

DECOMPOSITION OF CRYSTAL FAMILIES

AND

GRAPHICAL REPRESENTATIONS  
OF SPACE GROUPS AND ASYMPTOTIC  
ESTIMATES FOR LARGE DIMENSIONS

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The publication of the tables of Brown, Bülow, Neubüser, Wondratschek and Zassenhaus (1) has brought to an end one phase of  $n$ -dimensional crystallography : that of explicit enumeration of all space groups for low values of  $n$  . Further such explicit enumeration seems unlikely since, in the next case  $n = 5$ , the arithmetic crystal classes of holohedral primitive orthogonal and tetragonal groups alone contain 9608 and 11456 distinct space groups respectively . Similarly joint calculations by myself and Jarratt (3) show that the number of coloured groups is surprisingly large even for  $n = 2,3$  .

Future phases are more likely to concern the enumeration of families (for definitions see (1),(2),(6)) together with qualitative or asymptotic results for particular families ; these formed the subject matter for the two lectures given .

The first lecture gave an exposition of recent work of Jarratt. This introduces three invariants of a family : the number of degrees of freedom, the decomposition pattern, and the orthogonal decomposition pattern. Using these invariants Jarratt enumerates families for low values of  $n$  and is lead to the conjecture that the number  $F(n)$  of families in dimension  $n$  grows slowly with  $n$  :

CONJECTURE  $\lim_{n \rightarrow \infty} F(n)^{1/n}$  is finite .

Full details of this work are about to appear (2).

The second lecture showed how the results of (4) for orthogonal space groups can be extended to enumerate space groups belonging to families with higher symmetry, for example tetragonal or cubic orthogonal. Each space group is represented by a directed graph with  $n$  vertices and additional structure such as colouring of vertices. The numerical evidence obtained seems to support the conjecture that the number  $S(n)$  of space groups in dimension  $n$  grows rapidly with  $n$  :

CONJECTURE  $\lim_{n \rightarrow \infty} S(n)^{1/n^2}$  is finite .

Full details of this work are about to appear (5),(6).

(1) Crystallographic groups of four-dimensional space. H.Brown, R.Bulow, J.Neubuser, H.Wondratschek and H.Zassenhaus. John Wiley & Sons. New York 1978.

(2) The decomposition of crystal families. J.D.Jarratt. Math.Proc. Cambridge Phil.Soc. (in print).

- (3) Coloured plane groups. J.D.Jarratt and R.L.E.Schwarzenberger. Submitted to Acta Crystallographica.
- (4) The use of directed graphs in the enumeration of orthogonal space groups. R.L.E.Schwarzenberger. Acta Crystallographica A 32 (1976), 356-359.
- (5) Graphical representation of n-dimensional space groups. R.L.E. Schwarzenberger. Submitted to Iroc.London Math.Soc.
- (6) N-dimensional crystallography. R.L.E.Schwarzenberger. Pitman Publishing. London 1979.