Symmetry of icosahedral quasicrystals

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The symmetry groups of icosahedral quasicrystals are listed. The role played by scale transformations is determined. The patterns of extinctions on an x-ray diffraction pattern corresponding to nonsymmorphic groups are determined.

Many new quasicrystals belonging to the icosahedral symmetry group have recently been discovered. Diffraction experiments yield large numbers of sharp peaks of various intensities, which could in principle be used to determine the atomic structure of these substances. A structural analysis here, as for ordinary crystals, should begin with an identification of the type of symmetry. In the present letter we describe all possible symmetry groups of icosahedral quasicrystals. We show that these groups have important features which distinguish them from ordinary crystallographic groups.

Each symmetry group is related to a definite point group and a Bravais lattice. There are two different point groups: group Y, which consists of all rotational symmetries of an icosahedron (this group does not contain an inversion; it consists of 60 elements), and group Y', which consists of all symmetries of an icosahedron (it does contain an inversion, and it consists of 120 elements). The Bravais lattices of quasicrystals may be understood as translation groups which conserve the corresponding six-dimensional periodic structures. It can be assumed, as we will assume here, that a Bravais lattice describes the positions of the diffraction peaks in a three-dimensional k space and sum rules for them. It will accordingly be convenient to use three-dimensional notation for the six-dimensional integer vectors as introduced by Cahn *et al.*[1] We adopt three mutually perpendicular twofold symmetry axes of an icosahedron as the coordinate axes. With an appropriate choice of scale, the projection of any integer vector from R^6 can be written in these coordinates as

$$(k_1/k'_1, k_2/k'_2, k_3/k'_3), \qquad (k/k' = k + k'\tau, \ \ \tau = \frac{1}{2}(\sqrt{5}+1)), \qquad (1)$$

where k_i and k'_i are integers, and the sums $k_1 + k'_2, k_2 + k'_3, k_3 + k'_1$ are even the icosahedron is oriented with respect to the x,y,z axes in such a way that the vector (1/0,0/1,0/0) is a fivefold axis].

There exist three different Bravais lattices[2,3] which can be determined with the help of the conditions on vectors (1): a) A simple cubic lattice sc_6 (we are thinking of a six-dimensional cube), which consists of all vectors of the type in (1). b) A face-centered lattice fcc_6, which consists of those vectors of the type in (1) such that $k_1 + k_2 + k_3$ is even. c) A body-centered lattice bcc_6, which consists of those vectors of the type in (1) such that all the k_i are even, and the numbers $k_1 + k'_2, k_2 + k'_3$, and k_3

$+ k'_1$ generate identical remainders when divided by 4. A remarkable property of these lattices is that they are not single-valued in terms of the choice of Miller indices, because of scale invariance. For example, the fcc_6 and bcc_6 lattices do not change when the scale is changed by a factor of τ, while for the sc_6 lattice this scale factor is τ^3. The law specifying the conversion of indices upon a change of scale follows from the identity $\tau(k/k') = k'/(k'+k)$. Incorporating scale invariance is important in determining symmetry groups.

Any symmetry group which corresponds to a certain Bravais lattice L and a point group G consists of pairs (g,h_g), where g is an operation from G, and h is a vector defined within a vector of the lattice L. Symmetry transformations (g,h_g) act on the Fourier transform of the structure $\rho(k)$ in the following way:

$$\rho'(k) = \exp(2\pi i(k, h_g))\,\rho(g(k)). \tag{2}$$

Here (k,h_g) is a six-dimensional scalar product, which for $h_g = (h_1/h'_1, h_2/h'_2, h_3h'_3)$ is equal to $1/2\Sigma_i(k_ih_i + k'_ih'_i)$. For a complete description of this symmetry it is sufficient to specify the vector h_g for those elements of the point group which generate it through multiplication. The group Y is generated by two elements: a rotation A through an angle of 72° around the (1/0,0/1,0/0) axis and a rotation B through an angle of 120° around the (1/2,0/1,0/0) axis. There are three generating elements for the group Y': the transformations A and B and also the inversion.

