Identification of Three-Dimensional Crystal Lattices by Estimation of Their Unit Cell Parameters*

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Abstract. The problem of the identification of three-dimensional crystal lattices is considered in the article. Two matching methods based on estimation of unit cell parameters were developed to solve this problem. The first method estimates and compares main parameters of Bravais unit cells. The second method estimates and compares volumes of Wigner-Seitz unit cells. Both methods include normalised similarity measures: an edge similarity measure and an angle similarity measure for Bravais cells and a volume similarity measure for Wigner-Seitz cells. The results of computational experiments on the large set of simulated lattices showed that the developed methods allowed to achieve the identification accuracy above 90% for four lattice systems.

Keywords: crystal lattice, unit cell parameters, Monte Carlo method, similarity measure, structural identification

1 Introduction

One of the basic problems related to X-ray diffraction analysis is the identification of crystal lattices [5]. It is usually solved by comparing estimated parameters of analysed lattice with those of selected sample [2]. The lattice parameters either previously investigated or derived by modeling can be used as samples. Therefore the accurate identification of a crystal lattice requires a large data base of the preselected sample parameters.

Among the main methods for identification of three-dimensional crystal lattices the following ones can be singled out: NIST lattice comparator [1], identification on the basis of atomic packing factor [4] and centered cubic lattice

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comparison method [3]. These methods have a number of drawbacks limiting their application field: complexity of crystal preparation, high error in comparison of lattices, which are similar in volume, etc.

The new approach based on estimation of unit cell parameters attempts to avoid these drawbacks. The algorithms proposed in the work allow calculating a similarity measure for any two crystal lattices.

2 Models of Crystal Lattices

There are several methods to describe crystal lattices. The most widespread method was offered by Auguste Bravais [5]. Bravais unit cell is characterised by a set of six parameters: lengths of the three edges l_1, l_2, l_3 and values of the three angles between the edges $\alpha_1, \alpha_2, \alpha_3$ (Fig. 1).

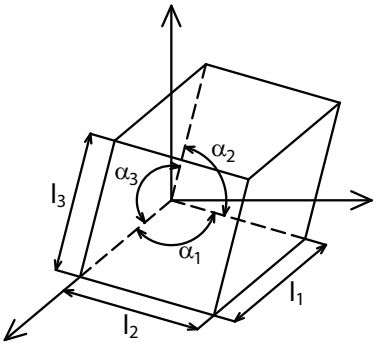

Fig. 1. The main parameters of Bravais unit cell

All Bravais lattices are subdivided into seven lattice systems. Table 1 shows characteristics of their unit cells.

Table 1. Characteristics of lattice systems

Lattice system	Symbol	Edge lengths	Angles
Triclinic	aP	$l_1 \neq l_2 \neq l_3$	$\alpha_1 \neq \alpha_2 \neq \alpha_3$
Monoclinic	mP	$l_1 \neq l_2 \neq l_3$	$\alpha_1 = \alpha_2 = 90^\circ \neq \alpha_3$
Orthorhombic	oP	$l_1 \neq l_2 \neq l_3$	$\alpha_1 = \alpha_2 = \alpha_3 = 90^\circ$
Tetragonal	tP	$l_1 = l_2 \neq l_3$	$\alpha_1 = \alpha_2 = \alpha_3 = 90^\circ$
Cubic	cP	$l_1 = l_2 = l_3$	$\alpha_1 = \alpha_2 = \alpha_3 = 90^\circ$
Rhombohedral	hR	$l_1 = l_2 = l_3$	$\alpha_1 = \alpha_2 = \alpha_3 \neq 90^\circ$
Hexagonal	hP	$l_1 = l_2 \neq l_3$	$\alpha_1 = 120^\circ; \alpha_2 = \alpha_3 = 90^\circ$

Another model of crystal lattices was offered by Jeno Wigner and Frederick Seitz [6]. Wigner-Seitz unit cell is characterised by a set of normal vectors which are drawn to limiting planes. In a three-dimensional space it is a polyhedron which contains inside itself one lattice node (Fig. 2).

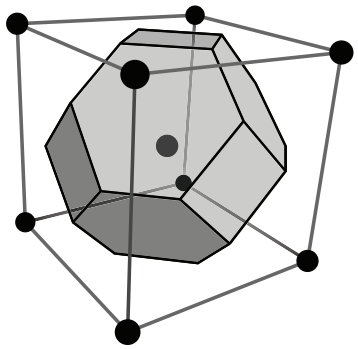

Fig. 2. Body-centered cubic Wigner-Seitz cell

3 Method of Crystal Lattice Identification on the Basis of Bravais Unit Cell Parameter Estimation

The initial data of the identification method are the set of radius-vectors determining the spatial position of crystal lattice nodes.

The following algorithm was designed to calculate the six main parameters of the Bravais unit cell:

1. Center the lattice.
2. Superpose the first radius-vector of minimal length with the axis OX.
3. Transfer the second radius-vector of minimal length into the plane XOY.
4. Select the third radius-vector of minimal length.
5. Calculate the main six parameters: $l_1, l_2, l_3, \alpha_1, \alpha_2, \alpha_3$.

Two normalised measures were introduced to determine separately the degree of the edge similarity and the degree of the angle similarity of two Bravais unit cells.

