

# The Modulated Structure of SrAuSn<sub>2</sub>

Saeid Esmailzadeh<sup>a</sup>, Rolf-Dieter Hoffmann<sup>b</sup>, and Rainer Pöttgen<sup>b</sup>

<sup>a</sup> Department of Inorganic Chemistry, Arrhenius Laboratory, Stockholm University, SE-106 91 Stockholm, Sweden

<sup>b</sup> Institut für Anorganische und Analytische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 36, D-48149 Münster, Germany

Reprint requests to R. Pöttgen. E-mail: pottgen@uni-muenster.de

Z. Naturforsch. **59b**, 1451 – 1457 (2004); received August 24, 2004

*Dedicated to Professor Hubert Schmidbaur on the occasion of his 70<sup>th</sup> birthday*

The ternary stannide SrAuSn<sub>2</sub> was synthesized by induction melting of the elements under an argon atmosphere in a sealed niobium ampoule in a water-cooled sample chamber of a high-frequency furnace. The structure of SrAuSn<sub>2</sub> was investigated by X-ray powder and single crystal diffraction. It was found to be favourable to describe as a commensurately modulated structure. The 3+1 dimensional superspace group symmetry  $P : Cmc m(\alpha, 0, 0) : 0s0$  with the unit cell dimensions  $a = 460.20(14)$ ,  $b = 2038.8(8)$ ,  $c = 460.34(19)$  pm and the modulation wave vector  $\mathbf{q} = 1/4 [100]^*$ . The Sn1 atoms were those with the strongest modulation while the rest of the atoms showed rather small deviations from the average structure. The SrAuSn<sub>2</sub> structure is closely related to the CeNiSi<sub>2</sub> type. Geometrically these structures are built up from distorted ThCr<sub>2</sub>Si<sub>2</sub> and AlB<sub>2</sub> slabs. The gold atoms are located in the ThCr<sub>2</sub>Si<sub>2</sub> slab. They have a distorted square pyramidal tin coordination at Au–Sn distances ranging from 266 to 294 pm. These pyramids are condensed *via* common edges forming two-dimensional layers. The latter are condensed *via* the Sn1 atoms within the AlB<sub>2</sub> slabs that form one-dimensional zigzag chains with Sn1–Sn1 distances ranging from 282 to 288 pm. These chains show the strong modulations. Together, the gold and tin atoms build up a three-dimensional [AuSn<sub>2</sub>] network, in which the strontium atoms fill distorted hexagonal channels.

**Key words:** Stannide, Crystal Structure, Modulated Structure

## Introduction

In recent years we have systematically analysed a series of alkaline earth (AE) and rare earth (RE) metal–transition metal (T)–stannides of compositions  $AETSn_2$  and  $RETSn_2$ .  $CaTSn_2$  (T = Rh, Pd, Ir) [1] and  $EuIrSn_2$  [2] crystallize with the  $MgCuAl_2$  type structure, a ternary ordered variant of the well-known  $Re_3B$  type. The tin substructure in these stannides consists of a three-dimensional, orthorhombically distorted tetrahedral network.  $LaRhSn_2$  and  $CeRhSn_2$  crystallize with their own structure type [3] where the two crystallographically different tin atoms form Sn<sub>2</sub> dumbbells.  $LaRhSn_2$  is a metallic conductor and Pauli paramagnetic while  $CeRhSn_2$  shows Kondo-like behaviour and orders ferromagnetically at 4 K [3]. This has been fully confirmed in a later study by Hossain *et al.* [4]. The latter stannides show all full occupancy of the atomic sites. This is different in the various orthorhombic CeNiSi<sub>2</sub> type stannides  $RET_{1-x}Sn_2$  [5, 6]. These

compounds have large defects on the transition metal sites, significantly influencing the electron count and thus the magnetic properties [6].

When searching for  $AEAuSn_2$  and  $REAuSn_2$  stannides with strontium and europium as the electropositive component we first got two compounds with different composition and different structural motifs. In the strontium based system we first synthesized the new stannide SrAuSn [7] with a complex superstructure that derives from the  $KHg_2$  type. Within the three-dimensional [AuSn] superstructure we observe a variety of Au–Au and Sn–Sn interactions. With europium we obtained the stannide  $Eu_2Au_2Sn_5$  [8]. This stannide has a slightly higher tin content and the structure may be considered as a superstructure of the well-known  $BaAl_4$  type.

