crystal structures (Smirnova, 1962), of Patterson diagrams (Koch & Hellner, 1971), of Dirichlet domains (Koch, 1973, 1984) and of sphere packings for subperiodic groups (Koch & Fischer, 1978*b*).

The 30 lattice complexes in two-dimensional space correspond uniquely to the 'henomeric types of dot pattern' introduced by Grünbaum and Shephard (*cf. e.g.* Grünbaum & Shephard, 1981; Grünbaum, 1983).

3.4.4.2. Relations between crystal structures

Different crystal structures frequently show the same geometrical arrangement for some of their atoms, even though their space groups do not belong to the same type. In such cases, the corresponding Wyckoff positions either belong to the same lattice complex or there exists a close relationship between them, *e.g.* a limiting-complex relation.

Examples

(1) The Fe atoms in pyrite FeS_2 occupy Wyckoff position 4*a* .$\bar{3}$. 0, 0, 0 of $Pa\bar{3}$ (descriptive symbol *F*) that belongs to the invariant lattice complex $Fm\bar{3}m$ *a*. Accordingly, the Fe atoms in pyrite form a face-centred cubic lattice, as do the Cu atoms in the element structure of copper.

(2) Cuprite Cu_2O crystallizes with symmetry $Pn\bar{3}m$. The oxygen atoms occupy Wyckoff position 2*a* $\bar{4}3m$ 0, 0, 0 (descriptive symbol *I*) and the copper atoms position 4*b* .$\bar{3}m$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ (descriptive symbol $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*). Position 2*a* belongs to lattice complex $Im\bar{3}m$ *a* and position 4*b* to $Fm\bar{3}m$ *a*. Therefore, the O atoms form a body-centred cubic lattice like the W atoms in the structure of tungsten, and the copper atoms form a face-centred cubic lattice. The tungsten configuration is shifted by $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ with respect to the copper configuration.

(3) K_2NaAlF_6 (elpasolite, *cf.* Morss, 1974) and $K_2PbNi(NO_2)_6$ (*cf.* Takagi *et al.*, 1975) crystallize with symmetry $Fm\bar{3}m$ and $Fm\bar{3}$, respectively.

K_2NaAlF_6

Al	4*a*	$m\bar{3}m$	0, 0, 0	*F*
Na	4*b*	$m\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}F$
K	8*c*	$\bar{4}3m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}P_2$
F	24*e*	4*m*.*m*	*x*, 0, 0	*F*6*z*
			$x = 0.219$	

$K_2PbNi(NO_2)_6$

Ni	4*a*	$m\bar{3}$.	0, 0, 0	*F*
Pb	4*b*	$m\bar{3}$.	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}F$
K	8*c*	23.	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}P_2$
N	24*e*	*mm*2..	*x*, 0, 0	*F*6*z*
			$x = 0.1966$	
O	48*h*	*m*..	0, *y*, *z*	*F*6*z*2*x*

As the descriptive lattice-complex symbols for the various atomic positions show immediately, the two crystal structures are very similar. The only difference originates from the replacement of the fluorine atoms in elpasolite by NO_2 groups in $K_2PbNi(NO_2)_6$, which causes the symmetry reduction from $Fm\bar{3}m$ to $Fm\bar{3}$.

(4) The crystal structure of CoU (Baenziger *et al.*, 1950) may be interpreted as a slightly distorted CsCl (or β-brass, CuZn)-type structure. CsCl corresponds to Wyckoff positions 1*a* and 1*b* of $Pm\bar{3}m$ with descriptive symbols *P* and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*, respectively; Co and U both occupy Wyckoff position 8*a* .3. *x*, *x*, *x* of $I2_13$ with $x = 0.0347$ for U and $x = 0.294$ for Co. As the descriptive symbol 2_12_1.. P_2Y^*1xxx shows, this Wyckoff position belongs to a Weissenberg complex with two invariant limiting complexes, namely *P* ($Pm\bar{3}m$ *a*) and Y^* ($I4_132$ *a*). $x = 0$ corresponds to P_2, $x = \frac{1}{4}$ to $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2, $x = \frac{1}{8}$ to $^+Y^*$ and $x = \frac{7}{8}$ to $^-Y^*$. Consequently, the uranium and cobalt atoms form approximately a P_2 and a $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2 configuration, respectively.

Publications by Hellner (1965, 1976*a*,*b*,*c*, 1977, 1979), Loeb (1970), Smirnova & Vasserman (1971), Sakamoto & Takahasi (1971), Niggli (1971), Fischer & Koch (1974*b*), Hellner *et al.* (1981) and Hellner & Sowa (1985) refer to this aspect.

3.4.4.3. Reflection conditions

Wyckoff positions belonging to the same lattice complex show analogous reflection conditions. Therefore, lattice complexes have also been used to check the reflection conditions for all Wyckoff positions in the space-group tables of this volume.

Example

The lattice complex *oF* consists of all face-centred point lattices with orthorhombic symmetry. For its characteristic Wyckoff position *Fmmm* 4*a*, only the general conditions for reflections *hkl* in space group *Fmmm* are valid, namely $h + k$, $h + l$, $k + l = 2n$ (*cf.* Chapter 2.3). The non-characteristic Wyckoff position *Ccce* 4*a* also belongs to this lattice complex. The general reflection condition for *Ccce* is *hkl*: $h + k = 2n$. This has to be combined with $k + l = 2n$, the special condition for Wyckoff position *a*. Together the two conditions produce $h + l = 2n$, the third condition for a face-centred point lattice.

The descriptive symbols may supply information on the reflection conditions. If the symbol does not contain any distribution-symmetry part, the reflection conditions of the Wyckoff position are indicated by the symbol of the invariant lattice complex in the central part (*e.g.* *P*4/*nmm g*: *C*4*xx* shows that the reflection condition is that of a *C* lattice, *hkl*: $h + k = 2n$). In cases where the site set consists of only one point, *i.e.* the Wyckoff position belongs to a Weissenberg complex, all conditions for general reflections *hkl* that may arise from special choices of the coordinates can be read from the central part of the symbol (*e.g.* *P*4/*nmm c*: $0\frac{1}{2}0$ ..2 *CI*1*z* indicates that, by special choice of *z*, either *hkl*: $h + k = 2n$ or *hkl*: $h + k + l = 2n$ may be produced).

3.4.4.4. Phase transitions

If a crystal undergoes a phase transition from a high- to a low-symmetry modification, the transition may be connected with a group–subgroup transition. In such cases, the comparison of the lattice complexes corresponding to the Wyckoff positions of the original space group on the one hand and of its various subgroups on the other hand very often shows which of these subgroups are suitable for the low-symmetry modification.

This kind of procedure will be demonstrated with the aid of the space group $R\bar{3}m$ and its three *translationengleiche* subgroups with index 2, namely *R*32, $R\bar{3}$ and *R*3*m*. In the course of the restriction to a subgroup, the Wyckoff positions of $R\bar{3}m$ behave differently: