σ_0	scattering given by a free electron
l	index labelling unit cells
k	index labelling atom within unit cell
f_k	scattering factor
W_k	Debye–Waller term $=(1/2N)\sum_\lambda (E/\omega^2)_\lambda \lvert \mathbf{K}\,.\,\mathscr{E}(k/\lambda)/m_k^{1/2}\rvert^2$
$\mathbf{K}$	scattering vector
$\mathbf{r}(lk)$	equilibrium coordinate of atom (lk)
λ	phonon state label $(\mathbf{q}j)$
$\mathbf{q}$	phonon wavevector
j	phonon branch index
ω_λ	phonon angular frequency
E_λ	average energy in phonon state $(\mathbf{q}j)$
m_k	mass of kth atom in unit cell
$\mathscr{E}(k/\lambda)$	(normalized) eigenvector for atom type k and phonon state λ

References

BORN, M. (1942). *Rep. Prog. Phys.* **9**, 294-333.
GHEZZI, C. & BOCCHI, C. (1982). *Thin Solid Films*, **88**, 1-8.
International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)
MARADUDIN, A. A., MONTROLL, E. W. & WEISS, G. H. (1963). *Theory of Lattice Dynamics in the Harmonic Approximation*, pp. 231-251. *Solid State Physics Suppl.* No. 3. London: Academic Press.
MATTHEW, J. A. D. & YOUSIF, S. Y. (1984). *Acta Cryst.* **A40**, 716-721.
ORLOVA, N. S. (1979*a*). *Phys. Status Solidi B*, **93**, 503-509.
ORLOVA, N. S. (1979*b*). *Sov. Phys. Crystallogr.* **24**, 516-518.
ORLOVA, N. S. (1981). *Phys. Status Solidi B*, **103**, 115-121.
REID, J. S. (1973). *Acta Cryst.* **A29**, 248-251.
REID, J. S. (1974). *Phys. Status Solidi B*, **64**, 57-64.
REID, J. S. (1983*a*). *Acta Cryst.* **A39**, 1-13.
REID, J. S. (1983*b*). *Acta Cryst.* **A39**, 533-538.
REID, J. S. & SMITH, T. (1970). *J. Phys. C*, **3**, 1513-1526.
ROBERTSON, B. F. & REID, J. S. (1978). *Acta Cryst.* **A35**, 785-788.
WALLER, I. (1928). *Z. Phys.* **51**, 213-231.
WILLIS, B. T. M. (1969). *Acta Cryst.* **A35**, 277-300.

Acta Cryst. (1985). **A41**, 528-530

A Note on the Superspace Groups for One-dimensionally Modulated Structures

BY AKIJI YAMAMOTO*

National Institute for Research in Inorganic Materials, Sakura-mura, Niihari-gun, Ibaraki, 305, *Japan*

T. JANSSEN AND A. JANNER

Institute for Theoretical Physics, University of Nijmegen, 6525 *ED Nijmegen, The Netherlands*

AND P. M. DE WOLFF

Vakgroep Fysische Kristallografie, Laboratory for Technical Physics, Technische Hogeschool, 2628 *CJ Delft, The Netherlands*

(*Received* 5 *December* 1984; *accepted* 10 *May* 1985)

Abstract

A computer generation of all the non-equivalent superspace groups for one-dimensionally modulated structures has been performed. Comparison of this result with the previous list by de Wolff, Janssen & Janner [*Acta Cryst.* (1981), **A37**, 625-636] shows that three superspace groups in this list are equivalent to others and that six groups had been overlooked. The new list contains 775 (3+1)-dimensional superspace groups. Some ambiguous points in the notation of the superspace groups and the selection of the wave vector are discussed.

* This work was partly done, while on leave, as a visiting member of the Institute for Theoretical Physics, University of Nijmegen.