The stannide SrAuSn<sub>2</sub> described herein has structural features of the CeNiSi<sub>2</sub> type. However, due to a modulation of the Sn1 positions, it represents a new, peculiar structure type in the series of  $AETSn_2$  stan-

nides. The synthesis and X-ray crystallographic characterization of the modulated structure of SrAuSn<sub>2</sub> is reported herein.

Modulated structures are usually described in the superspace using 3+n dimensional crystallography. Such crystal structures possess an average 3D structure and an additional periodic deviation from the basic structure. The periodicity of the deviation of the basic structure can be either commensurate or incommensurate with respect to the periodicity of the average structure. The modulation, either commensurate or incommensurate, can be compositional, positional or a combination of both. Commensurately modulated structures can also be described as 3D structures using a superstructure model. However the intensity distribution of the diffraction pattern usually makes a modulated model in 3+n D more favourable in terms of stability of the structure refinement and number of refined structure parameters. The choice of a modulated structure model or a superstructure model is dependent on the intensity distribution of the basic reflection data and the satellite reflections rather than the metrics of the satellites and whether the periodicity of the structure deviation and the basic crystal structure.

## Experimental Section

### Sample preparation

Starting materials for the preparation of SrAuSn<sub>2</sub> were small, redistilled strontium pieces (Johnson-Matthey, > 99.9%), gold wire (Degussa-Hüls,  $\varnothing$ 1 mm, > 99.9%), and tin granules (Heraeus, > 99.999%). The moisture sensitive strontium pieces were kept under argon in Schlenk tubes prior to the reactions. Pieces of the three elements were weighed in the ideal 1:1:2 atomic ratio and arc-welded in a small niobium ampoule ( $\varnothing$ 10 mm, *ca.* 1 cm<sup>3</sup>). Details about the arc-melting equipment are given in [9].

The niobium tube was then placed in a water-cooled sample chamber of a high-frequency furnace (HÜTTINGER TIG 1.5 / 300, 1.5 kW) under flowing argon [10]. The argon was purified over titanium sponge (900 K), silica gel and molecular sieves. The tube was first heated at about 1300 K for one minute. The reaction between the three elements was readily visible through a slight heat flash. The tube was subsequently annealed at about 870 K for another two hours followed by rapid cooling to room temperature within the water-cooled sample chamber by switching off the power of the high-frequency generator.

The silvery sample could easily be separated mechanically from the niobium ampoule. No reaction with the crucible material could be detected. Freshly cleaved fragments are silvery with metallic lustre, while powders are dark grey.

Table 1. Data collection and crystal parameters for SrAuSn<sub>2</sub>.

Chemical formula	SrAuSn <sub>2</sub>
Formula weight [g/mol]	522
Superspace group	$P : Cmc(\alpha 00)0s0$
t-Value	$1/16 + 4n$
<i>a</i> [pm]	460.2(1)
<i>b</i> [pm]	2038.8(8)
<i>c</i> [pm]	460.3(2)
Modulation wave vector	[0.25, 0 0]*
<i>V</i> [nm <sup>3</sup> ]	0.4319(3)
$\rho$ [g/cm <sup>3</sup> ]	8.025(5)
Crystal size [mm]	$0.02 \times 0.04 \times 0.04$
Diffractometer	STOE IPDS II
Radiation type	Mo-K $\alpha$
Wavelength [Å]	0.71073
No. of Images	360
$\phi$ Range	0 – 180°
2 $\theta$ Range	4 – 49.42
$\mu$ [mm <sup>-1</sup> ]	57.3
Data collection method	Phi rotation scans
Absorption correction	Numerical from crystal shape
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.094, 0.277
Measured reflections	6613
Independent reflections	857
Observed reflections	549
Independent satellites of 1 <sup>st</sup> order	417
Observed satellites of 1 <sup>st</sup> order	267
Independent satellites of 2 <sup>nd</sup> order	208
Observed satellites of 2 <sup>nd</sup> order	65
Criterion for observed reflections	$I \geq 3\sigma(I)$
<i>R</i> <sub>int</sub>	0.037
<i>h, k, l, m</i> Range	$-5 \leq h \leq 5$ $-23 \leq k \leq 23$ $-5 \leq l \leq 5$ $-2 \leq m \leq 2$
Refinement on	<i>F</i> <sup>2</sup>
<i>R</i> -factors of all observed reflections	0.021, 0.053
<i>R</i> , <i>wR</i>	
<i>R</i> -factors of observed main refls	0.015, 0.038
<i>R</i> , <i>wR</i>	
<i>R</i> -factors of observed satellites	0.032, 0.067
1 <sup>st</sup> order: <i>R</i> , <i>wR</i>	
<i>R</i> -factors of observed satellites	0.061, 0.135
2 <sup>nd</sup> order: <i>R</i> , <i>wR</i>	
Goodness of Fit	0.88
Reflections used in refinement	857
Parameters used in refinement	64
Weighting scheme	$1/(\sigma^2(I) + 0.0016 \cdot I^2)$
Residual electron density:	2.4, –2.9
max., min. [e/Å <sup>3</sup> ]	

The silvery single crystals are irregularly shaped. Larger pieces and well-shaped crystals of SrAuSn<sub>2</sub> are stable in moist air over longer periods of time. Fine powders deteriorate within some days.

