraction. Different types of disorder that occur in this structure type have been

found. On the other hand it should be noted that it is hard to distinguish between some disorder types with regular XRD methods. As the magnetic and electronic properties of Heusler compounds depend on the crystalline structure, these compounds should be investigated by many structure sensitive analysing methods.

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Figure Captions

Fig. 1

Crystal structures of the X₂YZ Heusler compounds.

The Cu₂MnAl (L2₁) structure and preferential types of disorder: The BiF₃ (DO₃), CsCl

(B2) and Tungsten (A2) structure. Note that all positions are shifted by (1/4, 1/4, 1/4)

with respect to the standard F m $\overline{3}$ m cell to make the CsCl superstructure visible.

Fig. 2

Crystal structure of the Heusler compounds in space group $F\overline{4}$ 3m.

The CuHg₂Ti-structure and the noncentrosymmetric LiMgPdSn-structure of XX'YZ compounds.

Fig. 3

Bärninghaus tree of the group-subgroup relationship of the Heusler structure and its disorder variants. The indices of *klassengleiche* (k) and *translationsgleiche* (t) as well as the unit cell transformations and the origin shifts are given.

Fig. 4

Simulated X-ray diffraction patterns measured with Mo K_{α} radiation for Co₂MnSi in different crystal structures: a) Cu₂MnAl-type (L2₁), b) CsCl-type (B2), c) BiF₃-type (DO₃), d) tungsten-type (A2), e) CuHg₂Ti-type (X) and f) NaTl-type (B32a) structure.

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Fig. 5

X-ray diffraction pattern of Cr₂CoGa measured with Cu K_{α} radiation.

The compound exhibits the CuHg2Ti-type structure. For comparison the theoretical diffraction pattern of the Cu₂MnAl-type structure is displayed as an inset.

Fig. 6

XRD pattern of $Co_2Mn_{0.95}Sc_{0.05}Ga$ measured with Mo K_{α} radiation.

Although the diffraction pattern shows the typical features of the tungsten-type structure, the degree of order cannot be determined since the intensity of the *fcc*-typical (111) and (220) reflexions is too weak.

Fig. 7

XRD pattern of NiCuScIn measured with Mo K_{α} radiation. The diffraction pattern shows the typical features of the Cu₂MnAl structure, the superlattice reflexions (111) and (200) are present. A differentiation between the Cu₂MnAl and the LiMgPdSn structure is not possible since the calculated XRD patterns of these two structures are almost identical.

Table captions

Table 1

Relation between ordered – disordered Heusler structures and different forms of notations.

Table 2

Relative intensities of the reflexions for Co₂MnSi in different structures.

Table 3

Structural properties ternary X_2YZ Heusler compounds.

Table 4

Structural properties of Co₂-based quaternary Heusler compounds.

Table 5

•

Structural properties quaternary XX'YZ Heusler compounds.



Fig. 1





Fig. 2







Fig. 4

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Fig. 5



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Fig. 6



Fig. 7

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site	general	structure type	SB	space group	Pearson
occupancy	formula	ICSD			
X, X', Y, Z	XX'YZ	LiMgPdSn	Y	$F \bar{4} 3m$ (no. 216)	cF16
X=X, Y, Z'	$X_2 YZ$	Cu ₂ MnAl	L2 ₁	$F m \overline{3} m$ (no. 225)	cF16
X, X'=Y, Z	XX' ₂ Z	CuHg ₂ Ti	X	$F \bar{4} 3m$ (no. 216)	cF16
X=X'=Y, Z	X_3Z	BiF ₃	DO ₃	$F m \overline{3} m (no. 225)$	cF16
X=X', Y=Z	X_2Y_2	CsCl	B2	$P m \overline{3} m$ (no. 221)	cP2
X=Y, X'=Z	<i>X</i> ₂ <i>X</i> ' ₂	NaTl	B32a	$F d \overline{3} m$ (no. 227)	cF16
<i>X=X'=Y=Z</i>	<i>X</i> ₄	W	A2	I m $\overline{3}$ m (no. 229)	cI2

Table 1

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Structure	(111)	(200)	(220)	(311)	(222)	(400)
		· · ·			· · /	· · /
Cu ₂ MnAl	4.30	4.67	100	2.01	1.30	16.46
CsCl	-	4.67	100	-	1.30	16.46
BiF ₃	0.79	0.41	100	0.33	0.09	16.58
Tungsten	-	-	100	-	-	16.58
CuHg ₂ Ti	6.53	2.27	100	3.26	0.57	16.46
NaTl	4.38	-	100	2.26	-	16.46

Table 2

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Compound	Structure	a / Å
Cr ₂ CoGa	CuHg ₂ Ti	5.81
Ni ₂ MgSb	Cu ₂ MnAl	6.06
Ni ₂ MoGa	W	6.25
Pd ₂ HfGa	Cu ₂ MnAl	6.34
Pd ₂ NbAl	CsCl	6.47
Pd ₂ MgSb	Cu ₂ MnAl	6.46
Pd ₂ MoAl	Cu ₂ MnAl	6.27
Pd ₂ ZrSn	Cu ₂ MnAl	6.55
Pt ₂ ScSn	Cu ₂ MnAl	6.54
Pt ₂ ZrIn	CsCl ¹)	6.56
Ru ₂ TiSi	Cu ₂ MnAl	5.95

¹) The Cu₂MnAl-type structure is possible but the (111) reflexion is not detectable due to the low scattering intensity.

