Modeling and identification of centered crystal lattices in three-dimensional space

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Abstract. The paper offers a method that allows to model crystal lattices in three dimensional space. The method is based on a description of crystal lattices in the six-dimensional Euclidean space G6. Transformations of three basic translation vectors from centered types to primitive types have been derived. Using these transformations, the proposed method provides a uniform way to model both primitive and centered Bravais lattices. On a set of simulated lattices, the possibility of structural identification of primitive and centered crystal lattices has been investigated. The previously developed parametric identification method based on estimation of Wigner-Seitz cell volume has demonstrated the best result of separation of centered lattices from primitive ones. In addition, this method allowed to identify the type of centering for five out of seven centered Bravais lattices.

Keywords: crystal lattice, primitive lattice, centered lattice, Bravais unit cell, Wigner-Seitz cell, structural identification, similarity measure

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1. Introduction

A three-dimensional crystal lattice is a mathematical model which does not only allow to describe a structure of any crystalline material, but also determines its basic physical and chemical properties.

The problem of structural identification of crystal lattices still remains one of the main problems related to X-ray diffraction analysis. In his paper, Kupriyanov [1] has proposed an efficient approach to its solution which consist of estimating a number of parameters in the lattices under investigation and their subsequent comparison with parameters of reference lattices. The lattices either previously investigated or derived by modeling can be used as samples. Thus, the accurate structural identification of crystal lattices requires a large database of predetermined reference parameters.

The analysis of existing methods to solve the problem of structural identification has shown that the methods are mainly studied for lattices of seven primitive types, while the centered lattices are completely ignored.

In this paper, we propose a modeling method for centered crystal lattices and investigate the possibility of structural identification of primitive and centered lattices by using the existing and developed parametric identification methods.

2. Modeling Method for Centered Crystal Lattices

A crystal lattice model used in previous researches was based on three translation vectors [2]. Its basic parameters are:

- three edge lengths l_1, l_2, l_3 and three angle values $\alpha_1, \alpha_2, \alpha_3$ of a unit cell (Fig. 1);
- a number of lattice points by each of the translation vectors N_1, N_2, N_3.

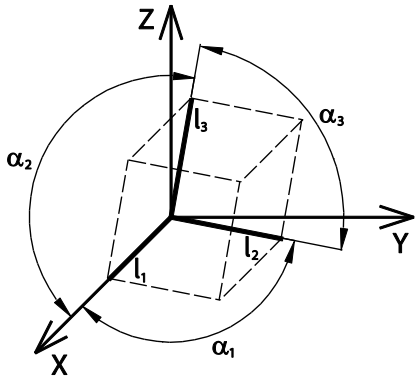

Fig. 1. – Unit cell model constructed on three basic translation vectors

This model has one significant disadvantage: it can only describe lattices of seven lattice systems – primitive Bravais lattices (index P). However, there are seven more centered Bravais lattices, which, in turn, are divided into the following three types [3]:

- body-centered (index I): one additional point at the center of the unit cell;
- base-centered (indices A, B, C): additional points at the centers of two parallel sides of the unit cell;
- face-centered (index F): additional points at the centers of each face of the unit cell.

Therefore, all crystal lattices can be assigned to one of the 14 Bravais lattice types (Fig. 2).

