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What are unit cells

Lawrence C. Andrews[a]* and Herbert J. Bernstein[b]

[a]*Ronin Institute, 9515 NE 137th St, Kirkland, WA, 98034-1820 USA, and* [b]*Ronin Institute, c/o NSLS-II, Brookhaven National Laboratory, Upton, NY, 11973 USA.*

E-mail: larry6640995@gmail.com

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Abstract

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Note: In his later publications, Boris Delaunay used the Russian version of his surname, Delone.

1. Introduction

The term “unit cell’ is now the most commonly used term for a smallest repeating unit of a crystal structure. It allows us to describe the crystal structure in terms of a simple geometric shape. This makes it easier to visualize the structure and to calculate its properties.

What is a unit cell? Conventionally, it is either thought

2. Conventional 3-space methods

2.1. Lattices as basis vectors

The fundamental understanding of crystals begins from the study of lattices. A typical lattice Λ in $\mathbb{R}^n$ thus has the form

$$\Lambda = \left\{ \sum_{i=1}^{n} a_i \mathbf{v}_i \middle| \, a_i \in \mathbb{Z} \right\},$$

where: $(\mathbf{v}_1, ..., \mathbf{v}_n)$ is a basis of the lattice. Conventionally, "the unit cell" is defined as the set of n vectors generated by $a_i = 1$.

In crystallography, we study the lattice in three-dimensional space (n=3 in the above equation). We use 3x3 matrices to create different unit cells by manipulating a vector of 3D vectors. These manipulations are usually described as happening in 3D space, but the vector of 3D vectors is actually a mathematical object with nine parameters in a space that can be described as $R^3 x R^3 x R^3$, which is a nine-dimensional space.

2.2. a,b,c,α,β,γ

The second conventional representation of unit cells is 2 triplets: 3 edge lengths of the basis vectors and the 3 angles between them. This is a 6-dimensional space: $R^3 x R^3$.

The problem with this representation occurs in the cases where the need is to compare two (or more) unit cells. The representation as $R^3 x R^3$ informs us that the two R^3 are not necessarily commensurate. Indeed, the edge lengths and the interaxial angles have no shared measure. (However, see Section 2.3.)

2.3. Polar coordinates

Section 2.2 alluded to the incommensurate nature of the two subspace of $R^3 x R^3$.

Delone *et* al. (1975) commented on the importance of the "opposite" scalars in the Bravais tetrahedron. Andrews *et* al. (2019) observed that the association of those opposites implied the association of each unit cell edge with the opposite interaxial angle:

$$(a, \alpha),\ (b, \beta),\ (c, \gamma).$$

They used that association to create a space C^3 (see Section 4.2). Using the above definition (2.3, we can define a 6-dimensional space P^3. Unlike the issue with the direct use of lengths and angles, polar coordinates are a well-known 2-dimensional object with the alternative representation as (x, y), the 2-dimensional plane, where we can immediately use Euclidean distance measure.

2.4. Dirac

Dirac cells are defined as one or more primitive unit cell between a pair of lattice plans. Physicists use Dirac cell in the computation of energy levels (Dirac, 1930).

3. Niggli space

4. Delone space

4.1. $\mathbf{S^6}$

4.2. $\mathbf{C^3}$

4.3. Linearized $\mathbf{S^6}$

Linearized $\mathbf{S^6}$ is defined as a vector for which then values are derived from the $\mathbf{S^6}$ representation of a lattice by taking the square root of each of the 6 elements. The advantage created is that the elements are now in Ångstrom units. The disadvantage is that there are no vectors beyond the boundaries, which have zero values; beyond the boundaries one or more of the elements of the vector would require the square root of a negative number. The consequence is that a Euclidean distance between to related points may greatly exceed the shortest measure that could be found.

4.4. Root Invariant

Root invariant is a lattice representation created by (Bright *et* al., 2021). Although it has several related definitions, the form for a general lattice is the same as linearized $\mathbf{S^6}$, except that a specific sorting of the elements of the vector are specified in order to create a unique vector. Linearized $\mathbf{S^6}$ has the properties that there are several (up to 24 in some lattices) sortings possible. The disadvantage of linearized $\mathbf{S^6}$ applies here also. Root invariant has been used to display meaningful representations of large numbers of experimentally determined lattices.

5. Wigner-Seitz space

6. Notation

7. Summary

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8. Availability of code

The C^{++} code for $\mathbf{C^3}$ and related software tools is available in github.com, in `https://github.com/duck10/LatticeRepLib.git`. The program CmdToC3 uses the required files.

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References

Andrews, L. C., Bernstein, H. J. & Sauter, N. K. (2019). Acta Cryst. A**75**(3), 593–599.
Bright, M., Cooper, A. I. & Kurlin, V. (2021). arXiv preprint arxiv:2109.11538, **2**.
Delone, B. N., Galiulin, R. V. & Shtogrin, M. I. (1975). J. Sov. Math. **4**(1), 79 – 156.
Dirac, P. A. M. (1930). The principles of quantum mechanics. Oxford University Press.

Synopsis

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