17-Symmetry and its Generalizations

MS-17.01.07 NEW APPROACH TO REPRESENTATIONS OF SPACE GROUPS AND SUBPERIODIC GROUPS. By V. Kopský, Department of Physics, University of the South Pacific, POBox 1168, Suva, Fiji.

It has been recently found that subperiodic groups appear as factor groups of reducible space groups (Kopský, V. (1989). Acta Cryst. A**45**, 805-815 and 815-823). This has immediate and useful consequences in the theory of representations of both space and subperiodic groups analogous to known relationship between space groups and corresponding point groups. The point group G of a space group $\mathcal{G}$ is isomorphic to the factor group $\mathcal{G}/T_G$ where T_G is the full translation subgroup of $\mathcal{G}$ and there exists a homomorphism $\sigma : \mathcal{G} \longrightarrow G$ with Ker $\sigma = T_G$. The lattice of equitranslational subgroups of $\mathcal{G}$ is isomorphic to the lattice of subgroups of G and representations of G engender those representations of $\mathcal{G}$, the kernel of which contains T_G. These are exactly the representations which correspond to wavevector $\mathbf{k} = 0$ and the kernels are the equitranslational subgroups of $\mathcal{G}$.
Let us now consider a reducible space group $\mathcal{G}$, the translation subgroup of which splits into a direct sum $T_G = T_{G1} \oplus T_{G2}$ of G- invariant subgroups $T_{G1} = T(\mathbf{a}, \mathbf{b})$ and $T_{G2} = T(\mathbf{c})$. These two groups are normal in $\mathcal{G}$ and the corresponding factor groups $\mathcal{G}/T(\mathbf{c})$, $\mathcal{G}/T(\mathbf{a}, \mathbf{b})$ have the structure of a layer group $\mathcal{L}$ with translation subgroup $T(\mathbf{a}, \mathbf{b})$ and of a rod group $\mathcal{R}$ with translation subgroup $T(\mathbf{c})$, respectively. Both the layer group $\mathcal{L}$ and the rod group $\mathcal{R}$ belong to the same geometric class G as the space group $\mathcal{G}$. There exist homomorphisms $\sigma_1 : \mathcal{G} \longrightarrow \mathcal{L}$ with Ker $\sigma_1 = T(\mathbf{c})$ and $\sigma_2 : \mathcal{G} \longrightarrow \mathcal{R}$ with Ker $\sigma_2 = T(\mathbf{a}, \mathbf{b})$.
The lattice of subgroups of the layer group $\mathcal{L}$ is isomorphic to the lattice of those subgroups of $\mathcal{G}$ which contain $T(\mathbf{c})$ and representations of $\mathcal{L}$ engender those representations of $\mathcal{G}$, the kernel of which contains $T(\mathbf{c})$.
The lattice of subgroups of the rod group $\mathcal{R}$ is isomorphic to the lattice of those subgroups of $\mathcal{G}$ which contain $T(\mathbf{a}, \mathbf{b})$ and representations of $\mathcal{R}$ engender those representations of $\mathcal{G}$, the kernel of which contains $T(\mathbf{a}, \mathbf{b})$.
The reciprocal space $\tilde{V}$ also splits into a direct sum of G-invariant subspaces $\tilde{V}_1 = \tilde{V}(\tilde{\mathbf{a}}, \tilde{\mathbf{b}})$ and $\tilde{V}_2 = \tilde{T}(\tilde{\mathbf{c}})$. Representations of $\mathcal{L}$, $\mathcal{R}$ and respective engendered representations of $\mathcal{G}$ correspond to wavevectors $\mathbf{k}_1 \in \tilde{V}_1$ and $\mathbf{k}_2 \in \tilde{V}_2$.
The best way to record ireps (irreducible representations) is to give their kernels and mapping of cosets onto matrix images. Kernels of ireps generate by intersections the lattice of normal subgroups which contains implicitly important information about mode interactions (Kopský, V. (1988). Comput. Math. Applic. 16, 493-505). These lattices are especially simple for irreducible space and subperiodic groups (Kopský, V. (1987). Czech. J. Phys. B**37**, 785-808) from which the systematic theory and recording develops. They have been actually derived already time ago by Fuksa & Kopský but so far unpublished; it is necessary to develop first a standard system of symbols for space and subperiodic groups which will include the specification of the origin, of nonstandard orientation and of translation subgroup.
It would be desirable to develop correlated standards of ireps for space and subperiodic groups to replace existing systems which are not quite compatible. Standards of subperiodic groups (pending Vol E of International Tables for Crystallography) correlated with standards of space groups will provide necessary background for this project including system of Hermann-Mauguin symbols which will suit the purpose.

PS-17.01.08 PERIODIC CLOSE PACKINGS OF IDENTICAL ELLIPSES. By Takeo Matsumoto*, Department of Earth Sciences, Faculty of Science, Kanazawa University, Kakuma-machi, Kanazawa 920-11, Japan.

In contrast with the closest packing of circles, with plane group p6mm, packings of ellipses with 6 contacting neighbours do not always have the maximum density $\rho = \pi/2\sqrt{3}$. Nowacki (1948) indicated five different densest packings of ellipses in 4 different plane groups: p2, c2mm, p2gg and p31m. In all of these packings, every ellipse is in contact with 6 neighbour ellipses. These packings could be considered to be the densest among the possible forms of ellipse packing.
Matsumoto (1968) and Matsumoto and Nowacki (1966) have shown that the first two of the above densest packings of ellipses, p2 and c2mm, always attain the above maximum density. That of the third, p2gg, cannot exceed this maximum density. Namely, the densest p2 and c2mm packings of identical ellipses are derived from the densest packing of circles by affine transformation, while the p2gg packing of ellipses can never attain the above maximum density ρ.
Tanemura and Matsumoto (1992) have shown that the density of p31m packings of ellipses, the fourth one of the above list, never exceeds the above maximum density ρ. Grünbaum and Shephard (1987) have published a fascinating book, in which 58 types of periodic patterns of ellipses are listed. Among them, 54 types are due to Nowacki (1948), and the other four are new packings, three of them with 6 contacting neighbours. Whether or not the density of these packings is limited to the value $\pi/2\sqrt{3}$ still remains to be established.

PS-17.01.09 DEFECTS OF HETEROSTRUCTURES CAUSED BY THE SYMMETRY DISCREPANCY (AN EXAMPLE OF HTS-LAYER ON PEROVSKITE-LIKE SUBSTRATES). By A.N.Efimov* and A.O.Lebedev, Ioffe Physical-Technical Institute, Petersburg, Russia.
Types of structural defects in heterostructures "layer on non-isomorphic substrate", causes of their origin and their density as a function of techniques and crys-

Table 1

Indexes of substrate	Expected types of defects	Parameters determining the density of defects
{111}	90° -twins (an angle between "c"-axes of twins is 90°)	density of nucleation
{001}	45° -twins (axes "a" and "b" of twins replace each other) coherent polysynthetic twins with interface on (110) or (110), incoherent interfaces between them,	density of nucleation
	antiphase domains	angular deflection of the substrate plane from singular one
{110}	antiphase domains	density of nucleation
{hhl}	45° -twins coherent polysynthetic twins with interface on (110) or (110)	density of nucleation
	antiphase domains	density of nucleation and angular deflection of the substrate plane from (001)
{0kl}, {hkl}	antiphase domains	density of nucleation and angular deflection of the substrate plane from (001)

