substance: $CrSi_2$
property: crystal structure of $CrSi_2$ and other TSi_2 phases

The hexagonal $CrSi_2$ structure and the tetragonal $MoSi_2$ type structure belong to the same family of polytypic structures as does the orthorhombic $TiSi_2$ 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 $MoSi_2$, three (ABC) in hexagonal $CrSi_2$ and four (ACBD) in orthorhombic $TiSi_2$. The $MoSi_2$ 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. $ReSi_2$ crystallizes in a slightly distorted $MoSi_2$ structure, isopuntal with orthorhombic $MoPt_2$. In $CrSi_2$ Si has 2 + 3 close Cr neighbors and 2 + 3 Si neighbors at 2.48 and 2.56 Å. $FeSi_2$ (so-called β phase) is stable only below 950...970°C. At this temperature it decomposes into FeSi + $Fe_{\approx 0.8}Si_2$ (so-called α-$FeSi_2$). The structure of $FeSi_2$ is of the orthorhombie $OsSi_2$ type [71D] which can be described as a distorted CaF_2 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:

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72P Pearson, W. B.: "The Crystal Chemistry and Physics of Metals and Alloys", Wiley, New York 1972.