### X-ray powder investigation

SrAuSn<sub>2</sub> was characterized through its Guinier powder pattern using Cu-K $\alpha_1$  radiation and  $\alpha$ -quartz (*a* = 491.30,

$c = 540.46$  pm) as an internal standard. The Guinier camera was equipped with an image plate system (Fujifilm, Basread-1800). The lattice parameters ( $a = 458.3(4)$ ,  $b = 2029(1)$ ,  $c = 458.5(3)$  pm) match those of the single crystal work (Table 1).

#### Single crystal work

Small single crystals of SrAuSn<sub>2</sub> were isolated from the crushed sample. These crystals were first examined by use of a Buerger camera equipped with an image plate system (Fujifilm BAS-1800) in order to establish suitability for intensity data collection. The intensity data were collected on a Stoe IPDS II image plate diffractometer with monochromatized Mo-K $\alpha$  radiation in oscillation mode (140 mm detector distance, 15 min. exposure time,  $\omega$  range 0–180°,  $\Delta\omega = 0.5^\circ$ ). The integration parameters were  $A = 15.6$ ,  $B = 3.2$ , and  $EMS = 0.03$ . All relevant data concerning the data collection are listed in Table 1.

## Results and Discussion

### Structure refinement

The single crystal X-ray diffraction data collected for the SrAuSn<sub>2</sub> crystal was used for the determination of the crystal structure. An average crystal structure model was obtained from the software SHELXS [11] by using structure factors corresponding to the unit cell  $a = 460.20(14)$ ,  $b = 2038.8(8)$ ,  $c = 460.34(19)$  pm and with the space group symmetry  $Cmcm$ . The average structure was found to be closely related to the structure of CeNiSi<sub>2</sub> where Sr replaces Ce, Au on the Ni positions and Sn on the Si positions. However, this structure refinement yielded high  $R$ -values and the model was found to be most unsatisfactory for the Sn atoms, indicating that the strongest modulation is to be found for Sn. A superstructure model was then applied with  $a_{\text{super}} = 4a_{\text{sub}}$ . However, the structural refinement of this model was found to be very unstable due to the large number of absent satellite reflections of higher order. Part of the diffraction pattern is illustrated in Fig. 1. Strong basic structure reflections as well as first and second order satellite reflections can be viewed in this diffraction pattern.

An attempt was therefore made to refine the structure as a commensurately modulated structure. The structure refinement software package JANA2000 [12] was used for this purpose. The 4D  $hklm$  data including the diffraction data of the average structure as well as the satellites were analysed in detail in order to determine a superspace group symmetry. The following

Table 2. Atomic positions and anisotropic displacement parameters of the basic structure of SrAuSn<sub>2</sub>.  $U_{23}$ ,  $U_{13}$  and  $U_{12}$  are fixed to zero by symmetry.

Atom	$x$	$y$	$z$	$U_{11}$	$U_{22}$	$U_{33}$
Sr	0	0.11160(7)	$1/4$	0.0156(4)	0.0190(7)	0.0149(6)
Au	0	0.334037(18)	$1/4$	0.0196(2)	0.0150(2)	0.0182(3)
Sn1	0	0.46403(3)	$1/4$	0.0397(5)	0.0120(4)	0.0109(4)
Sn2	0	0.74968(4)	$1/4$	0.0128(3)	0.0145(4)	0.0118(4)