0108-7673/85/060528-03$01.50

1. Corrections to the former list

A list of (3+1)-dimensional superspace groups has been given by de Wolff, Janssen & Janner (1981), hereafter referred to as I. The list was calculated partly by computer, partly by hand. Although the calculation was done carefully and employing two independent methods, errors are almost unavoidable in computations of such length by hand. For that reason we have once more executed the calculations of the non-equivalent superspace groups in which all the steps were performed by means of a computer. Furthermore, in order to remove errors in programming, superspace groups have been generated by two independent programs based on the same theory (Janner & Janssen, 1979). As a result, several discrepancies have been found between the new list and

Table 1. *List of corrections to Table 2 in de Wolff, Janssen & Janner* (1981)

The first and second columns indicate the basic space group, the third the (3+1)-dimensional Bravais class specifying the position of the correction. The last two columns give the entry as stated in I and that by which it should be replaced.

(1) Corrections involving groups that were missing or listed twice in I

Basic space group		Bravais class	in I	should be
24.	$I2_12_12_1$	12	1	12
45*b*.	$I2cb$	12	1	12
46*c*.	$I2cm$	12	1	12
43*a*.	$Fdd2$	17	123*	12
43*b*.	$F2dd$	17	12†	1
70.	$Fddd$	17	123*	12
67*a*.	$Cmma$	13	12	123
67*a*.	$Cmma$	14	12	123
120.	$I\bar{4}c2$	21	1	12
(2) Other errors				
117.	$P\bar{4}b2$	20	1	3
118.	$P\bar{4}n2$	20	1	3
Heading above 12*b*. $B2/m$			$B^{2/m}_{1\ \bar{1}}$	$B^{B2/m}_{\ \ 1\ \bar{1}}$
Heading above 44*a*. $Imm2$			$4:1s1$	$4:1ss$
Heading above 42*b*. $F2mm$			$1:\bar{1}s\bar{1}$	$2:\bar{1}s\bar{1}$
Heading above 115. $\bar{4}m2$			—	add $3:\bar{1}q\bar{1}$
Group 88.			$I4/a$	$I4_1/a$

* Bottom lines 1 and 3 are equivalent.
† Bottom lines 1 and 2 are equivalent.

that in I. Besides a number of misprints, the present result shows that three superspace groups in the list in I are equivalent with other groups in the list while six superspace groups do not occur in I. This result has been confirmed also by hand calculations. All the corrections to be made are listed in Table 1. Finally we get 775 superspace groups for one-dimensionally modulated structures belonging to 24 Bravais classes, 31 geometric crystal classes and 116 arithmetic crystal classes (in 3+1 dimensions).

2. Ambiguity of certain symbols

Some superspace groups are not uniquely determined by their two-line symbol as described in I: the same symbol may denote two non-equivalent superspace groups with the same basic space group given by the top line. This ambiguity occurs because satellites can be indexed in more than one way. For example, in the Bravais class $P^{I\,mmm}_{\ \ 1\,1\,\bar{1}}$ it has been tacitly assumed in I that (for a choice $\mathbf{q}=\gamma\mathbf{c}^*$) the general reflection condition is $h+k+l=2n$. Now consider $P^{I\,2cb}_{\ \ \bar{1}s\bar{1}}$, which belongs to this Bravais class. Its basic space group $I2cb$ has two glide planes a and c normal to $\mathbf{b}$. In the superspace group they correspond to elements denoted by $\binom{a}{s}$ and $\binom{c}{s}$, respectively. The corresponding reflection conditions are $h+m=2n$ or $l+m=2n$ for $h0lm$. For the equivalent choice $\mathbf{q}=(1-\gamma)\mathbf{c}^*$, which in practical cases may be preferable, the general reflection condition becomes $h+k+l+m=2n$ and the parallel symmetry elements are now $\binom{c}{1}$ and $\binom{a}{s}$ (and the reflection conditions $l=2n$ or $h+m=2n$ for $h0lm$) so that the symbol for the superspace group in this setting could be written as $P^{I\,2cb}_{\ \ \bar{1}1\bar{1}}$. This is identical to the symbol used in I for the non-equivalent group, which has $\binom{a}{1}$ instead of $\binom{a}{s}$ and reflection condition $h=2n$ for $h0lm$!