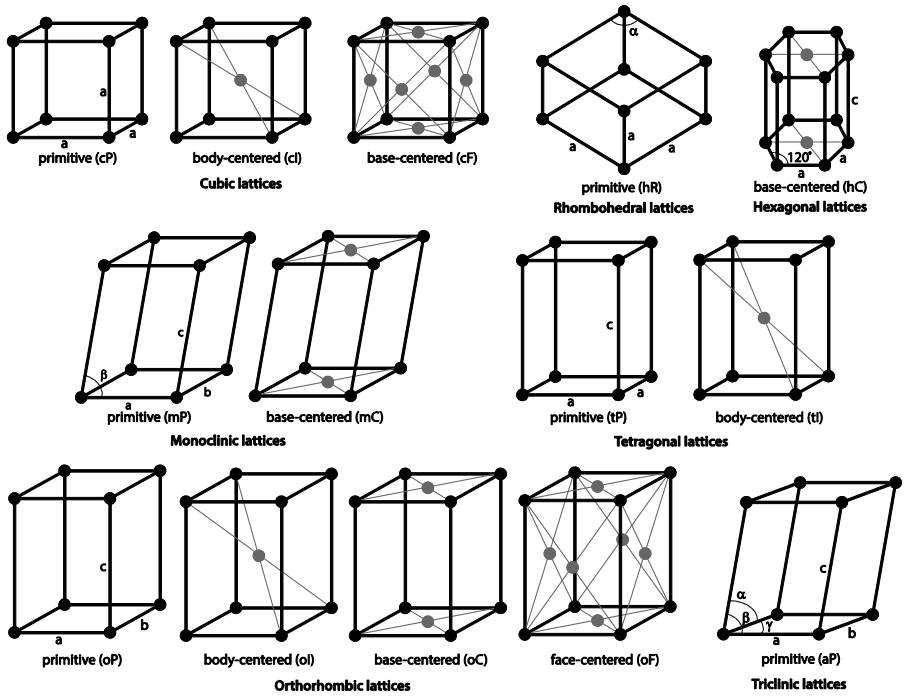

Fig. 2. – Primitive and centered types of Bravais lattices

To describe centered lattices, the used model has to be expanded by adding up to three translation vectors (Fig. 3). Doubling the number of parameters makes the model overly complicated.

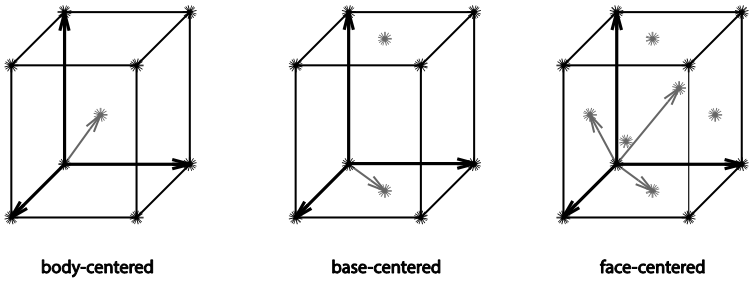

Fig. 3. – Choice of extra translation vectors within a centered lattice

An analogue of this model was suggested by Andrews and Bernstein [4]. It describes the lattice in the form of a six-dimensional vector $\bar{g}$ in the space G6. In addition, Andrews and Bernstein proved that each centered lattice $\bar{g}_T$ might be transformed to a primitive representation $\bar{g}_P$ by the following transformation:

$$\bar{g}_P = \mathrm{A} \cdot \bar{g}_T. \quad (1)$$

Each centered type has its own general form of the transformation matrix A. By solving the system of linear equations (1) with respect to basic translation vectors $\bar{a}_1, \bar{a}_2, \bar{a}_3$, we deduced the following solutions:

$$\begin{cases} \bar{a}_{1P} = \bar{a}_{1I} \\ \bar{a}_{2P} = \bar{a}_{2I} \\ \bar{a}_{3P} = 0.5\bar{a}_{1I} + 0.5\bar{a}_{2I} + 0.5\bar{a}_{3I} \end{cases}; \begin{cases} \bar{a}_{1P} = \bar{a}_{1C} \\ \bar{a}_{2P} = 0.5\bar{a}_{1C} + 0.5\bar{a}_{2C} \\ \bar{a}_{3P} = \bar{a}_{3C} \end{cases}; \begin{cases} \bar{a}_{1P} = 0.5\bar{a}_{1F} + 0.5\bar{a}_{2F} \\ \bar{a}_{2P} = 0.5\bar{a}_{1F} + 0.5\bar{a}_{3F} \\ \bar{a}_{3P} = 0.5\bar{a}_{2F} + 0.5\bar{a}_{3F} \end{cases}. \quad (2)$$

In other words, the transformations (2) make a choice of three new translation vectors. These vectors also allow to simulate all lattice points, however their parameters correspond to a primitive lattice that can be allocated within a centered lattice (Fig. 4).

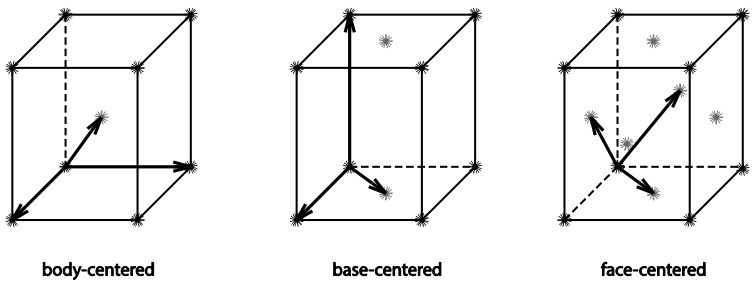

Fig. 4. – Selection of translation vectors of a primitive lattice within a centered lattice

This result gives a completely different look at the problem of modeling crystal lattices. On the one hand, if it is necessary to model a large set of random lattices, this set can be simulated by changing each parameter of a unit cell (lengths of the edges and values of the angles) independently in a specified range with a given partition. The resulting set of lattices will cover all primitive as well as centered lattices.