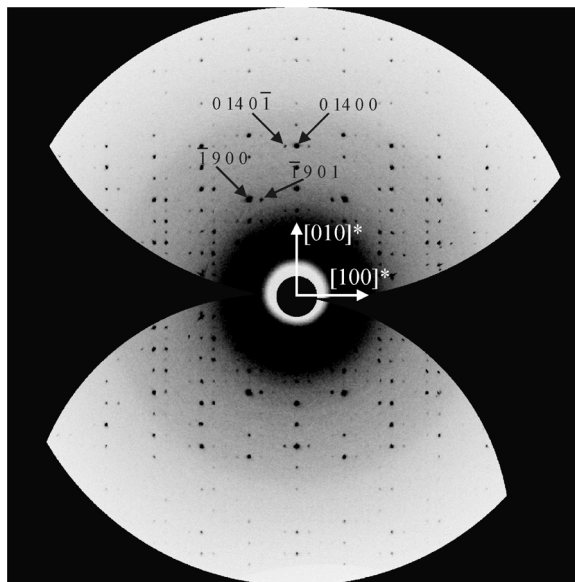


Fig. 1. The single crystal X-ray diffraction pattern of SrAuSn<sub>2</sub> extracted from the IPDS raw data. This pattern illustrates the reciprocal layer  $hk0$  containing both basic reflections and satellite reflections of first and second order.

systematic extinction conditions were found:  $F_{hklm} = 0$  if  $h + k \neq 2j$ ,  $F_{hk0m} = 0$  if  $h + k \neq 2j$  and  $F_{hk0m} = 0$  if  $m \neq 2j$ . The superspace group symmetry was determined to be  $Cmcm(\alpha, 0, 0)0s0$  with the modulation vector  $\mathbf{q} = [0.25, 0, 0]^*$ .

Since SrAuSn<sub>2</sub> has a commensurately modulated structure, a supercell and the origin of the  $t$ -value must be defined. By defining these parameters a 3D space group is obtained for the structure and the best refinement for SrAuSn<sub>2</sub> was obtained by using a  $t$ -value fixed to  $1/16 + n/4$ , which results in the 3D space group  $Pbnm$ .

The average structure determined by using the software program SHELXS was used as an initial model. All atoms were refined with anisotropic displacement parameters. The largest displacement parameters were obtained for Sn1, indicating the largest modulations. First and second order sinusoidal functions were used

