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Random-Generation Model for Statistical Distribution of Point Groups

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Abstract

The point groups which have C_{2h} as a subgroup are frequently observed in crystal data. A random-generation model of point groups gives a possible reason for the statistical distribution among the point groups in the class of crystals containing elements and alloys. By the addition of possible symmetry operations to point group C_{2h}, new point groups of higher symmetry can be generated. The computer simulation of the random-generation model seems to explain the higher frequencies of occurrence of O_h and D_{6h}, the lower frequencies of C_{4h} and C_{6h} and the moderately high frequencies of the remaining five point groups which have C_{2h} as a subgroup.

The symmetry of three-dimensional periodic structure is described by the 230 space groups. The statistical distribution of the 230 space groups for crystals may aid the assignment of the symmetry of a crystal under study (Nowacki, Matsumoto & Edenharter, 1967; Bel'skii & Zorkii, 1971; Matsumoto & Nowacki, 1966; Matsumoto, 1988). The number of space groups that should be observed is estimated by a statistical study on ordered abundances (MacKay, 1967).

Statistical distributions on graphs or algebraic structures can be a convenient tool for various fields of science (Itoh, 1979). A random-generation model of groups gives a possible reason for the frequent observation of point groups in the structures of oxide and hydroxide crystals (Itoh, 1986). Here we give another random-generation model to explain the statistical distribution for the class of elements and alloys (Nowacki, Edenharter, & Matsumoto, 1967) whose structures are closely related to hexagonal closest packing or cubic closest packing. The symmetry of a crystal is determined by physical and chemical processes, which are composed of a large number of mutually interacting factors. These factors may give a reason for the use of the stochastic model for statistical distributions.

To carry out the statistical study we must make clear the concept of the species of a crystal. Although

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there are good databases on crystals, for example ICSD, it is not easy to define the species to obtain the population for the statistical study. Here we make use of the paper by Nowacki, Edenharter & Matsumoto (1967), since we could not find a statistical study following their work. There are 32 crystallographic point groups for three dimensions. It is remarkable that the frequently observed point groups have as a subgroup the point group C_{2h} $(2/m)$. Although the theory for the phase transition of the second kind (Landau & Lifshitz, 1968) suggests a random suppression model, the random suppression of elements from point groups of higher symmetry will not explain this. We make a random-generation model to explain this statistical observation.

Consider a point group X as the initial point group and take possible symmetry operations which can be added to X at random. Assume the number N of operations is given by the probability $\Pr(N = n)$. Add the operations to the point group X and we get a point group generated by the operations and X. We take C_{2h} as the initial point group X. We start from a set of four spheres, of equal radius, which are mutually tangential with each other. There is one way for constructing regular cubic closest packing, using the set of spheres, while there are four ways for hexagonal closest packing. Hence, there are altogether five ways of regular closest packing starting from the mutually tangential four spheres. This consideration will provide a good basis for our stochastic model.

We represent O_h $(m\bar{3}m)$ and D_{6h} $(6/mmm)$ by 3×3 matrices. Place the eight nodes of the cube at $(\pm 1, \pm 1, \pm 1)$. Consider all the possible orthogonal transformations which keep the set of eight nodes invariant. These transformations are represented by 48 matrices from the geometrical meaning (Brown, Bulow, Neubuser, Wondratschek & Zassenhaus, 1978). We choose a representation of D_{6h} which has the largest number of common matrices with the 48 matrices. Then the representation of D_{6h} has 12 of the 24 matrices which are common to the 48 matrices of O_h. The 12 matrices represent the point group D_{3d} $(\bar{3}m)$. There are four possible such representations of D_{6h}. Thus, we have 96 matrices altogether for these representations of O_h and D_{6h}, corresponding to the above five ways of regular closest packing.

In the ${}_{96}C_4$ possible combinations of four matrices out of the 96 matrices, 25 combinations represent the point group C_{2h}. Noting that the point group C_{2h} consists of $1, \bar{1}, 2$ and $\bar{2}$, we consider the 25 combinations of the four elements which represent C_{2h}. Then take a combination at random out of these 25 combinations. Add N elements which are obtained by random sampling with replacement from the 96 matrices where the probability is given by a distribution $\Pr(N = k + 1) - (a^k/k!)e^{-a}$, which is a Poisson distribution with shift. Consider the point group generated by the C_{2h} and the N elements. We can determine the point group by the order of elements, and by the trace and the determinant of the representation of each element. There are combinations of the matrices, taken from the 96 matrices, which do not form a close set through our method of generation. We name this set of matrices the 33rd group G_{33}.

