

prism composition and type of linkage of the octahedron columns. Formulae framed by rectangles with full lines correspond to structures containing only columns of antiprisms and octahedra, those by rectangles with dashed lines to structures containing additional M atoms in between the antiprisms columns. In this latter case the additional atoms assure that the T elements participating in the antiprisms have an octahedral M surrounding; these M-octahedra, however, do not form face-shared octahedron columns.

| antiprism composition linkage   | (R <sub>4</sub> T <sub>4</sub> )M <sub>2</sub> antiprism columns  | (R <sub>6</sub> T <sub>2</sub> )M <sub>2</sub> antiprism columns   | R <sub>6</sub> M <sub>2</sub> antiprism columns   |
|---|---|--|---|
| M <sub>6</sub> T <sub>2</sub><br>isolated octahedron columns  | R <sub>4</sub> T <sub>6</sub> M <sub>8</sub><br><span style="border: 1px solid black; padding: 2px;">Zr<sub>2</sub>Ru<sub>3</sub>Si<sub>4</sub></span>  | R <sub>6</sub> T <sub>4</sub> M <sub>8</sub>   | R <sub>8</sub> T <sub>2</sub> M <sub>8</sub>  |
| 2 (M <sub>2</sub> M <sub>4/2</sub> )T <sub>2</sub><br>octahedron columns edge-connected with 2 others | R <sub>4</sub> T <sub>8</sub> M <sub>10</sub><br><span style="border: 1px solid black; padding: 2px;">Sc<sub>2</sub>Cr<sub>4</sub>Si<sub>5</sub></span> | R <sub>6</sub> T <sub>6</sub> M <sub>10</sub><br><span style="border: 1px dashed black; padding: 2px;">ZrFeSi<sub>2</sub></span><br><span style="border: 1px dashed black; padding: 2px;">ZrMnSi<sub>2</sub></span><br><span style="border: 1px dashed black; padding: 2px;">LuMnGe<sub>2</sub></span> | R <sub>8</sub> T <sub>4</sub> M <sub>10</sub>   |
| 4 (M <sub>6/2</sub> )T <sub>2</sub><br>octah. columns edge-connected with 3 others                    | R <sub>4</sub> T <sub>12</sub> M <sub>14</sub>  | R <sub>6</sub> T <sub>10</sub> M <sub>14</sub>   | R <sub>8</sub> T <sub>8</sub> M <sub>14</sub><br><span style="border: 1px solid black; padding: 2px;">Zr<sub>4</sub>Co<sub>4</sub>Ge<sub>7</sub></span> |

The structure of Zr<sub>2</sub>Ru<sub>3</sub>Si<sub>4</sub> will be compared with ScRe<sub>2</sub>Si<sub>3</sub> and Sc<sub>3</sub>Re<sub>2</sub>Si<sub>3</sub>. The latter has a similar unit cell and identical atom sites (except for one unoccupied Si position). A detailed account of this work will be published in Acta Crystallographica.

08.3-11 A NEUTRON POWDER DIFFRACTION INVESTIGATION OF LANTHANUM HEXABORIDE. By M.M. Korsukova, V.N. Gurin, A.F. Ioffe Physical-Technical Institute, Academy of Sciences of the USSR, Leningrad, USSR

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It has been established that the cell dimensions of LaB<sub>6</sub> do not vary with composition (Storms, Mueller, J. Phys. Chem. (1978) 82, 51). Nevertheless, the chemical analyses indicate that a relatively extensive range of homogeneity occurs. Several explanations have been presented as regards the atomic mechanism behind this composition variation. The most obvious suggestion is the occurrence of vacancies at the lanthanum position for boron-rich compositions. Another explanation (Storms, Mueller, J. Phys. Chem. (1978) 82, 51) anticipates the occurrence of separate phases with different compositions (LaB<sub>6</sub> and LaB<sub>9</sub>) but with identical unit cells as well as identical diffraction intensities.

In the present study an attempt was made to evaluate the occurrence of vacancies in the La- or B-sublattice using the neutron powder diffraction technique.

The crystals were prepared by solution growth from an Al melt using a <sup>11</sup>B-enriched (93-96%) boron. The B/La ratio in the melt was 9/1. The neutron powder diffraction study was made using the Rietveld-type profile refinement technique.

The results of these investigations will be presented and discussed.