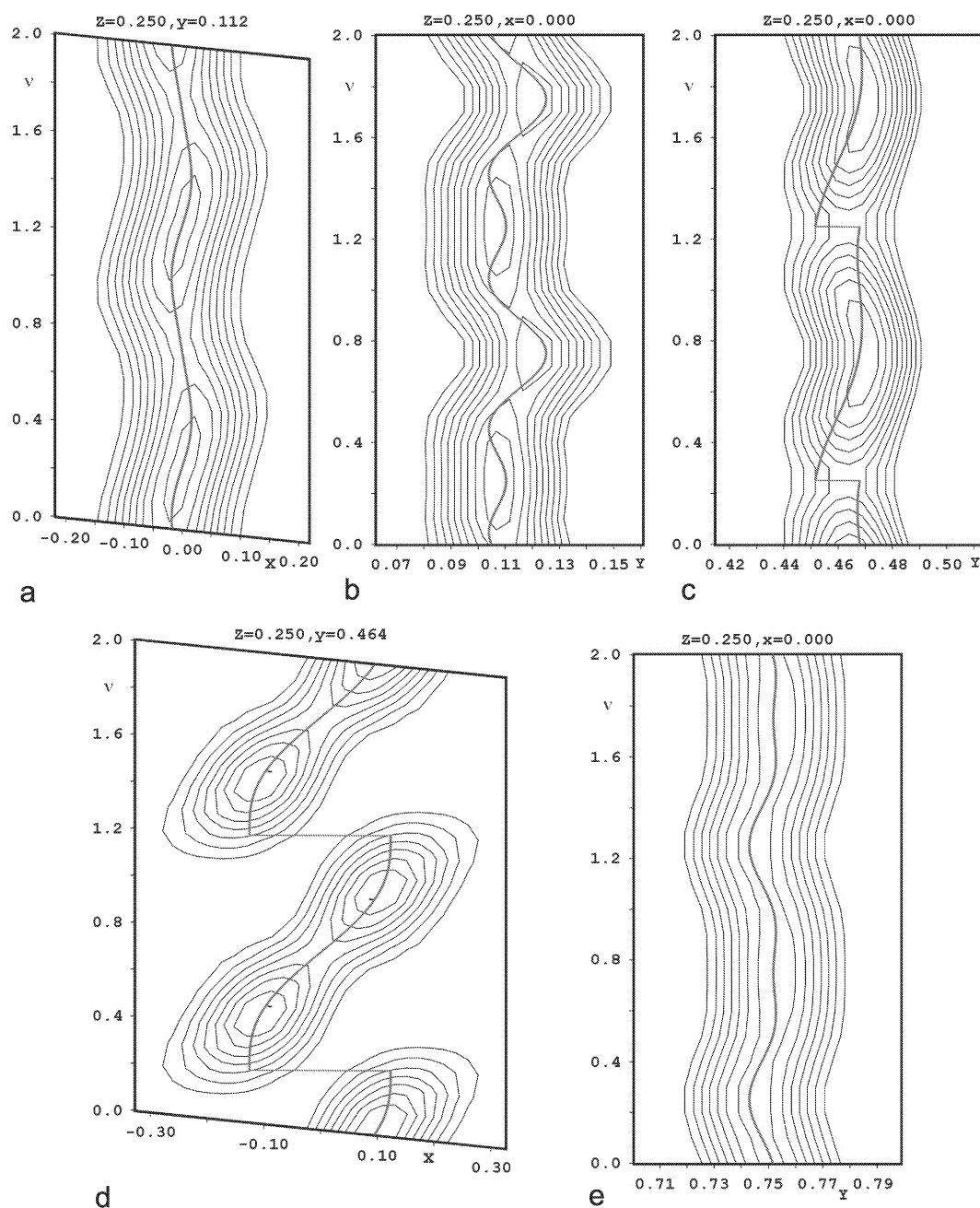


Fig. 2. Selected electron density maps of SrAuSn<sub>2</sub> calculated from  $F_{\text{obs}}$ , centred at the atomic position of (a, b) Sr, (c, d) Sn1 and (e) Sn2. The refined atomic modulation function of each atom is illustrated in the figures.

for modelling the modulation of all atoms initially. However the Sn1, which showed the strongest modulation, was found to be modelled best by combining one sinusoidal function and a saw tooth function. The refined modulation functions and the electron density

distribution of the different atoms are illustrated for selected crystallographic directions in Fig. 2.

The structure refinement merged to a final  $R1$  value of 0.021 for all reflections, including basic reflections as well as first and second order reflections. A total

Atom		<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>11</sub>	<i>U</i> <sub>22</sub>	<i>U</i> <sub>33</sub>	<i>U</i> <sub>23</sub>	<i>U</i> <sub>13</sub>	<i>U</i> <sub>12</sub>
Sr	sin1	0	−0.00740(9)	0	−0.0007(7)	−0.0061(9)	0.0006(9)	0	0	0
Sr	cos1	−0.0163(3)	0	0	0	0	0	0	0	0.0017(6)
Sr	sin2	−0.0027(11)	0	0	0	0	0	0	0	−0.0044(13)
Sr	cos2	0	−0.00633(18)	0	0.0019(17)	−0.0034(11)	0.000(2)	0	0	0
Au	sin1	0	−0.00343(3)	0	−0.0024(3)	0.0002(3)	−0.0013(4)	0	0	0
Au	cos1	−0.01130(14)	0	0	0	0	0	0	0	0.0003(6)
Au	sin2	0.0031(8)	0	0	0	0	0	0	0	0
Au	cos2	0	−0.00047(10)	0	−0.0015(13)	−0.0002(5)	0.0012(10)	0	0	0
Sn1	sin1	0	−0.00408(6)	0	−0.0091(9)	−0.0003(5)	−0.0011(9)	0	0	0
Sn1	cos1	0.0400(6)	0	0	0	0	0	0	0	0.0004(4)
Sn1	sin2	—	—	0	0	0	0	0	0	−0.0034(5)
Sn1	cos2	—	—	0	−0.0271(11)	0.0009(11)	−0.0019(15)	0	0	0
Sn2	sin1	0	−0.00443(5)	0	−0.0001(4)	0.0009(5)	−0.0002(6)	0	0	0
Sn2	cos1	−0.00251(18)	0	0	0	0	0	0	0	0.0000(4)
Sn2	sin2	−0.0019(13)	0	0	0	0	0	0	0	0.0019(10)
Sn2	cos2	0	0.00209(14)	0	0.001(2)	0.0017(10)	−0.0018(17)	0	0	0

Table 3. Positional and anisotropic displacement modulation wave parameters for SrAuSn<sub>2</sub>. The sawtooth function parameters used for Sn1 are: ax: 0.1253(8); ay: 0; az: 0; c: −1/4 and w: 1.

number of 64 refineable structural parameters were used in the refinement.

A final difference Fourier synthesis was flat and did not reveal significant residual peaks. The results of the structure refinement are summarized in Table 1. Atomic coordinates and the anisotropic displacement parameters are given in Table 2, the atomic modulation functions are given in Table 3 and the interatomic distances are listed in Table 4. Further details on the structure refinement are available\*.