Table 1. *Random generation model and statistical data for elements and alloys*

Point group	Observed frequency	Expected frequency	Simulation
O_h	388	402	1380
T_h	32	37	126
D_{6h}	217	216	741
D_{4h}	138	58	199
C_{6h}	1	18	62
D_{3d}	36	100	344
C_{4h}	3	5	18
D_{2h}	109	83	285
C_{2h}	26	31	108
Totals	950	950	3263

The observed 181 crystals not listed in this table are distributed in the remaining 23 point groups (Nowacki, Edenharter & Matsumoto, 1967).

We compare the frequencies among the point groups which have C_{2h} as a subgroup with the results of simulations in Table 1 for the class of elements and alloys (Nowacki, Edenharter & Matsumoto, 1967). The parameter of the shifted Poisson distribution is taken as $a = 3{\cdot}0$ to obtain a good fit to the data. We carried out 50 000 trials. Of them, 46 737 trials generated elements which do not form a close set by our method of generation of groups, and hence do not correspond to any crystal structure. That is to say, each of the 46 737 trials generated G_{33}. We assume that each crystal is a realization of the stochastic model. Hence, each of the groups obtained by the remaining 3263 trials, given in Table 1, is assumed to represent the symmetry of a crystal. The expected frequencies in Table 1 are taken to be proportional to the frequencies obtained by our simulation. Our model explains, as given in Table 1, the higher frequencies of O_h and D_{6h}, the lower frequencies of C_{4h} and C_{6h} and the moderately high frequencies of the remaining five point groups. Our model explains that, although T_h has the same number of elements as that of D_{6h}, it has lower frequency. This applies also to the case for the D_{3d} and C_{6h} pair and to the D_{2h} and C_{4h} pair. Thus our model seems to explain the data fairly well, and hence suggests a possible process for each crystal of adapting its symmetry.

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A Novel Algorithm for a Quasiperiodic Plane Lattice with Fivefold Symmetry

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Abstract

Conventionally, Penrose tilings with fivefold symmetry are constructed with the aid of two characteristic rhombic tiles and sets of rules based on either matching of markings on the tiles or their subdivision. Both these procedures involve decision making when tiling is to be done extensively. In the present communication, a fool-proof method of producing Penrose tilings using a set of operations that can be repeated *ad infinitum* is described. The steps in the present procedure are akin to conventional crystallographic operations and can be expressed in simple mathematical terms which bring out some interesting aspects of Penrose tilings.

Introduction

The pioneering work of Penrose (1974) on tiling a floor (Gardner, 1977) to generate patterns exhibiting fivefold rotational symmetry, extension of these ideas to three dimensions by Mackay (1981) and the subsequent discovery by Shechtman, Blech, Gratias & Cahn (1984) of quasicrystals with icosahedral symmetry have generated world-wide interest. Several methods are now available for the generation of two-dimensional aperiodic tilings with forbidden rotational symmetry. These range in approach from the empirical matching rules of Penrose, the geometrical approach of Sasisekharan (1986) and dualization of periodic pentagrids to projection from higher-dimensional space (de Bruijn, 1981). The procedure of tiling due to Penrose involves assembling two types of rhombs, *viz* a prolate (or thick) rhomb with acute angle $2\pi/5$ and an oblate (or thin) rhomb with acute angle $\pi/5$, or a set of kites and darts. For example, the process of building an infinitely large tiling with these two types of rhombs consists of marking them and laying them edge to edge such that the markings match according to set rules so that aperiodicity and fivefold symmetry are ensured. The matching rules are an expression of the self-similarity transformation of the Penrose tiling. Hitherto, this transformation has been exploited to generate a large cluster of tiles from a cluster of a smaller number of tiles obeying the matching rules by subdividing each of its rhombs according to a set pattern. The resultant tiling then

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