Table 3

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Compound	Structure	a / Á
Co ₂ Fe _{0.76} Sc _{0.24} Ga	cubic	5.73(6)
Co ₂ Fe _{0.7} Ti _{0.3} Ga	cubic	5.77(5)
Co ₂ Fe _{0.45} Ti _{0.55} Ge	Cu ₂ MnAl	5.79(1)
Co ₂ Fe _{0.6} V _{0.4} Ga	cubic	5.75(9)
Co ₂ MnAl _{0.5} Ge _{0.5}	CsCl ²)	5.75(1)
Co ₂ MnAl _{0.5} Si _{0.5}	Cu ₂ MnAl	5.70(1)
Co ₂ Mn _{0.5} Fe _{0.5} Sn	Cu ₂ MnAl	5.96(3)
Co ₂ Mn _{0.5} V _{0.5} Si	Cu ₂ MnAl	5.65(3)
Co ₂ MnGa _{0.5} Ge _{0.5}	Cu ₂ MnAl	5.76(1)
Co ₂ MnGa _{0.5} Si _{0.5}	CsCl ²)	5.70(9)
Co ₂ Mn _{0.95} Sc _{0.05} Ga	cubic	5.76(5)
Co ₂ Mn _{0.7} Sc _{0.3} Sn	Cu ₂ MnAl	6.00(7)
Co ₂ Mn _{0.935} Ti _{0.065} Ga	cubic	5.80(8)
Co ₂ Mn _{0.6} Ti _{0.4} Ge	Cu ₂ MnAl	5.77(1)
Co ₂ Mn _{0.9} V _{0.1} Ga	cubic	5.80(3)
Co ₂ Ti _{0.5} Fe _{0.5} Si	Cu ₂ MnAl	5.67(8)
Co ₂ Ti _{0.5} Fe _{0.5} Sn	Cu ₂ MnAl	6.05(3)
Co ₂ Ti _{0.5} Mn _{0.5} Si	Cu ₂ MnAl	5.70(6)
Co ₂ Ti _{0.5} Mn _{0.5} Sn	Cu ₂ MnAl	6.03(3)

Co ₂ Ti _{0.5} V _{0.5} Sn	Cu ₂ MnAl	5.98(5)

²) The Cu₂MnAl-type structure is possible but the (111) reflexion is not detectable due

to the low scattering intensity.

Table 4

	2	<i>.</i>
Compound	Structure ³)	a / Å
$(Ni_{0.5}Ag_{0.5})_2ScAl$	Cu ₂ MnAl	6.52
$(Ni_{0.5}Cu_{0.5})_2ScAl$	Cu ₂ MnAl	6.16
$(Ni_{0.5}Cu_{0.5})_2ScGa$	Cu ₂ MnAl	6.05
$(Ni_{0.5}Cu_{0.5})_2ScIn$	Cu ₂ MnAl	6.30
$(Pd_{0.5}Ag_{0.5})_2ScAl$	Cu ₂ MnAl	6.48
$(Pd_{0.5}Ag_{0.5})_2ScIn$	Cu ₂ MnAl	6.58
$(Pd_{0.5}Ag_{0.5})_2YIn$	Cu ₂ MnAl	6.79
$(Pd_{0.5}Au_{0.5})_2ScIn$	Cu ₂ MnAl	6.57

³) The XRD pattern of the structure LiMgPdSn does not differ significantly from one of the Cu₂MnAl structure. Therefore it is not possible to determine whether the compounds are ordered at X and X' positions.

Table 5



Crystal structures of the X2YZ Heusler compounds. The Cu2MnAl (L21) structure and preferential types of disorder: The BiF3 (DO3), CsCl (B2) and Tungsten (A2) structure. Note that all positions are shifted by (1/4, 1/4, 1/4) with respect to the standard F m m cell to make the CsCl superstructure visible. 254x190mm (600 x 600 DPI)







Bärninghaus tree of the group-subgroup relationship of the Heusler structure and its disorder variants. The indices of klassengleiche (k) and translationsgleiche (t) as well as the unit cell transformations and the origin shifts are given. 247x233mm (600 x 600 DPI) Page 33 of 36

Simulated X-ray diffraction patterns measured with Mo Kα radiation for Co2MnSi in different crystal structures: a) Cu2MnAl-type (L21), b) CsCl-type (B2), c) BiF3-type (DO3), d) tungsten-type (A2), e) CuHg2Ti-type (X) and f) NaTl-type (B32a) structure. 81x115mm (600 x 600 DPI)

X-ray diffraction pattern of Cr2CoGa measured with Cu K α radiation. The compound exhibits the CuHg2Ti-type structure. For comparison the theoretical diffraction pattern of the Cu2MnAl-type structure is displayed as an inset. 43x56mm (600 x 600 DPI)

XRD pattern of Co2Mn0.95Sc0.05Ga measured with Mo K α radiation. Although the diffraction pattern shows the typical features of the tungsten-type structure, the degree of order cannot be determined since the intensity of the fcc-typical (111) and (220) reflexions is too weak. 86x111mm (600 x 600 DPI)

ZAAC

XRD pattern of NiCuScIn measured with Mo K α radiation. The diffraction pattern shows the typical features of the Cu2MnAl structure, the superlattice reflexions (111) and (200) are present. A differentiation between the Cu2MnAl and the LiMgPdSn structure is not possible since the calculated XRD patterns of these two structures are almost identical. 86x111mm (600 x 600 DPI)