### Crystal chemistry

SrAuSn<sub>2</sub> crystallizes with a peculiar new structure type. The average structure of SrAuSn<sub>2</sub> is closely related to the CeNiSi<sub>2</sub> type, space group *Cmcm* [13]. This orthorhombic structure type occurs also for ternary stannides; *i.e.* rare earth metal and alkaline earth metal–transition metal stannides *RETSn*<sub>2</sub> and *AETSn*<sub>2</sub> (*RE* = rare earth metal; *AE* = alkaline earth metal) [5]. As an example for the ideal structure we present a drawing of the BaCuSn<sub>2</sub> unit cell [14] in Fig. 3. This structure can be described as an intergrowth of distorted BaAl<sub>4</sub> and AlB<sub>2</sub> slabs. The Sn1 atoms within the AlB<sub>2</sub> slabs of BaCuSn<sub>2</sub> form zigzag chains running along the *c*-axis at Sn1–Sn1 distances of 285 pm.

In the modulated structure of SrAuSn<sub>2</sub> we observe only small structural distortions in the BaAl<sub>4</sub> slabs, while the Sn1–Sn1 zigzag chains within the AlB<sub>2</sub> slabs are responsible for the strong modulation. All gold

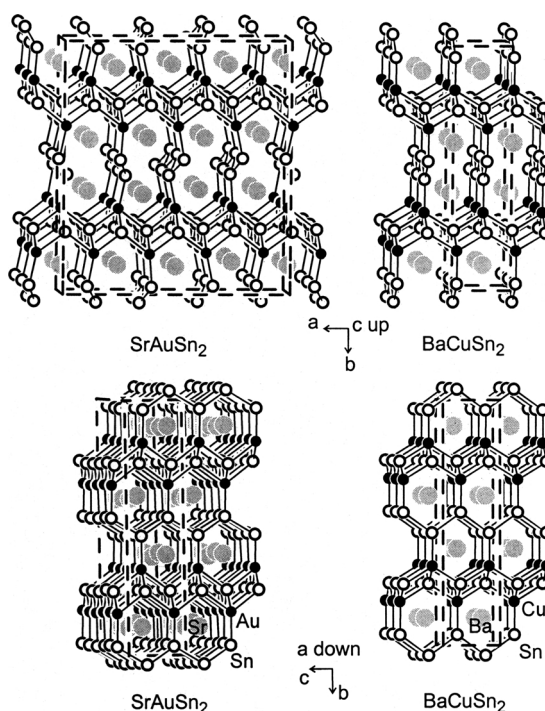


Fig. 3. Crystal structure of SrAuSn<sub>2</sub> illustrated along the *c*-axis and the structure of BaCuSn<sub>2</sub>. The open circles represent the Sn atoms, the black filled atoms are Au(Cu) and the grey atoms are Sr(Ba).

atoms are located within the BaAl<sub>4</sub> slabs. They have five tin neighbours in a distorted square pyramidal coordination at Au–Sn distances ranging from 266 to 294 pm. This larger range results from the modulation. The Au–Sn2 distances within the BaAl<sub>4</sub> slabs range from 278 to 294 pm, and they compare well with the sum of the covalent radii of 274 pm [15]. Sim-

\*Details may be obtained from: Fachinformationszentrum Karlsruhe, D-76344 Eggenstein-Leopoldshafen (Germany), by quoting the Registry No. CSD-414298.