08.3-12 CRYSTAL STRUCTURE OF NEW PHASES IN THE Ca-Au, Sr-Au AND Ba-Au SYSTEMS

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About the existence and the crystal structure of intermetallic compounds in the systems formed by Ca, Sr and Ba with Au a few data are available in the literature. Concerning the range 0-50% at. of gold, three phases were reported in the Ca-Au diagram and five in the Sr-Au diagram, all of these with unknown structure. For the same range in the Ba-Au system no information are given (M. Hansen & K. Anderko, "Constitution of Binary Alloys", McGraw-Hill, 1958; R.P. Elliott, "Constitution of Binary Alloys, 1st Supplement", McGraw-Hill, 1965). Recently CaAu was found to be isotypic with the CrB type (F. Merlo, J. Less-Comm. Met. 86, 1982, 241-6).

In this work we present the crystal structure determination of the intermetallic compounds Ca<sub>7</sub>Au<sub>3</sub>, Ca<sub>5</sub>Au<sub>3</sub>, Ca<sub>5</sub>Au<sub>4</sub>, Sr<sub>7</sub>Au<sub>3</sub>, Sr<sub>3</sub>Au<sub>2</sub>, SrAu and BaAu.

They were identified by single crystal methods and the structures determined and refined by single crystal diffractometer data.

Ca<sub>7</sub>Au<sub>3</sub>, oP80, orthorhombic, Pbcu, a=20.742(8), b=18.036(8), c=6.665(2) Å, Z=8, is a new structure.

It can be derived from the hexagonal Th<sub>7</sub>Fe<sub>3</sub> - type, with the following relationships:

$$a = 2 a_{\text{Th}_7\text{Fe}_3} ; \quad b = \sqrt{3} a_{\text{Th}_7\text{Fe}_3} ; \quad c = c_{\text{Th}_7\text{Fe}_3}$$

The structure is built up by packing four layers along the short axis. Two of these, formed by Ca atoms only, are identical to those formed by Th atoms in Th<sub>7</sub>Fe<sub>3</sub>; two other layers containing both Ca and Au are rearranged, so that the calcium octahedra assume two possible orientations, one rotated 60° about the short axis relative to the other.

Ca<sub>5</sub>Au<sub>3</sub>, tI32, tetragonal, I4/mcm, a=7.867(3), c=14.39(1) Å, Z=4, is isotypic with Cr<sub>5</sub>B<sub>3</sub>.

Ca<sub>5</sub>Au<sub>4</sub>, mP18, monoclinic, P2<sub>1</sub>/c, a=8.028(3), b=8.019(6), c=7.727(3) Å, beta=109.16(6)°, Z=2, is a new structure. It is closely related to the Pu<sub>5</sub>Rh<sub>4</sub>-type.

Sr<sub>7</sub>Au<sub>3</sub>, hP20, hexagonal, P6<sub>3</sub>mc, a=11.07(1), c=7.161(4) Å, Z=2, is isotypic with Th<sub>7</sub>Fe<sub>3</sub>.

Sr<sub>3</sub>Au<sub>2</sub>, hR15, rhombohedral, R $\bar{3}$ , a=9.604(4), c=18.36(1) Å, Z=9, is isotypic with Er<sub>3</sub>Ni<sub>2</sub>.

SrAu, mP40, monoclinic, P2<sub>1</sub>/m, a=40.13(3), b=4.697(1), c=6.192(4) Å, beta=94.21(6)°, Z=20, is a new structure. It belongs to the family of the stacking variants of the CrB-FeB types, with stacking symbol hch<sub>2</sub>ch<sub>2</sub>chc and Zhdanov notation (2)21(2)12.

BaAu, oP8, orthorhombic, Pnma, a=8.338(8), b=4.925(3), c=6.390(7) Å, Z=4, is isotypic with FeB.

In these structures gold is always surrounded by a trigonal prism formed by alkaline earth atoms. Through the lateral faces of the prism other waist contacts with alkaline earth or gold atoms are also possible, so that we find Au-Au pairs in Ca<sub>5</sub>Au<sub>3</sub>, Ca<sub>3</sub>Au<sub>4</sub> and Sr<sub>3</sub>Au<sub>2</sub>, and Au zig-zag chains in SrAu<sub>5</sub> and BaAu.