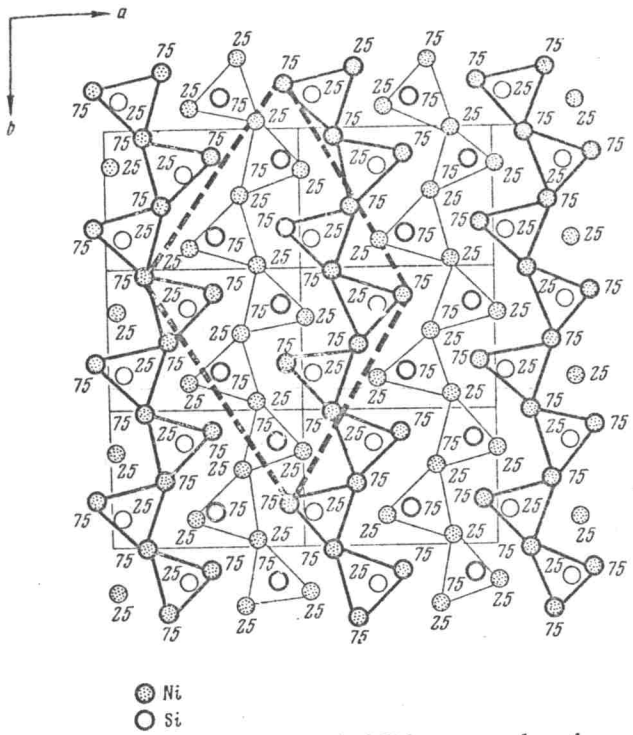


Fig. 1. Projection of the $Ni_2Si$ (anti-$PbCl_2$) structure along the c axis in the Pbnm–$D_{2h}^{16}$ aspect. The dashed lines are sections $a\,a$ of the proposed hexagonal unit cell for $Mg_2SnII$; 25 is the coordinate z = 0.25 for the corresponding atom.

ature modification having the fluorite structure and the low-temperature form having the hexagonal structure mentioned above.

It is interesting that the $NaNdF_4$ structure is little different in essence from the hexagonal $Fe_2P$ structure; they would be identical if we assume that Na atoms randomly occupying 2(h) positions in the $P\bar{6}$ group, 1/3, 2/3, z; 1/3, 3/2, $\bar{z}$ (z = 0.656), settle into 1(f) positions, 1/3, 2/3, 1/2. In turn, the $Fe_2P$ and $PbCl_2$ structure types are mutually related by a simple translation.

Thus there are a number of crystal structures with nearly identical motifs for the atomic arrangement which are quite extensive among the intermetallic compounds and are characterized by identical coordination polyhedra (nine vertices) differently linked with respect to each other. It can be suggested on this basis that the hexagonal $Mg_2$ · SnII unit cell proposed in this work, having parameters $a_0$ = 13.18 ± 0.02 and $c_0$ = 6.99 ± 0.04 Å, is not the result of arbitrary indexing. If we choose the period $a_{hex}$ in a pseudohexagonal network of Ni atoms in the $Ni_2Si$ structure, as shown in Fig. 1, and set $c_{hex} = 2c_{rhomb}$, then we obtain unit cell parameters close to those given above. However, if we preserve the $Ni_2Si$ unit cell as structural motif we should have z = 18, which does not agree with $\rho_e$ whose value gives z = 15 or 16. This condition can be satisfied if, in addition to the nine Si atoms which are contained in the chosen unit cell of the $Ni_2Si$ structural motif, we put another six Si atoms in place of the six Ni atoms which occupy sites on the edges (2) and on the three-fold axes (4). Thus with a doubling of $c_{rhomb}$ we find 30 Ni atoms per unit cell.

Figure 2 shows one of two possible atomic arrangements which differ by c/2. It should be noted that the proposed structure model is obtained not only by the distortion of $Ni_2Si$–type structures described above, but also in analyzing the intensities by construction of cross sections perpendicular to

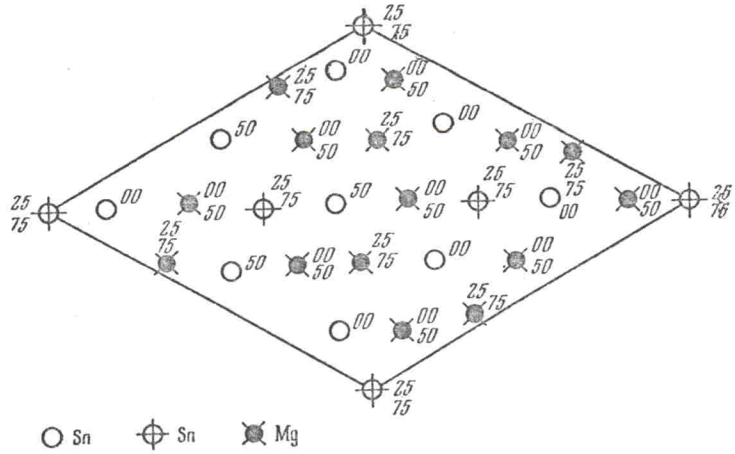


Fig. 2. Projection of the assumed structure model for $Mg_2SnII$ along the c axis. The dark circles and the oblique crosses are Mg atoms at various heights, and the circles and plain crosses are Sn atoms at various heights.