Sr							
t = 1/16		t = 5/16		t = 9/16		t = 13/16	
Sn1	337.2(3)	2Au	338.4(3)	2Sn1	340.2(3)	2Sn1	332.9(3)
2Au	342.6(3)	2Au	343.6(3)	2Au	342.2(3)	2Au	337.9(2)
2Sn1	353.0(3)	Sn1	345.8(4)	2Au	352.3(3)	2Sn1	339.6(3)
2Au	353.7(3)	Sn1	351.2(4)	Sn1	357.8(3)	2Au	341.9(2)
Sn2	370.6(4)	Sn2	361.6(4)	Sn2	366.5(4)	Sn2	348.8(4)
2Sn2	371.3(2)	2Sn2	364.3(3)	2Sn2	367.7(2)	Sn2	351.9(4)
Sn2	376.0(4)	Sn2	365.7(4)	Sn2	368.6(4)	2Sn2	355.7(3)
2Sn1	383.8(4)	2Sn1	373.1(2)	2Sn1	390.8(4)	Sn1	398.4(3)
		2Sn1	382.7(3)				
Au							
t = 1/16		t = 5/16		t = 9/16		t = 13/16	
Sn1	271.2(2)	Sn1	269.6(2)	Sn1	269.9(1)	Sn1	266.1(2)
Sn2	278.8(4)	Sn2	284.7(2)	Sn2	280.5(3)	2Sn2	284.1(2)
2Sn2	288.5(1)	2Sn2	286.3(2)	2Sn2	287.6(1)	Sn2	286.1(3)
Sn2	294.3(3)	Sn2	292.3(3)	Sn2	292.0(4)	Sn2	289.7(4)
2Sr	341.9(3)	2Sr	337.9(2)	2Sr	338.4(3)	2Sr	343.6(3)
2Sr	342.6(3)	2Sr	342.2(3)	2Sr	353.2(3)	2Sr	353.7(3)
Sn1							
t = 1/16		t = 5/16		t = 9/16		t = 13/16	
Au	271.2(2)	Au	269.6(2)	Au	269.9(1)	Au	266.1(2)
2Sn1	287.9(2)	2Sn1	282.2(1)	2Sn1	287.9(2)	2Sn1	282.2(2)
2Sr	339.6(3)	2Sr	332.9(3)	Sr	337.2(3)	2Sr	353.0(3)
Sr	345.8(4)	Sn1	349.7(5)	2Sr	340.2(3)	Sr	357.8(3)
Sn1	349.7(5)	Sr	351.2(4)	2Sr	382.7(3)	2Sr	373.1(2)
2Sr	383.8(4)	2Sr	390.8(4)			Sr	398.4(3)
Sn2							
t = 1/16		t = 5/16		t = 9/16		t = 13/16	
Au	284.7(4)	2Au	284.1(2)	Au	278.8(4)	Au	280.5(3)
2Au	287.6(1)	Au	292.3(3)	2Au	288.5(1)	Au	286.1(3)
Au	292.0(4)	Au	294.3(3)	Au	289.7(4)	2Au	286.3(2)
2Sn2	323.1(4)	2Sn2	324.5(3)	2Sn2	324.5(3)	2Sn2	326.4(3)
2Sn2	326.5(3)	2Sn2	326.4(3)	2Sn2	326.3(4)	2Sn2	326.5(3)
Sr	365.7(4)	2Sr	355.7(3)	Sr	351.9(4)	Sr	348.8(4)
2Sr	367.7(2)	Sr	361.6(4)	2Sr	371.3(2)	2Sr	364.3(3)
Sr	368.6(4)	Sr	370.6(4)	Sr	376.0(4)	Sr	366.5(4)

Table 4. The interatomic distances given in pm, calculated at the four possible t-values in the SrAuSn<sub>2</sub> structure.

ilar Au–Sn distances occur in related stannides, *i.e.* SrAuSn (279–312 pm [7]), YbAuSn (272–315 pm [16]), Eu<sub>2</sub>Au<sub>2</sub>Sn<sub>5</sub> (272–301 pm [8]), or Li<sub>2</sub>AuSn<sub>2</sub> (273 pm [17]).

The Sn1 atoms form homoatomic bonds. Due to the modulation we observe a small range of Sn1–Sn1 distances from 282 to 288 pm, close to the Sn–Sn distance in  $\alpha$ -tin (281 pm) [18]. Such Sn–Sn distances are typically observed in tin-rich stannides with related structures, *e.g.* Eu<sub>2</sub>Au<sub>2</sub>Sn<sub>5</sub> (295–348 pm [8]) or Li<sub>2</sub>AuSn<sub>2</sub> (296 pm [17]).

Together, the gold and tin atoms build up a three-dimensional [AuSn<sub>2</sub>] network in which the strontium atoms fill distorted channels (Fig. 3). While the Au and Sn2 atoms remain almost at their ideal positions within the BaAl<sub>4</sub> slabs, the strontium atoms react on the strong modulation of the Sn1 chains through shifts

in the  $\pm y$  direction. Due to the modulation, the Sn1 atoms strongly shift in the  $\pm x$  direction, thus violating the mirror plane at 0yz in the average subcell structure.