On the other hand, if the experiment requires a certain number of lattices for each type of centering, it would be possible to obtain a necessary number of lattices using the above transformations (2).

In the framework of new ideas, three basic translation vectors are to be sufficient to describe any crystal lattice in three-dimensional space. It is only needed to supplement them with the transformations (2) allowing to simulate a lattice of a particular centered type.

3. Methods of Crystal Lattice Parametric Identification

The basic methods among the existing crystal lattice parametric identification methods are the following:

- parametric identification method based on estimation of atomic packing factor [5];

- parametric identification method based on estimation of distances between isosurfaces [6].

In the parametric identification method based on estimation of atomic packing factor, each unit cell is represented as close packing of spheres (Fig. 5). The atomic packing factor can be calculated by dividing volume of atoms in unit cell by volume of unit cell.

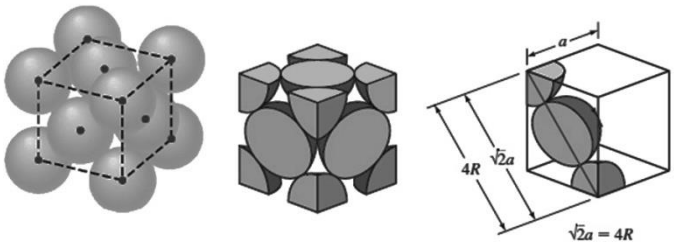

Fig. 5. – Close packing of spheres

In the parametric identification method based on estimation of distances between isosurfaces, a set of isosurfaces are constructed for each unit cell (Fig. 6). Then the root mean square distance and the Hausdorff distance between the isosurfaces are calculated.

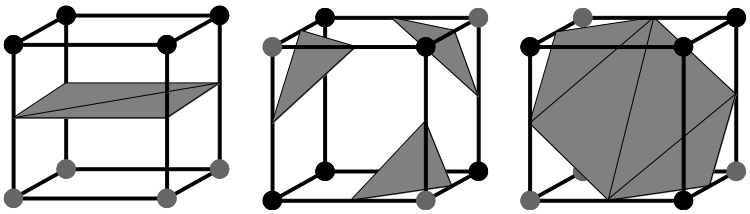

Fig. 6. – Types of isosurfaces constructed for a cubic lattice

The investigation of above two methods has shown that they have a number of disadvantages: a strong dependence of the crystal lattice identification accuracy from the type of the crystal system and a high sensitivity to distortions of coordinates of crystal lattice points. In order to eliminate these drawbacks, we have developed two new parametric identification methods.

The first of the developed method is based on estimation of Bravais unit cell parameters (lengths of three edges and values of three angles between the edges). By using the rotation of the analyzed lattice about coordinate axes, the proposed algorithm chooses three lattice points and calculates lengths of their radius vectors and angles between them. The radius vectors of the chosen points are non-coplanar and have minimum lengths [7].

The second of the developed method is based on estimation of Wigner-Seitz cell volume. The proposed algorithm uses Monte Carlo method to calculate the volume. It

constructs planes limiting Wigner-Seitz cell and scatters randomly a great number of points in the lattice area. The amount of points that fall into the limited area determines the Wigner-Seitz cell volume [8].

All the methods listed above use normalized similarity measures to compare estimated parameters with reference parameters. The similarity measures take the greatest value of unit when parameters completely coincide.

4. Identification of Centered Crystal Lattices

We conducted a series of computational experiments in order to investigate the possibility of separation centered lattices from primitive ones, as well as the possibility of delimiting types of centering.

Using the developed modeling method, crystal lattices of 11 Bravais types were simulated: monoclinic (mP, mC), orthorhombic (oP, oC, oI, oF), tetragonal (tP, tI) and cubic (cP, cI, cF). Triclinic, rhombohedral and hexagonal crystal systems were excluded from our consideration since all lattices of these systems are primitive. As simulation parameters we used the parameters of crystal lattices of natural minerals which have the unit cells similar in volume.

Then, the identification methods were used to estimate parameters of each crystal lattice and to calculate similarity measures between parameters of primitive and centered lattices. The results of computational experiments in the form of diagrams are presented below in Fig. 7 and Fig. 8.

