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A rigorous proof on the crystallographic restriction theorem

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Abstract
With respect to the crystallographic restriction theorem, although there is a famous proof which is concurred and used by a lot of books in solid state physics, this paper analyses some incorrect or inappropriate arguments in the proof, for example, the possible value of m= 1from the proof is in contradiction with eq.(1); the argument of that the length of B'A' must be the integral multiples of that of AB is not clear for real lattices of solids, and is required to be proved for various crystal lattices. On the basis of the viewpoint of that the inexistence of C_5 axis of symmetry is equivalent of that pentagons are impossible to fill all the space with a connected array of pentagons, using a purely mathematical approach the paper rigorously proves the crystallographic restriction theorem.

Keywords: the crystallographic restriction theorem, pentagons, n-sided(n≥7) polygons, proper rotation

Introduction

It is well - known that the axes of symmetry of the crystal can merely exist C_1, C_2, C_3, C_4 and C_6, this is the so - called crystallographic restriction theorem [1, 4]. Among various proofs of this theorem, there is a famous proof which is generally concurred by those people who are familiar with the solid state physics. Although the well - known proof of the theorem has been applied in many famous books [2- 3], it is not satisfactory at least due to the following two reasons. First, considering an n-fold (n is an integer) rotation of the crystal in the two - dimensional space, as shown as Fig.1 [2],

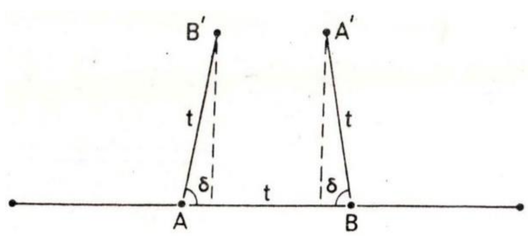

Fig 1: The point B' is one of the points generated by an n-fold rotation axis through point A operating on lattice point B with angle δ, and the point A' by a similar axis through point B inversely operating on lattice point A with angle δ. The value of angle δis equal to $\frac{2\pi}{n}$.

in terms of the famous proof, because of the periodicity of lattice structure, the length of B'A' must be equal to the integral multiples of that of AB, namely.

$$B'A' = m\,t. \qquad (1)$$

However, in the viewpoint of mathematics, eq. (1) is not clear as an argument for the 14 different Bravais lattice structures of real crystals, but not the supposing Bravais lattice, all of the 14 lattices should be respectively demonstrated in order to support eq. (1).

Second, the calculation from eq.(1) in accordance with Fig.1 demonstrates that the possible values of m are −1, 0, 1, 2, and 3, nevertheless, if m takes the value of −1, neither of the lengths of B'A' and t in eq.(1) can be significant to be negative.
Therefore, it is necessary to find a more satisfactory proof of the crystallographic restriction theorem.

2 The inexistence of C_5 axis

The inexistence of C_5 axis is equivalent of that pentagons are impossible to fill all the space with a connected array of pentagons [3], and this can be easily generalized to all the cases of C_n (n≥7) axis. At first, let us consider two congruent regular pentagons respectively noted with A_5 and B_5 in the two - dimensional space, as shown as Fig.2.

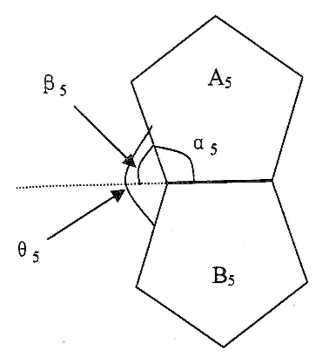

Fig 2: Two congruent regular pentagons fit together.

In Fig. 2, α_5 and β_5 respectively note the interior angle and the exterior angle of the pentagon, and θ_5 is the clipped angle between the side of A_5 and the side of B_5. Because the sum of all the exterior angles of a polygon is always equal to 360°, thus, it can be written

$$\beta_5 = \frac{360^\circ}{5} = 72^\circ, \quad (2)$$

hence,

$$\alpha_5 = 180^\circ - \beta_5 = 108^\circ. \quad (3)$$

It is clear from Fig. 2 that if the other one or more pentagons just can fill the space within the scope of θ_5 with no "gaps " between pentagons, it requires that one or more interior angles can just fill θ_5 angle with no "gaps" between them, or the size of θ_5 must be just equal to the integral multiples (positive) of the size of an interior angle, namely,

$$\theta_5 = m\alpha_5 \ (m = 1, 2, 3\ldots\ldots). \quad (4)$$

Nevertheless, using eq.(2), the size of θ_5 is given by

$$\theta_5 = 2\beta_5 = 2\times 72^\circ = 144^\circ, \quad (5)$$

from eq.(5) and eq.(3), it can be found

$$\theta_5 = \frac{4}{3}\alpha_5, \quad (6)$$

in terms of eq. (4), C_5 axis can not exist. Fig.3 depicts the "gaps" between pentagons in the scope of θ_5 in a close packing of congruent regular pentagons in the two-dimensional space [3].