One way to avoid this ambiguity is, of course, to mention the reflection conditions explicitly. An alternative solution is to choose a form of the top line that makes the bottom line independent of $\mathbf{q}$. For instance, in our example the basic space group is equally well denoted by $I2ab$. Then the bottom lines $\bar{1}1\bar{1}$ and $\bar{1}s\bar{1}$ yield unambiguous symbols for the two different groups involved. In Table 2 suitable alternative symbols are listed for the 16 basic space groups for which the problem occurs.

Table 2. *Alternative symbols for basic space groups with symmetry elements with intrinsic translations in the direction of the modulation vector* $\mathbf{q}$ (*which is chosen along the c axis*), *together with parallel elements without such a translation*

The first symbol is the standard one. For the Bravais class mentioned in the first column the standard symbol gives rise to ambiguities that are avoided by using the alternative symbol.

Bravais class	Basic group		Alternative symbol
12	24.	$I2_12_12_1$	$I2_12_12$
12	45*b*.	$I2cb$	$I2ab$
12	46*c*.	$I2cm$	$I2am$
12	72*b*.	$Imcb$	$Imab$
12	73.	$Ibca$	$Ibaa$
12	74*b*.	$Icmm$	$Ibmm$
15	39*c*.	$Ac2m$	$Ab2m$
15	41*c*.	$Ac2a$	$Ab2a$
15	64*c*.	$Acam$	$Abam$
15	67*b*.	$Acmm$	$Abmm$
15	68*b*.	$Acaa$	$Abaa$
21	108.	$I4cm$	$I4bm$
21	110.	$I4_1cd$	$I4_1bd$
21	120.	$I\bar{4}c2$	$I\bar{4}b2$
21	140.	$I4/mcm$	$I4/mbm$
21	142.	$I4_1/acd$	$I4_1/abd$

It should be stressed that what causes concern here is the double meaning of symbols. The fact that the bottom line as well as the reflection conditions (both general and special) depend on the choice of $\mathbf{q}$ is not in itself a serious drawback (*cf.* § 3).

3. Non-unique symbols

For the superspace group symbol described in I, it is worth mentioning that, apart from the dependence on $\mathbf{q}$ just discussed, there are still other cases for which the bottom line is not unique. For operators denoted in the top line that leave $\mathbf{q}$ invariant (modulo reciprocal-lattice vectors) this bottom line represents $\tau=\delta-\mathbf{q}_r.\mathbf{s}$, where δ and $\mathbf{s}$ are translations in internal and external space, respectively, and $\mathbf{q}_r$ is the rational component of the modulation wave vector. Possible values of τ are $0, \frac{1}{2}, \pm\frac{1}{3}, \pm\frac{1}{4}$ or $\pm\frac{1}{6}$ (mod 1), for which

Table 3. *Examples of equivalent superspace groups*

The first column indicates some space groups as they are listed in Table 2 of I. The remaining columns are the equivalent groups obtained from those in the first column by employing the wave vector shown in the heading.

$\mathbf{q}=\gamma\mathbf{c}^*$	$\mathbf{q}=(\gamma-1)\mathbf{c}^*$	$\mathbf{q}=(\gamma-2)\mathbf{c}^*$	$\mathbf{q}=(\gamma-3)\mathbf{c}^*$
$P^{Pmcn}_{s1\bar{1}}$	$P^{Pmcn}_{ss\bar{1}}$		
$P^{P4_122}_{1\bar{1}\bar{1}}$	$P^{P4_122}_{q\bar{1}\bar{1}}$	$P^{P4_122}_{s\bar{1}\bar{1}}$	
$P^{P6_1}_{1}$	$P^{P6_1}_{h}$	$P^{P6_1}_{t}$	$P^{P6_1}_{s}$
P^{Fdd2}_{111}	P^{Fdd2}_{qq1}	P^{Fdd2}_{ss1}	
$P^{I4_1/a}_{1\bar{1}}$	$P^{I4_1/a}_{q\bar{1}}$	$P^{I4_1/a}_{s\bar{1}}$	

