

substance: FeSi₂

property: crystal structures of FeSi₂ and other TSi₂ phases

The hexagonal CrSi₂ structure and the tetragonal MoSi₂ type structure belong to the same family of polytypic structures as does the orthorhombic TiSi₂ structure. These three structure types can be generated from close-packed layers in bcc [110] stacking [72P]. Of the four possible stacking positions ABCD two (AB) are involved in tetragonal MoSi₂, three (ABC) in hexagonal CrSi₂ and four (ACBD) in orthorhombic TiSi₂. The MoSi₂ cell contains three bc tetragonal ($c/a < 1$) pseudo-cells. Thus, Si pairs in c direction result which however are connected with four Si atoms of the adjacent pseudo-cell at virtually the same distance. The metal atom is coordinated to 10 Si atoms. ReSi₂ crystallizes in a slightly distorted MoSi₂ structure, isopuntal with orthorhombic MoPt₂. In CrSi₂ Si has 2 + 3 close Cr neighbors and 2 + 3 Si neighbors at 2.48 and 2.56 Å. FeSi₂ (so-called β phase) is stable only below 950...970°C. At this temperature it decomposes into FeSi + Fe_{≈0.8}Si₂ (so-called α -FeSi₂). The structure of FeSi₂ is of the orthorhombic OsSi₂ type [71D] which can be described as a distorted CaF₂ type derivative, i.e. a distorted arrangement of Si cubes half of which are occupied by Fe atoms. The deformation leads to distorted Fe tetrahedrons around each Si atom. At the same time the Fe atoms as well as the Si atoms approach each other. Fe atoms cluster to a square with distances of 2.97 Å and the Si atoms acquire 5 Si neighbors as close as 2.45...2.59 Å.

References:

- 71D Dusauroy, Y., Protas, J., Wandji, R., Roques, B.: *Acta Crystallogr. B* 27 (1971) 1209.
- 72P Pearson, W. B.: *"The Crystal Chemistry and Physics of Metals and Alloys"*, Wiley, New York 1972.