Crystal structure of cobalt chromium germanium, CoCrGe

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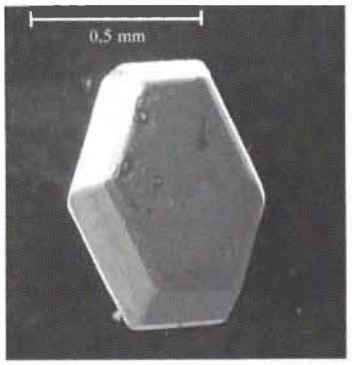

Fig. 1. A single crystal of CoCrGe.

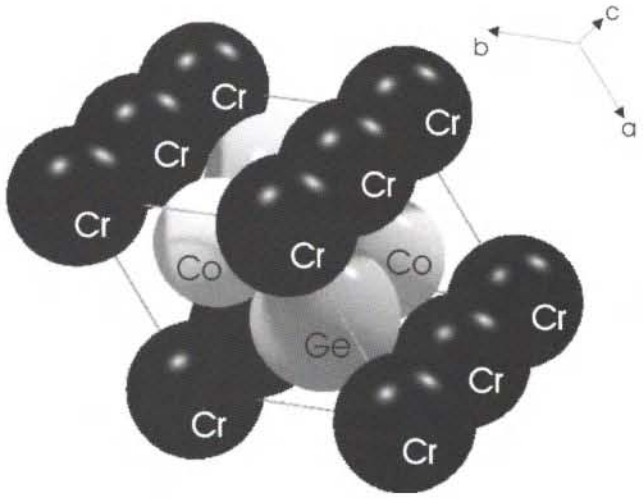

Fig. 2. Unit cell of CoCrGe.

Abstract

CoCrGe, hexagonal, $P6_3/mmc$ (No. 194), $a = 4.092(1)$ Å, $c = 5.145(2)$ Å, $V = 74.6$ Å^3, $Z = 2$, $R_{gt}(F) = 0.049$, $wR_{all}(F^2) = 0.097$, $T = 300$ K.

Source of material

Single crystals of cobalt chromium germanium were grown by chemical vapour transport in a closed quartz ampoule. Iodine was used as transporting agent. The metals and the transporting agent were heated at 1148 K for seven days to homogenize the source material. The chemical vapour transport was performed at 1073 K → 1223 K. After seven days, the deposition of single crystals with different compositions can be observed in the crystallisation zone. Within these products crystals of the composition CoCrGe (EDX-analysis) were found and isolated.

The figure shows an euhedral crystal of about 0.5 mm diameter. For the data collection a smaller crystal without well developed faces was used.The empirical absorption correction was based on a function of the mean intensity of the imaging plate versus angle phi using program DECAY of the Stoe IPDS software package. A spherical absorption correction with $\mu R = 1.8$ was applied too using program SPHERE of the PROMETHEUS system [1]. The absorption correction improved the R_{int} from 0.187 to 0.142.

Discussion

The structure of CoCrGe can be derived from the Ni_2In type. From our X-ray analysis we conclude that position 2*a* is occupied by Cr, 2*c* by Co and 2*d* by Ge. Co and Ge may be interchanged. The high temperature phase of CoGeMn, e.g., is known to have this structure [2]. According to the TYPIX database [3] the structure belongs to the BeZrSi-type, but BeZrSi has a much higher *c*/*a* ratio. Related phases in the binary system Co-Ge are $Co_{1.78}Ge$ (called "Co_2Ge" [4]) and Co_5Ge_3, but in these phases at least one occupation factor for Co is <1. Therefore these phases have a smaller cell volume. The lattice constants of "Co_2Ge" are reported as $a = 3.940$ Å and $c = 5.018$ Å. The higher displacement factor of Co and the lower one of Cr suggest that there might be a mixed occupation of positions 2*a* and 2*c*, for instance (0.9 Cr + 0.1 Co) on 2*a* and (0.9 Co + 0.1 Cr) on 2*c*. But trials to refine this model yield only very small amounts of the minor element in both positions with large errors and no significant reduction of the $U(2c)/U(2a)$ ratio. A similar $U(2c)/U(2a)$ ratio is observed in CoGeMn (HT) (see [2], where an explanation is given for the large value of B_{Co}). If one refines anisotropic displacement parameters thermal ellipsoids are obtained which are comparable to those in CoGeMn (HT), namely elongated ellipsoids for Co and Ge and a flattened ellipsoid for the 2*a* metal with respect to the hexagonal *c* axis. For this comparison the parameters of CoGeMn (HT) given in [2] have to be transformed by an origin shift of 0 1/4 1/4 followed by a multiplication with matrix 002/011/-100, because in [2] the structure is described in terms of an orthorhombic cell which simplifies the comparison to the low temperature phase of CoGeMn. The refinement of anisotropic displacement parameters improves the *R* values considerably, but because of the small number of observed reflections in the unique data set the isotropic structure model is preferred in this work.

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Table 1. Data collection and handling.

Crystal:	metallic grey, irregular shape, size 0.06 × 0.09 × 0.13 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	374.49 cm^{-1}
Diffractometer:	Stoe IPDS, 100 exposures, $\Delta\varphi = 2°$
$2\theta_{max}$:	55.38°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	741, 50
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 29
$N(param)_{refined}$:	5
Programs:	PROMETHEUS [1], SHELXL-93 [5], CIF2SX [6], DIAMOND [7]

Table 2. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{iso}
Ge(1)	2*d*	1/3	2/3	3/4	0.013(2)
Co(1)	2*c*	1/3	2/3	1/4	0.018(2)
Cr(1)	2*a*	0	0	0	0.007(1)

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