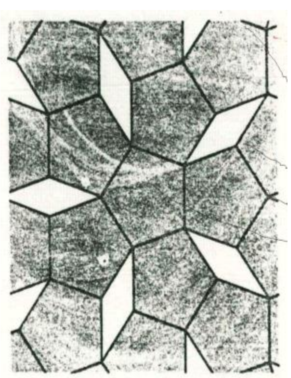

Fig 3: C_5 axis of symmetry does not exist.

3 The inexistence of C_n (n≥7) axis

Assuming to substitute two congruent regular n –sided (n≥7) polygons such as A_n and B_n respectively for A_5 and B_5 in Fig. 2, accordingly, θ_n (or β_n) for θ_5 (or β_5), and α_n for α_5. Thus, an exterior and an interior angles of the n - sided (n≥7) polygon are respectively written

$$\beta_n = \frac{360^\circ}{n} = \frac{2}{n}\times 180^\circ, \quad (7)$$

and

$$\alpha_n = 180^o - \beta_n = 180^o - \frac{360^\circ}{n} = \frac{n-2}{n}\times 180^\circ, \quad (8)$$

in accord with Fig. 2,

$$\theta_n = 2\beta_n = 2\times\frac{360^\circ}{n} = \frac{4}{n}\times 180^\circ. \quad (9)$$

Comparing eq. (9) with eq. (8), obviously, if n≥7, the inequality

$$\theta_n < \alpha_n \quad (10)$$

holds true, thus

$$\theta_n \neq m\alpha_n \ (m = 1, 2, 3\ldots\ldots), \quad (11)$$

therefore, C_n (n≥7) axis can not exist.

4 The proper rotation axes

In the viewpoint of mathematics, C_1, C_2, C_3, C_4 and C_6 axes must also be discussed. At first, it is clear that C_1 axis represents an one-fold rotation with the rotation angle 0° or 360°, and will certainly remain the crystal invariant.

We separately consider an oblique Bravias lattice in the two-dimensional space, if a two-fold rotation with the rotation angle of 180° through any lattice point in a primitive cell, the primitive cell will remain invariant, this is also true for equivalent points in other primitive cells [3]. Therefore, C_2 axis for a crystal based on such a primitive cell can exist.

Differing from the case of pentagons, in Fig. 2, If assuming respectively to substitute two congruent regular triangles such as A_3 and B_3, tetragons such as A_4 and B_4 and hexagons such as A_6 and B_6 for A_5 and B_5, accordingly, θ_k (or β_k) (k=3,4, 6) for θ_5 (or β_5), and α_k (k=3, 4, 6) for α_5, it is easy to calculate out:

$$\theta_3 = 4\alpha_3,\ \theta_4 = 2\alpha_4,\ \theta_6 = \alpha_6, \quad (12)$$

in terms of eq.(4), it is clear to recognize that C_3, C_4, and C_6 axes are allowable for the crystal rotation.

5 Conclusions

With respect to the crystallographic restriction theorem, the paper proposed different opinions on a famous proof concurred and used by many famous books about solid state physics or crystallography. Due to the periodicity of the lattice structure, the inexistence of C_5 axis is equivalent of that pentagons are impossible to fill all the space with a connected array of pentagons, for example, in Fig.2, if one or more other congruent regular pentagons can fill all the space within the scope of θ_5 with no "gaps" between them, the value of θ_5 must be the integral multiples of the value of an interior angle of the congruent regular pentagon. Nevertheless, from the present calculation it can be found that the value of θ_5 is impossible an integral multiple of that of α_5, therefore, C_5 axis do not exist.

Similarly, if assuming to substitute two congruent regular n-sided (n≥7) polygons for the two pentagons in Fig.2, the similar calculation demonstrates that the value of θ_n (n≥7) is smaller than that of the interior angle of the n-sided ($n \geq 7$) polygon, no possible to be its integral multiple. But rather, if assuming to substitute the two pentagons in Fig. 2 with two congruent regular triangles, or tetragons, or hexagons, it is easy to calculate out that$\theta_3 = 4\alpha_3$, $\theta_4 = 2\alpha_4$, $\theta_6 = \alpha_6$, they are consistent with eq.. Moreover, it is clear that C_1 and C_2 are compatible with translational symmetry. Therefore, the possible axes of rotation of the crystal are merely C_1, C_2, C_3, C_4 and C_6.

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