substance: Ru_2Si_3
property: crystal structure, chemical bond of Ru_nSi_{2n-m} compounds

The structures of the Nowotny chimney-ladder compounds $T_n(IV)_{2n-m}$ (T: transition element) are derived from the $TiSi_2$ type. The Ti atoms in orthorhombic $TiSi_2$ and the T atoms in tetragonal $T_n(IV)_{2n-m}$ 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 the (III)-or (IV)-atoms is stretched up along *c* as compared with the $TiSi_2$ 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.

In Ru_2Si_3 Si has no like neighbors within bonding distance in contrast to the Mn_nSi_{2n-m} phases, where Si chain fragments are formed even in Mn_4Si_7, thus reducing the number of valence electrons available for Mn – Si bonding to about 5 per Mn atom. Unfortunately, there is no clear-cut separation between bonding and nonbonding Si – Si distances.

The tetragonal high-temperature structures Ru_2Si_3, Ru_2Ge_3 and Ru_2Sn_3 undergo second-order transitions to orthorhombic symmetry (D_{2h}^{14} – Pbcn; Z = 8) at 1300 K (Ru_2Si_3), 800 K (Ru_2Ge_3), and < 100 K (Ru_2Sn_3). Os_2Si_3 and Os_2Ge_3 are known only in the latter structure.

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