Similarity measure of edges:

$$\|\boldsymbol{l}_1 - \boldsymbol{l}_2\| = 1 - \frac{\sqrt{(l_{11} - l_{21})^2 + (l_{12} - l_{22})^2 + (l_{13} - l_{23})^2}}{\max\left\{\sqrt{(l_{11})^2 + (l_{12})^2 + (l_{13})^2}, \sqrt{(l_{21})^2 + (l_{22})^2 + (l_{23})^2}\right\}} \quad (1)$$

Similarity measure of angles:

$$\|\boldsymbol{\alpha}_1 - \boldsymbol{\alpha}_2\| = 1 - \max\left\{\sin\left(|\alpha_{11} - \alpha_{21}|\right), \sin\left(|\alpha_{12} - \alpha_{22}|\right), \sin\left(|\alpha_{13} - \alpha_{23}|\right)\right\} \quad (2)$$

4 Method of Crystal Lattice Identification on the Basis of Wigner-Seitz Unit Cell Volume Estimation

The initial data of the identification method are the number of scattering points L and the set of radius-vectors determining the spatial position of crystal lattice nodes.

The following algorithm was designed to calculate the volume of the Wigner-Seitz cell:

1. Center the lattice.
2. Determine the normal vectors from central lattice node to the planes limiting Wigner-Seitz cell.
3. Calculate the volume of cell limited by planes with the use of the Monte Carlo method.
   (a) Generate L-values of three-dimensional random vectors which are uniformly distributed in the whole lattice volume.
   (b) Count the number of vectors that hit in the region limited by planes and calculate the volume of cell based on the fact that the probability of hit in the Wigner-Seitz cell region is proportional to its measure (volume).

A normalised measure was introduced to determine the degree of the volume similarity for two Wigner-Seitz unit cells:

$$\|V_1 - V_2\| = 1 - \frac{\sqrt{(V_1 - V_2)^2}}{\max\{V_1, V_2\}} \quad (3)$$

The following computational experiments of crystal lattice identification on the large set of simulated three-dimensional lattices were conducted to analyse the efficiency of the introduced similarity measures.

5 Results of Experimental Computations

The initial data for experiments were 7,000 lattices (1000 lattices of each lattice system) obtained by simulation. The lengths of edges and values of angles were determined by values of a uniformly distributed random variable.

Each lattice was matched with all the rest lattices in pairs: two lattices were considered to be similar in edges or in angles, if the value of the corresponding similarity measure was no less than 0.95. Selection of this limiting value relates to the fact that currently the error of lattice parameter determination is no less than 5% [1].

Two lattices in the first experiment were brought into comparison only by the value of the edge similarity measure. Matching of two lattices in the second experiment was carried out only by the value of the angle similarity measure. However, the derived values of the percentage of lattice exact identification were near 14% for all lattice system in both experiments. These results show that the partitioning of all Bravais crystal lattices into seven lattice systems by using only the edge similarity measure or the angle similarity measure is not uniform and separable.

Consequently more exact lattice identification requires the simultaneous application of both similarity measures. For this reason in the third experiment two lattices were considered to be similar if values of the edge similarity measure and the angle similarity measure were no less than 0.95. Table 2 shows the results.

Table 2. Percentage of lattice exact identification for the main lattice systems by simultaneous edges and angles comparison

Estimated cell	Sample cell						
	aP	*mP*	*oP*	*tP*	*cP*	*hR*	*hP*
aP	98	1	1	0	0	0	0
mP	7	39	36	14	1	0	3
oP	6	36	39	14	1	1	3
tP	5	26	26	34	4	4	1
cP	4	12	12	23	26	23	0
hR	11	2	2	3	4	78	0
hP	12	3	3	2	0	0	80

Table data show average percent of coincidence of the estimated lattices with sample lattices (both similarity measures are no less than 0.95). For example the set of sample lattices which have coincided with one of the rhombohedral lattices in the third experiment consists on the average of 11% triclinic, of 2% monoclinic, of 2% orthorhombic, of 3% tetragonal, of 4% cubic, of 78% rhombohedral and of 0% hexagonal.

The use of the volume similarity measure of Wigner-Seitz unit cells was the last step to increase the identification accuracy. Matching of two lattices in the final fourth experiment was conducted with the application of all three similarity measures simultaneously: edges and angles of Bravais unit cells and volumes of Wigner-Seitz unit cells. Table 3 shows the results of the experiment.

According to Table 2 and Table 3 data it can be concluded that the accuracy of lattice identification increased by average 15%. The maximum increase of accuracy was achieved for monoclinic lattices by 51%. However, there is a separate group (orthorhombic, tetragonal, cubic) with the low percentage of lattice exact identification and, therefore, the problem of delimiting these three lattice systems cannot be considered as solved.

Table 3. Percentage of lattice exact identification for the main lattice systems by simultaneous edges, angles and volumes comparison

Estimated cell	Sample cell						
	aP	*mP*	*oP*	*tP*	*cP*	*hR*	*hP*
aP	99	1	0	0	0	0	0
mP	2	90	4	3	0	0	1
oP	2	22	54	20	1	1	0
tP	1	10	34	44	6	5	0
cP	0	3	15	26	30	26	0
hR	1	0	2	3	4	90	0
hP	1	7	0	0	0	0	92

6 Conclusion

The developed methods of crystal lattice identification allowed to achieve the identification accuracy above 90% for four lattice systems (triclinic, monoclinic, rhombohedral and hexagonal).

Basing on the performed calculation it can be concluded that the best way to identify the lattice system for the generated set of 7,000 lattices is simultaneous application of all three introduced similarity measures.

Identification accuracy of the remaining three lattice systems (orthorhombic, tetragonal and cubic) is not still sufficiently high. They require further research for the purpose of finding additional similarity measures (for example, comparison of isosurfaces, tensor representation of unit cells, etc.).

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