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Bravais Lattices: Why Lattices Are Not Classified Based On Shape

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ABSTRACT

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Keywords: Bravais Lattices Crystal System Classification Shape Questions This paper aims to demonstrate reasons why lattices are not classified on the basis of shape. To achieve this, a review of the terms related to the Bravais lattices was carried out and the 7 crystal systems and 14 Bravais lattices were also illustrated in order to provide structural insight into the subject of this paper. The issue of classifying lattices based on shapes introduced several questions put forward by researchers and due to these questions, different structures of the Bravais lattices were analyzed in this research paper in order to proffer a panacea to the issue.

1. Introduction

Classification of the Bravais lattices based on symmetry has been a norm over the years [1]. Recently, university students, researchers, and scientists have questioned the origination of this norm and have come up with questions like "why has the classification of lattices based on shape been refuted when each crystal has a defined lattice shape e.g. cubic, hexagonal, monoclinic, orthorhombic etc. just to mention a few, and if such lattice shapes do exist, then there should be a probable classification of lattices based on shape [2, 3]. Other questions like "why do only 14 Bravais lattices exist when 28 lattices are possible, and why is the base/end centered cubic Bravais lattice absent?" were also accommodated [4, 5]. These questions create an agitation for more research on the issue. It is with this in mind that this paper reports the issues pertaining to the classification of Bravais lattices based on shape. The objective of this paper is to give a simple and clear understanding of the crystal lattice system, illustrate reasons why the classification based on shape for Bravais lattices was refuted and give answers to the growing questions of university students, researchers, and scientists.

1.1. The Crystal Lattice System

Lattices or "crystal skeletons" are the internal structure or framework on which the crystal is generated. The three dimensional array formed by the unit cells of a crystal is called a lattice [6]. Sometimes termed the foundation of the crystal, a lattice can be defined as a three-dimensional periodic arrangement of points in space [7]. To form a crystal, these points are associated with a group of atoms called the Motif or Basis of the crystal.

A crystal is a solid whose constituent atoms or molecules are arranged in a systematic geometric pattern [8]. Two points can be drawn from this definition to give a clear understanding of the origin of a lattice in a crystal system;

- Constituent atoms or molecules,
- Systematic geometric pattern.

The constituent atoms or molecules describes the motif or basis that are associated with each lattice point in the crystal while the systematic geometric pattern describes the lattice or crystal structure that can generate the entire crystal by repetition.

Simply put, a crystal can be defined as:



Figure 1: Illustration of a Crystal = Lattice + Motif

1.2. The Unit Cell and Crystal Co-ordinate System

Unit cells for most crystal structures are parallelepipeds or prisms having three sets of parallel faces; one is drawn within the aggregate spheres, which in this case happens to be a cube. Thus, the unit cell is the basic structural unit or building block of the crystal structure and defines the crystal structure by virtue of its geometry and the atom positions within [9]. A unit cell is also defined as a region of space which can generate the entire lattice (or Crystal) by repetition through lattice translation [10]. Any vector from one lattice point to another lattice point is known as Lattice Translation [11]. This lattice translation covers a distance (length a, b and c) from one point to another at given inter-axial angles (α , β , and γ) collectively known as lattice parameters. These parameters form the crystal co-ordinate system. In the case of a three-dimensional lattice, a primitive unit cell has the shape of a parallelepiped defined by 3 non collinear and not all in the same plane primitive translation vectors \overline{a} , \overline{b} , and \overline{c} .



Figure 2: A 3-D representation of (a) the crystal co-ordinate system and (b) the unit cell with its parameters

Where;

• \bar{a}, \bar{b} , and \bar{c} represents the unit vectors/lengths of the unit cell

- α represents the angle between vectors \overline{b} and \overline{c}
- β represents the angle between vectors \overline{c} and \overline{a}
- γ represents the angle between vectors \overline{a} and \overline{b}

1.3. The 7 Crystal Systems and 14 Bravais Lattices

The Bravais lattice is the basis from which all crystals can be constructed. In 1850, Mathematician Auguste Bravais (1811-1863) discovered that there were 14 different groups of points, which are known as Bravais lattices [12, 13]. Based on the length of each unit vector and their corresponding orientations, a total number of 7 crystal systems can be obtained and with three categories called face, body and base/end centers added to these crystal systems, 14 different types of 3-dimensional lattices known as Bravais lattices can be generated.

The 7 Crystal systems are illustrated below;

1. Cubic



2. Tetragonal



3. Orthorhombic



4. Monoclinic



A simple representation of the 7 crystal systems and 14 Bravais lattices are shown in Table 1;

S/N	Crystal Systems	Bravais Lattices				
1.	Cubic	Р	I	F		
2.	Tetragonal	Р	I			
3.	Orthorhombic	Р	Ι	F	С	
4.	Hexagonal	Р				
5.	Trigonal	Р				
6.	Monoclinic	Р			С	
7.	Triclinic	Р				

Table 1: The 7 Crystal Systems and 14 Bravais Lattices

Table 1 shows the Bravais lattices being represented with letters "P" denoting the simple Bravais lattice, "I" denoting the body centered Bravais lattice, "F" denoting the face centered Bravais lattice and "C" denoting the base/end centered Bravais lattice system. The simple Bravais system shows that lattice points are located only at the corners of the unit cell, the body-centered Bravais system shows that lattice points are located at corners as well as the center of the unit cell, the face centered Bravais system shows that lattice points are located Bravais are located at corners as well as the center of the unit cell, the face centered Bravais system shows that lattice points are located Bravais system shows that lattice points are located at corners as well as all face centers of the unit cell while the base or end centered Bravais system shows that lattice points are located at corners as well as a pair of parallel face centers of the unit cell.