Once an indexing of the Bravais lattice has been chosen, the symmetry groups which are not equivalent to each other can be found quite easily either numerically[4] or analytically[3] [as usual, two symmetry groups are regarded as equivalent if one can be obtained from the other through a change in the origin of coordinates: $h'_g = h_g + h_g + g(a) - a$]. As an example, we show the results for the case $L = sc_6$, $G = Y$. There are five groups, which are specified by the vectors h_A and h_B:

$$h_A = \frac{m}{5}(1/\bar{1}, 1/1, \bar{1}/\bar{1}), \quad h_B = 0, \quad (m = 0, \dots, 4). \tag{3}$$

We now consider scale transformations. Calculations show that an extension by a factor of τ^3 acts on groups (3) in the following way: $m \to 2m(\text{mod}5)$. We see that incorporating scale transformations reduces the number of nonequivalent groups to two, since any two groups of the type in (3) with $m \neq 0$ can be sent into each other by a scale transformation. In this case we thus have only two symmetry groups: a symmorphic group ($h_A = 0$, $h_B = 0$) and a nonsymmorphic group, for which h_A and h_B can be specified by relations (3) with $m = 1$.

With a different choice of point group and Bravais lattice, the situation turns out to be similar: The consideration of an equivalence gauge transformation is important and leads to the identification of a large fraction of the symmetry groups. The number of nonequivalent groups remaining after this identification is fairly small. There is one symmorphic group ($h_A = 0, h_B = 0$) and one nonsymmorphic group ($h_A \neq 0, h_B = 0$) for each point group G and Bravais lattice L except $G = Y'$, $L = fcc_6$. For the latter case, there is only the symmorphic group. Here are the vectors h_A for the nonsymmorphic groups: 1—$G = Y$. a) $L = sc_6$, $h_A = 1/5(1/\bar{1},1/1,\bar{1}/\bar{1})$; b) $L = fcc_6$, $h_A = 1/$

$10(1/\bar{1},6/1,\bar{1}/\bar{6}$; c) $L = \mathrm{bcc}_6$, $h_A = 1/10(1/\bar{1},6/1,\bar{1}/\bar{6}$. 2—$G = Y'$. a) $L = \mathrm{sc}_6$, $h_A = 1/2(\bar{1}/0,1/1,0/\bar{1}$; b) $L = \mathrm{bcc}_6$, $h_A = 1/4(1/0,1/\bar{1},0/\bar{1})$. There is accordingly a total of 11 groups.

The nonsymmorphic symmetry groups, as in the case of ordinary crystals, lead to the extinction of certain peaks on an x-ray diffraction pattern which are allowed by the lattice sum rules. These extinctions occur either on fivefold symmetry axes (if $G = Y$) or in twofold symmetry planes (if $G = Y'$). Here are the coordinates of extinguished peaks: 1) $G = Y$, $L = \mathrm{sc}_6$, fcc_6, bcc_6: $(m - n/2n,2n/m + n,0/0)$, where m and n are integers, and m is not divisible by 5. 2) $G = Y'$, $L = \mathrm{sc}_6$: $(m/n,0/0,q/r)$, where n and q are odd, while m and r are even integers. 3) $G = Y'$, $L = \mathrm{bcc}_6$: $(2m/2n,0/0,2q/2r)$, where m and r are even, and n and q are odd. We have listed here only those peaks which lie on one of the axes or symmetry planes (the others can be found from them by applying the point-group operations). Interestingly, the families of extinctions in all cases except $L = \mathrm{bcc}_6$, $G = Y'$ are invariant under scale transformations of the corresponding lattices. For $L = \mathrm{bcc}_6$, $G = Y'$ the extinction pattern is invariant under extensions by a factor of τ, while there is no invariance under scale transformations of the bcc_6 lattice (with a factor of τ).

We conclude by pointing out that the role played by scale transformations was ignored in Ref. 4. As a result, some erroneous conclusions were drawn: Many of the symmetry groups found in Ref. 4 are equivalent to each other.

Comment. For comparison with other studies we should stress that our lattices sc_6, fcc_6, and bcc_6 are defined not in x space, as they usually would be, but in k space. The corresponding lattices in x space are found in the following way: $\mathrm{sc}\frac{x}{6} = 2\pi\mathrm{sc}_6$, $\mathrm{fcc}\frac{x}{6} = \pi\mathrm{bcc}_6$, $\mathrm{bcc}\frac{x}{6} = \pi\mathrm{fcc}_6$.

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