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Lawrence C Andrews and Herbert J Bernstein

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Co-editor:

Professor M.I. Aroyo

Física de la Materia Condensada, Facultad de Ciencia y Tecnología, Universidad del País Vasco, Apartado 644, 48080 Bilbao

Email: mois.aroyo@gmail.com

Submitting author:

Lawrence C Andrews

Ronin Institute For Independent Scholarship Incorporated, 9515 NE 137th St, Kirkland, WA, 98034, United States

Email: larry6640995@gmail.com

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

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

E-mail: lawrence.andrews@ronininstitute.org

lattice "unit cell" reduction

Abstract

Several attributions exist for the reduced cells of lattices and for the reduction processes to produce them. The actual origins of the terms are compared and a taxonomy created. The terms "Niggli reduction", "Niggli cell", "Delaunay reduction", and "Delaunay cell" most accurately describe the crystallographic usages of reduced cells and reduction methods.

An alternative spelling of Boris Delaunay's name, adopted by him later in life, is Delone.

1. Introduction

Niggli (1928) and Delaunay (1932) first described the solutions to the problem of recognizing the appropriate Bravais lattice type of a particular unit cell by the procedures of reduction. They used the mathematical techniques developed for the studies of matrices and polynomials.

In recent literature, various names are associated with the reduction methods used to produce "reduced cells" in crystallography. Oishi-Tomiyasu (2012)[1] uses the term "Minkowski reduction" for the process often referred to as "Niggli reduction". Andrews *et al.* (2019)[2] use the term "Selling reduction", which is often referred to as "Delaunay reduction".

In an attempt to clarify the relationships and meanings of the various methods of reduction, we have prepared a table of hierarchy of the types and describe their origins.

It should be noted that the terms used to describe these cells vary, often being named "region", "domain", "parallelohedron", "parallelopiped", or "zone of influence". In the particular case of lattices, they all describe objects that tile space, in no way differing from the concept of unit cell.

The choice of a reduction technique is an important early step in measuring the similarities among lattices and in classifying lattices (Andrews & Bernstein, 2023) (Andrews *et al.*, 2023).

2. Types of reduction

Table 1 list the types of reductions commonly encountered. The table progresses (left to right) from general/n-dimensional to three dimensional, to more specific (sorted).

[1] Introduced a matrix-based system for rapid determination of Bravais lattice type.
[2] Introduces the space $\mathbf{S}^6$ and also $\mathbf{C}^3$.

2.1. Taxonomy

Table 1. *Types of reduction*

algebraic	n-dimensional/geometric	three-dimensional	sorted
Seeber (1831)/Eisenstein (1851)	Minkowski (1905)	Buerger (1960)	Niggli (1928)
Selling (1874)		Delaunay (1932)	
Dirichlet (1850)	Voronoi (1908*a*)	Wigner & Seitz (1933)	

2.2. The specific types

- Buerger reduction (Buerger, 1960): The Buerger reduced cell is defined as the cell with edge vectors that are the shortest, non-coplanar set of three vectors in the lattice. This is a special case of Minkowski reduction. No sorting of the sizes of the lengths or angles is specified, and no special conditions are described for the issues of equalities of values.
- Delaunay (aka Delone) reduction (Delaunay, 1932): Delaunay used Selling reduction to derive his specific reduction for three dimensions. Six scalars are used, which are the dot products of the base vectors and their negative sum. The lattice is reduced when all of the scalars are non-positive. The reduced cell is not unique in several ways. First, in the general case, there are 24 permutations of the values that all specify the same lattice. Also, for cases where some of the scalars are zero, there are alternative cells.
- Dirichlet reduction (Dirichlet, 1850): Dirichlet described the reduction of positive quadratic forms.
- Eisenstein reduction (Eisenstein, 1851): Eisenstein derived reduction conditions for positive ternary quadratic forms.
- Minkowski reduction (Minkowski, 1905): Minkowski defines a reduced cell in an n-dimensional vector space as a cell with the shortest non-linearly-dependent lengths. Neither length sorting or description of how equalities are to be resolved are required.

- Niggli reduction (Niggli, 1928): Niggli used the formalism of Eisenstein to derive the set of conditions to define a unique unit cell in three dimensions. The lengths of the edges are sorted, and special conditions are defined for cases of ambiguity.
- Seeber reduction (Seeber, 1831): Seeber derived reduction conditions for three-dimensional lattices, which were adopted by Eisenstein and subsequently by Niggli, so a Niggli reduced cell is a Seeber reduced cell.
- Selling reduction (Selling, 1874): Selling derived reduction conditions for binary and ternary quadratic forms. The Selling cell differs from the Minkoski cell by being based on introduction of a fourth vector $d = -a - b - c$ and reducing by requiring all six angles between the four vectors to be obtuse or right angles.
- Voronoi domains (Voronoi, 1908*b*): Voronoi was concerned with the "regions of influence" of points in space. The term Voronoi domain is used to describe the regions of a Delaunay triangulation of a set of points. Voronoi (1908*b*) addresses quadratic forms and polyhedral tesselations. For a lattice, a Voronoi cell is the set of points at least as close to a chosen lattice point as they are to any other lattice point. This defines a cell around each lattice point that tiles the entire space. Such a Voronoi cell of a lattice is also called a Dirichlet cell or a Delaunay cell or a Wigner-Seitz cell.
- Wigner-Seitz cell (Wigner & Seitz, 1933): The authors define the cell for the face-centered lattice of sodium. As defined, it is the Voronoi cell in three dimensions. Although this cell was defined only for face-centered cubic lattices, it apparently has been adopted by the physics community as the name of the Dirichlet cell in general. As Hart *et al.* (2019) has shown, the Wigner-Seitz cell centered on a given lattice point is contained entirely within the convex envelope of the immediate neighbors of a given lattice point, which are most efficiently found by starting with Minkowski-, Buerger-, or Niggli-reduction, rather than Delaunay

reduction (Bernstein *et al.*, 2023). The Wigner-Seitz cell (for the above case) is a truncated octahedron, and in general has six, eight, ten, twelve, or fourteen sides. (Fig. 1).

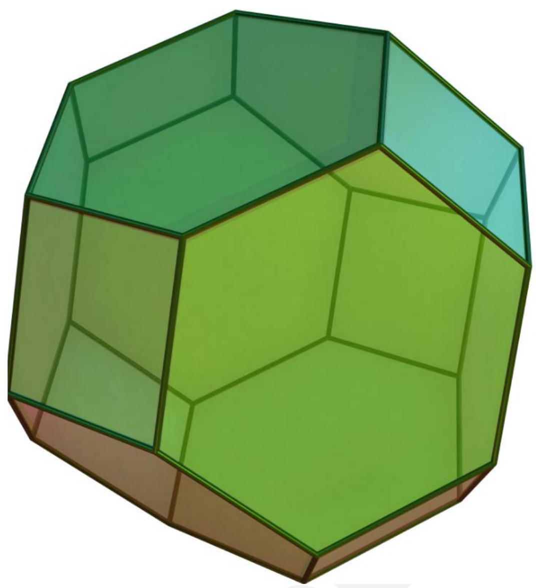

Fig. 1. Truncated octahedron (Wikipedia, 2017)

3. Summary

An attempt is made to make more explicit the relationships of the various types of unit cell reduction used in crystallography.

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Synopsis

The hierarchy of types of unit cell reduction is discussed.