Finally we need to comment on the structural peculiarities of the CeNiSi<sub>2</sub> type and related compounds. There exist two different branches for the CeNiSi<sub>2</sub> intermetallics. The silicides and some germanides crystallize with the ideal composition [5], while most germanides and the stannides show large ranges of homogeneity  $RE_{1-x}Ge_2$  and  $RE_{1-x}Sn_2$  [6, 19, 20]. Furthermore, some of the stannides with nickel and manganese as transition metal component reveal defects on the tin positions leading to phases  $RENi_{1-x}Sn_{2-y}$  and  $REMn_{1-x}Sn_{2-y}$  [6]. The defects and the homogeneity ranges have significant influence on the magnetic properties of these phases. The strong modulation of the Sn1 atoms observed here for SrAuSn<sub>2</sub> is a further structural peculiarity in this family of intermetallics.

The electronic nature of this behaviour is not yet understood.

#### Acknowledgements

We thank Birgit Heying for experimental help and the Degussa-Hüls AG for a generous gift of gold wire. Professor Sven Lidin is acknowledged for valuable discussions. This work was financially supported by the Deutsche Forschungsgemeinschaft. S.E. acknowledges the Swedish science foundation (vetenskapsrådet) for financial support.

- 
- [1] R.-D. Hoffmann, D. Kußmann, U.Ch. Rodewald, R. Pöttgen, C. Rosenhahn, B. D. Mosel, *Z. Naturforsch.* **54b**, 709 (1999).
  - [2] R. Pöttgen, R.-D. Hoffmann, M. H. Möller, G. Kotzyba, B. Künnen, C. Rosenhahn, B. D. Mosel, *J. Solid State Chem.* **145**, 174 (1999).
  - [3] D. Niepmann, R. Pöttgen, B. Künnen, G. Kotzyba, C. Rosenhahn, B. D. Mosel, *Chem. Mater.* **11**, 1597 (1999).
  - [4] Z. Hossain, L. C. Gupta, C. Geibel, *J. Phys.: Cond. Matter.* **14**, 9687 (2002).
  - [5] P. Villars, L. D. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases*, Second Edition, American Society for Metals, Materials Park, OH 44073 (1991), and Desk Edition (1997).
  - [6] R. V. Skolozdra, *Stannides of Rare-Earth and Transition Metals*, in K. A. Gschneidner (Jr.), L. Eyring (eds.): *Handbook on the Physics and Chemistry of Rare Earths*, Vol. 14, chapter 164, Elsevier, Amsterdam (1997).
  - [7] R.-D. Hoffmann, R. Pöttgen, D. Kußmann, D. Niepmann, H. Trill, B. D. Mosel, *Solid State Sci.* **4**, 481 (2002).
  - [8] D. Kußmann, R. Pöttgen, U.Ch. Rodewald, C. Rosenhahn, B. D. Mosel, G. Kotzyba, B. Künnen, *Z. Naturforsch.* **54b**, 1155 (1999).
  - [9] R. Pöttgen, Th. Gulden, A. Simon, *GIT-Laborfachzeitschrift* **43**, 133 (1999).
  - [10] D. Kußmann, R.-D. Hoffmann, R. Pöttgen, *Z. Anorg. Allg. Chem.* **624**, 1727 (1998).
  - [11] G.M. Sheldrick, *SHELXL-97*, Program for Crystal Structure Refinement, University of Göttingen, Germany (1997).
  - [12] V. Petricek and M. Dusek, *Jana2000*. The crystallographic computing system. Institute of Physics, Praha, Czech Republic (2000).
  - [13] O.I. Bodak, E.I. Gladyshevskii, *Sov. Phys. Crystallogr.* **14**, 859 (1970).
  - [14] W. Dörrscheidt, G. Savelsberg, J. Stöhr, H. Schäfer, *J. Less-Common Met.* **83**, 269 (1982).
  - [15] J. Emsley, *The Elements*, Clarendon Press, Oxford (1989).
  - [16] R.-D. Hoffmann, R. Pöttgen, D. Kußmann, R. Müllmann, B. D. Mosel, *Chem. Mater.* **13**, 4019 (2001).
  - [17] Zh. Wu, B. D. Mosel, H. Eckert, R.-D. Hoffmann, R. Pöttgen, *Chem. Eur. J.* **10**, 1558 (2004).
  - [18] J. Donohue, *The Structures of the Elements*, Wiley, New York (1974).
  - [19] M. François, G. Venturini, B. Malaman, B. Roques, *J. Less-Common Met.* **160**, 197 (1990).
  - [20] G. Venturini, M. François, B. Malaman, B. Roques, *J. Less-Common Met.* **160**, 215 (1990).
  - [21] A. Szytuła, J. Leciejewicz, *Handbook of Crystal Structures and Magnetic Properties of Rare Earth Intermetallics*, CRC Press, Boca Raton, Florida (1994).