1, *s*, *t*, *q* or *h* is written in the bottom line. For superspace groups with non-zero $\mathbf{q}_r$, which are denoted by *A*, *B*, *C*, *L*, *M*, *N*, *U*, *V*, *W* and *R* in the prefix of the symbol, several values of τ are possible. For example, we consider A^{Pmmm}_{111}, which has $\mathbf{q}_r = \mathbf{a}^*/2$. By the convention in I, the first $({}^{m}_{1})$ represents a (hyper-) mirror plane perpendicular to the *a* axis with $\tau=0$. On the other hand, the same group also has a mirror plane parallel to this but a distance $a/2$ apart because of the lattice translation **a**. The value of τ corresponding to the latter is then $\frac{1}{2}$. Hence the symbol for this plane is $({}^{m}_{s})$. Thus $A^{Pmmm}_{s1\bar{1}}$ represents the same group as $A^{Pmmm}_{11\bar{1}}$. This is analogous to the situation in three dimensions, where, for example, *Ammm* could also be written as *Ancb*. However, conventions such as those that give preference to *Ammm* have not yet been formulated for superspace groups. Notice that, just as in the three-dimensional case, the non-uniqueness of the symbol does not play a role in the reflection conditions and is of no practical consequence.

4. Equivalent superspace groups

The **q** dependence of the superspace group symbol is related to the equivalence of superspace groups. For example, consider $P^{Pmcn}_{ss\bar{1}}$ with $\mathbf{q}=\gamma\mathbf{c}^*$, which is the superspace group appearing in the incommensurate phase of K_2SeO_4 (Janner & Janssen, 1980). For the choice $\mathbf{q}=(\gamma-1)\mathbf{c}^*$, the superspace group becomes $P^{Pmcn}_{s1\bar{1}}$ because δ is invariant and $\mathbf{q}_r$ is $-\mathbf{c}^*$ in this case. Thus a different choice of **q** may lead to a different superspace group. This is however always equivalent to the original one (Janner & Janssen, 1979). For the sake of the practical problem encountered in the determination of the superspace group, several examples of equivalent superspace groups are shown in Table 3.

In addition, there are many equivalent superspace groups that are related to the choice of the basic vectors **a**, **b**, **c**. Consider again $P^{Pmcn}_{ss\bar{1}}$. This is equivalent to $P^{Pnam}_{\bar{1}ss}$: the latter is obtained from the former by exchanging the *a* and *c* axes. Such a kind of equivalence relation is similar to that in the usual space groups.

One of the authors (AY) is indebted to the Faculty of Science, University of Nijmegen, for financial support.

References

JANNER, A. & JANSSEN, T. (1979). *Physica (Utrecht)*, **99A**, 47-76.
JANNER, A. & JANSSEN, T. (1980). *Acta Cryst.* **A33**, 399-408.
WOLFF, P. M. DE, JANSSEN, T. & JANNER, A. (1981). *Acta Cryst.* **A37**, 625-636.

Acta Cryst. (1985). **A41**, 530-540

Space Groups of Coincidence-Site Lattice Dichromatic Patterns in the Cubic System

BY D. S. VLACHAVAS

3 *Kristalli Str.*, *GR*-111 41 *Athens*, *Greece*

(*Received* 16 *July* 1984; *accepted* 22 *April* 1985)

Abstract

The determination of the full space symmetry of two interpenetrating lattices in a coincidence-site lattice orientation is discussed. The considered coincidence-site lattices are formed by two primitive cubic, face-centred cubic or body-centred cubic lattices. The two interpenetrating lattices form a dichromatic pattern and its symmetry is investigated by combining the three-dimensional periodicity of the coincidence-site lattice with the point-symmetry operations of the motif characterizing the particular dichromatic pattern. This provides a very concise formulation for treating this subject, especially if antisymmetry (two-coloured symmetry) is used. The translational symmetry of coincidence-site lattices with $\Sigma < 50$ is specified by determining the finest common sublattice of the two interpenetrating lattices. The point symmetry is determined by using the principle of the symmetry of composites and it is shown that the

0108-7673/85/060530-11$01.50