08.3–3 X-RAY INVESTIGATION OF CRYSTALLIZATION AND THERMAL EXPANSION OF $AuSn_4$, $PdSn_4$ AND $PtSn_4$.

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Isomorphic crystal structures of $AuSn_4$, $PdSn_4$ and $PtSn_4$ are described by the orthorombic space group Aab2 (Schubert & Roesler, Z. Metallkd. (1950) 41,298; Kubiak & Wołcyrz, J. Less-Comm. Met. (1984) 97,265). The investigation of crystallization process of $AuSn_4$ (Kubiak, J. Less-Comm. Met. (1981) 80, P53) revealed the existence of the relationship between the speed of crystallization and the formation of superstructure (with 6-fold extension of c-parameter).
In the present work the single crystals of all the three compounds were obtained in order:
(i) to check whether crystallization process of $PdSn_4$ and $PtSn_4$ can also lead to the superstructure formation,
(ii) to compare the thermal expansion of all three compounds.

The results are following:
(i) Contrary to $AuSn_4$, attempts to obtain $PdSn_4$ and $PtSn_4$ single crystals from stoichiometric alloys were unsuccessful. Therefore, single crystals of $PdSn_4$ and $PtSn_4$ were obtained by the fast cooling of the melted mixtures of the pure metals with the excess of tin, which then was etched. As a result of this procedure, single crystals were obtained with a shape of rectangular plates. X-ray photographs were taken but gave no evidence of the superstructure.
(ii) Thermal expansion coefficients were calculated on the basis of presice lattice parameters measurements performed with a Bond-type diffractometer (Łukaszewicz et al., Krist. Tech (1978) 13,561) equiped with the high- and low-temperature attachment. Lattice parameters are almost linear vs. temperature. Numerical values of the linear (α_i) and volume (β_v) thermal expansion coefficients calculated at T = 298 K are presented below.

		lattice param. at 298 K	temp. range T [K]	α_i $[10^{-5}\ K^{-1}]$	β_v $[10^{-5}\ K^{-1}]$
$AuSn_4$	a	6.5124(1)	300 - 473	2.292	5.904
	b	6.5162(1)		2.212	
	c	11.7065(1)		1.400	
$PdSn_4$	a	6.3888(1)	194 - 500	1.281	5.391
	b	6.4415(1)		1.292	
	c	11.4462(2)		2.818	
$PtSn_4$	a	6.3823(1)	295 - 499	1.265	4.920
	b	6.4190(1)		1.241	
	c	11.3666(2)		2.414	

The results presented above show distinctly different behaviour of $AuSn_4$ in comparison with the two other compounds. For $AuSn_4$ the difference between the lattice parameters a and b is much less than for $PdSn_4$ and $PtSn_4$. Therefore in $AuSn_4$ stacking faults can appear relatively easy and possibility of superstructure formation does exist. This leads probably also to the different character of the thermal expansion of $AuSn_4$.
As it was stated, in the case of the fast crystallization $AuSn_4$ shows superstructure which disappeares when the sample is heated and homogenized. This phenomenon can be a reason of different superconduction critical temperatures measured for the thin film of $AuSn_4$ obtained by sputtering of tin and gold on the cooled substrate (Klokholm & Chion, Acta Met. (1966) 14,565) and for the bulk and homogenized sample (Raub, Z. Metallkd. (1964) 55,195).

08.3–4 ANOMALOUS SCATTERING PHENOMENA APPLIED TO THE STUDY OF SHORT-RANGE ORDER IN TERNARY ALLOYS.

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Intensity measurement of diffuse scattering from a short-range-ordered Cu-20at%Ni-24at%Zn alloy single crystal has been carried out using a monochromatic radiation selected from a band of continuous spectrum of synchrotron orbital radiation now available at KEK. A simple mathematical treatment of the three sets of intensity data obtained with the three wavelengths lying near the absorption edges of the component atoms enables one to divide the observed intensity into the partial intensities arising from the spatial correlation of the three different pairs of atoms, Cu-Ni, Ni-Zn and Zn-Cu. It has been found that a specific pair of atoms in ternary alloy does not behave in the same manner as it does in binary alloy. Attempts have also been made to divide the diffuse scattering intensity around a fundamental reflection into components arising from displacements of atoms and from clustering of atoms.

08.3–5 THE STRUCTURE OF THE TERNARY CARBIDE $Ho_2Cr_2C_3$. By R.K. Behrens and W. Jeitschko, Anorganisch-Chemisches Institut, Universität Münster, D-4400 Münster, West Germany.

The new compounds $R_2Cr_2C_3$ with R = Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, Lu were prepared by arc melting the stoichiometric mixtures of the elemental components and subsequent annealing at 900°C. They crystallize with a new structure type which was determined from single crystal X ray data of $Ho_2Cr_2C_3$. It has monoclinic symmetry, space group C2/m and the lattice constants: a = 10.480(2) Å, b = 3.3623(5) Å, c = 5.533(1) Å, β = 106.37(1)°, V = 187.1 Å³, Z = 2. The least squares refinement resulted in a residual of R = 0.027 for 24 variables and 739 independent F values. The structure may be derived from a body centered cubic metal lattice by distortion and ordering of the metal atoms (Fig. 1). One fourth of the (distorted) octahedral voids is filled with carbon atoms. The refinement of the occupancy factors of the two independent carbon positions resulted in almost the ideal values (occupancy parameters of 97 ± 4 and 94 ± 3 %). Each Ho atom is surrounded by 6 Ho (at distances from 3.36 to 3.59 Å), 5 Cr (3.00 to 3.15 Å) and five carbon atoms (2.41 to 2.63 Å). The Cr atoms have coordination number 11 (5 Ho, 2 Cr, and 4 C atoms). The two different carbon atoms have 2 Cr + 4 Ho and 3 Cr + 3 Ho neighbors with Cr-C distances varying between 1.91 and 2.03 Å. The structure is closely related to that of orthorhombic $UMoC_2$ (Cromer, Larson & Roof, Acta Cryst. (1964) 17, 272). The latter structure can also be derived from a body centered cubic metal lattice by ordering of the metal atoms and filling (in this case one third) of the octahedral voids by carbon