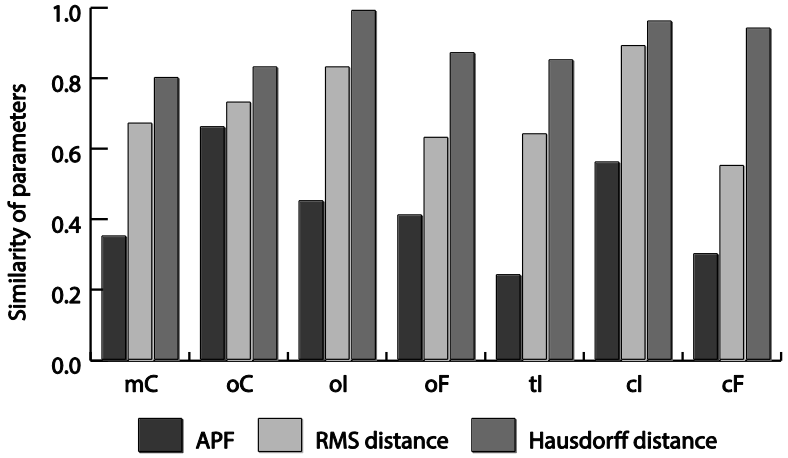

Fig. 7. – Similarity between centered and primitive Bravais lattices. Comparing atomic packing factors and distances between isosurfaces

Fig. 7 shows that RMS and Hausdorff distances are weakly dependent on the type of centering. Moreover, for two centered lattices, the value of their similarity with primitive lattices was about 0.95. Thus, the identification method based on estimation of distances between isosurfaces is not applicable to separate centered lattices from primitive ones. The obtained result can be explained by the fact that this method

estimates the maximum and the average distances between lattice points, whereas the centering has the greatest influence on the minimum distance. A similar situation can be observed in Fig. 8 for the identification method based on estimation of Bravais unit cell parameters (edges and angles).

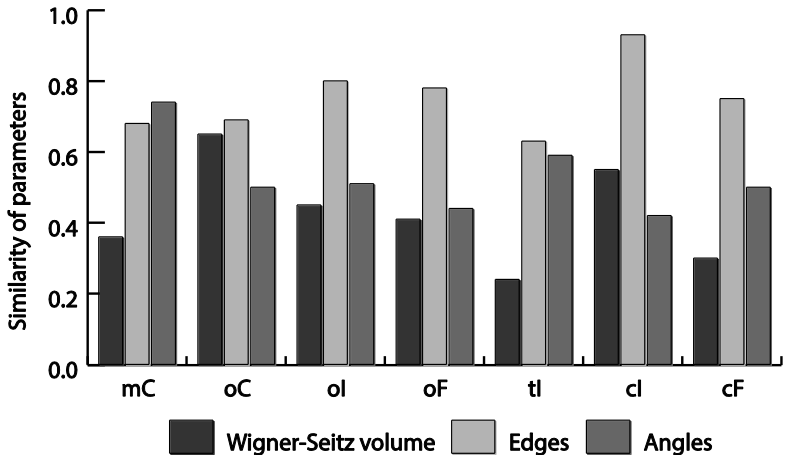

Fig. 8. – Similarity between centered and primitive Bravais lattices. Comparing edges and angles of unit cell and Wigner-Seitz cell volumes

The identification methods based on estimation of atomic packing factor and Wigner-Seitz cell volume have demonstrated the best result among other identification methods. The maximum value of their similarity with the primitive types was 0.66 and the average value of difference between the centered types was 0.2. Therefore, these methods allow to identify the type of centering with high accuracy. However, for orthorhombic system, it proved to be impossible to separate body-centered lattices from base-centered lattices.

It should be noted that the parametric identification method based on estimation of Wigner-Seitz cell volume does not require any information about basic translation vectors of a unit cell. As a consequence, this method is more universal than the parametric identification method based on estimation of atomic packing factor. At the same time, the parametric identification method based on estimation of Wigner-Seitz cell volume has the highest computational complexity because of the Monte Carlo method taken as its basis.

5. Conclusion

The developed crystal lattice modeling method allows to simulate any primitive or centered lattice in three-dimensional space. Besides, by changing each parameter of a unit cell (lengths of the edges and values of the angles) independently, a large set of lattices can be simulated to cover all 14 types of Bravais lattices. This set is a necessary condition for correct structure identification of crystal lattices.

The performed investigation of possible identification of centered crystal lattices has demonstrated that the parametric identification method based on estimation of Wigner-Seitz cell volume allows to separate with the high accuracy the centered lattices from the primitive lattices. In addition, it can identify the type of centering for five out of seven centered Bravais lattices (mC, oF, tI, cI, cF).

As it has been shown in previous papers, the parametric identification method based on estimation of Bravais unit cell parameters provides the high accuracy of lattice system identification. However, the Bravais type is determined not only by the lattice system but also by the type of centering. Therefore, it is essential to use both developed methods for the most accurate structural identification of crystal lattices.

Acknowledgements

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