

**substance: Os<sub>2</sub>Si<sub>3</sub>**

**property: crystal structure, chemical bond of Os<sub>n</sub>Si<sub>2n-m</sub> compounds**

The structures of the Nowotny chimney-ladder compounds T<sub>n</sub>(IV)<sub>2n-m</sub> (T: transition element) are derived from the TiSi<sub>2</sub> type. The Ti atoms in orthorhombic TiSi<sub>2</sub> and the T atoms in tetragonal T<sub>n</sub>(IV)<sub>2n-m</sub> occupy a β-Sn-like array of sites with a strongly increased axial ratio  $c/a$ . The number  $n$  in the formula corresponds to the number of white-tin-like pseudocells stacked along  $c$ . According to the (IV)-deficiency the distribution of (III)- or (IV)-atoms is stretched up along  $c$  as compared with the TiSi<sub>2</sub> structure [70N, 71D, 72P, 74B, 76D].

The electronegativity of the transition element is larger than that of the group IV element. Thus the T atoms act as anions so that the bonding is similar to that in the transition-element carbonyls. According to Jeitschko and Parthe [67J, 69P, 70N, 77J] semiconductor behavior and hence filled energy bands occur with 14 valence electrons per T atom.

The tetragonal high-temperature structures Ru<sub>2</sub>Si<sub>3</sub>, Ru<sub>2</sub>Ge<sub>3</sub> and Ru<sub>2</sub>Sn<sub>3</sub> undergo second-order transitions to orthorhombic symmetry (D<sub>2h</sub><sup>14</sup> – Pbcn; Z = 8) at 1300 K (Ru<sub>2</sub>Si<sub>3</sub>), 800 K (Ru<sub>2</sub>Ge<sub>3</sub>), and < 100 K (Ru<sub>2</sub>Sn<sub>3</sub>). Os<sub>2</sub>Si<sub>3</sub> and Os<sub>2</sub>Ge<sub>3</sub> are known only in the latter structure.

## References:

- 67J Jeitschko, W., Parthé, F.: Acta Crystallogr. 22 (1967) 417.
- 69P Parthé, F.: in "Developments in the Structural Chemistry of Alloy Phases" (B. C. Giessen, ed.), Plenum New York 1969, p. 49.
- 70N Nowotny, H.: in "The Chemistry of Extended Defects in Non-Metallic Solids", North Holland 1970, p. 223.
- 71D De Ridder, R., Amelinckx, S.: Mat. Res. Bull. 6 (1971) 1223.
- 72P Pearson, W. B.: "The Crystal Chemistry and Physics of Metals and Alloys"; Wiley, New York 1972.
- 74B Boller, H.: Monatsh. Chem. 105 (1974) 934.
- 76D De Ridder, R., van Tendebo, G., Amelinckx, S.: Phys. Status Solidi (a) 33 (1976) 383.
- 77J Jeitschko, W.: Acta Crystallogr. B33 (1977) 2347.