2. Methodology

Several questions were raised in the introduction of this paper. Hence, this section gives an analysis of those questions.

This section makes use of the Pythagorean Theorem.

Pythagoras' theorem:



Figure 3: The Pythagoras' Theorem

2.1. Why do only 14 Bravais Lattices exist when 28 lattices are possible? And why is the Base Centered Cubic Lattice Absent?

If there are 7 crystal systems and 4 Bravais systems (simple, face, body and base centered), there should be 7 x 4 = 28 total Bravais lattices. Then why are there only 14? Examining a specific question like why is the base centered cubic Bravais lattice absent would provide reasons for the other empty spaces in the Bravais lattice system.

• Analyzing the Base/End Centered Cubic Lattice



Figure 4: Analysis of the End Centered Cubic Lattice Structure

The illustration above represents two base centered cubic lattices placed side by side and from the illustration you would see that it is possible to create a new unit cell based on shape for the same lattice.

Recalling the conditions for a cubic crystal system;

$$a = b = c$$
 and $\alpha = \beta = \gamma = 90^{\circ}$

Since all the sides of a cube are equal, we can assume that the sides of the cube be represented by one length "a" and the basis vector a', b', and c' are the lengths of the new unit cell and all angles are equal i.e. $\alpha = \beta = \gamma = 90^{\circ}$. Using the Pythagoras theorem, the basis vectors of the new unit cell are;

$$a' = \frac{a}{\sqrt{2}}; \ b' = \frac{a}{\sqrt{2}}; \ c' = a$$

The inter-axial angles of the base centered crystal lattice and new crystal lattice obtained are the same i.e. $\alpha = \beta = \gamma = 90^{\circ}$. Therefore, analyzing the new lattice obtained it was found to have the following conditions;

$$a' = b' \neq c'$$
 and $\alpha = \beta = \gamma = 90^{\circ}$

Comparing these conditions with that of each of the 7 crystal systems, the new crystal lattice obtained was found to have the shape of a Tetragonal unit cell and noticing that the lattice points of the new unit cell obtained are only located at the corners of the cell, it is termed a Simple Tetragonal Unit Cell. Therefore if we classify lattices based on shape, we can say that;

Base Centered Cubic Lattice (Cubic C) = Simple Tetragonal Lattice (Tetragonal P) ... (1)

S/N	Crystal Systems	Bravais Lattices				
1.	Cubic	Р	Ι	F	C×	
2.	Tetragonal	Р✓	Ι			
3.	Orthorhombic	Р	Ι	F	С	
4.	Hexagonal	Р				
5.	Trigonal	Р				
6.	Monoclinic	Р			С	
7.	Triclinic	Р				

 Table 2: Tabular Illustration of Cubic C being replaced by Tetragonal P

From equation 1 and Table 2 above, it is detected that the base /end centered cubic lattice (Cubic C) is absent but was replaced by the simple tetragonal lattice structure (Tetragonal P). Why was this done? In order to have an in depth clarification, a lattice (FCC Lattice) which is already present in the Bravais system is analyzed.

• Analyzing the Face Centered Cubic Lattice (Cubic F);



Figure 5: Analysis of the Face Centered Cubic Lattice Structure

Applying the same procedure to the Face centered cubic (FCC) lattice as we did for the base centered cubic (BCC) lattice, an identical unit cell was obtained in the process i.e. a Tetragonal unit cell. Now the difference here is the location of lattice points in the unit cell. For the new unit cell obtained, the lattice points are located at the corners as well as at the center of the unit cell; it is then called a Body centered Tetragonal Unit cell. Hence, if we classify Bravais lattices based on shape, we can also say that;

Face Centered Cubic Lattice = Body Centered Tetragonal Lattice (2)

If we approve of this equation (2), there would be a problem. The face centered cubic lattice and the body centered cubic lattice are both present in the Bravais lattice system and this is an issue because when classifying Bravais lattices, two lattices of the same structure cannot be present on the Bravais list i.e. one lattice must replace the other.

3. Results and Discussion

So why can't the face centered cubic lattice (Cubic F) be considered as a Body Centered Tetragonal lattice (Tetragonal I)? From research on Basic Crystallography carried out by Professor Rajesh Prasad in the Indian Institute of Technology, this is simply because the Bravais lattices were not classified based on shape (but on symmetry) and the reason for this is due to the non-uniqueness of the unit cell [14]. A unit cell being the building block of a crystal lattice can be in different shapes and sizes [15].

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Figure 6: The Non-Uniqueness of the Unit cell in a Lattice

Hence, unit cell shape cannot be the basis for classification of lattices because the unit cell of a lattice is not unique i.e. in a lattice, an infinite number of unit cells with different shapes are possible.

4. Conclusion

The questions put forward by university students, researchers and scientists like; why has the classification of lattices based on shape been refuted? [16, 17], why do only 14 Bravais lattices exist when 28 lattices are possible? [18, 19], and why is the base/end centered cubic Bravais lattice absent? [20, 21] are quite debatable because a crystal has a defined lattice shape (i.e. cubic hexagonal, tetragonal etc.) but if we were to classify lattices based on shape we would experience issues as proven in section 2. Therefore, as stated in the results of this research, the sole reason why there are only 14 Bravais lattices present and why the base centered cubic lattice is absent is because the Bravais lattices were classified based on symmetry [22] and also the reason why a lattice cannot be classified based on shape is due to the fact that there is an unlimited number of possible unit cell types with different shapes in a lattice [23].

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6. Conflict of Interest

There is no conflict of interest associated with this work.

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