APPLICATION OF GRADIENT STEEPEST DESCENT METHOD TO THE PROBLEM OF CRYSTAL LATTICE PARAMETRIC IDENTIFICATION

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Abstract. The objective of this paperwork is the development of a crystal lattice parameter identification algorithm, which allows obtaining a more accurate solution compared to the Bravais unit cell estimation algorithm. To achieve the objective, we suggest solving the parameter identification problem using the steepest descent gradient method. The study of the parameter identification accuracy was conducted on a large number of modeled crystal lattices using the edges and angles similarity measures for Bravais unit cells.

Keywords: crystal lattice, Bravais unit cell, Wigner-Seitz unit cell, similarity measure, translation vector, parameter identification, gradient steepest descent method.

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Introduction

Nowadays, much attention has been concentrated on reconstruction of three-dimensional objects [1, 2, 3]. In particular in crystallography, reconstruction of a three-dimensional crystal lattice structure is related directly to a parameter identification problem, which is one of the basic problems of X-ray diffraction analysis [4, 5]. Unfortunately, such methods either lack sufficient accuracy or fail to describe comprehensively the crystal properties [4, 6-10]. The majority of universal methods aimed at the solution of the parameter identification problem with high accuracy are based on estimating parameters of a unit cell [6-8].

The most well-known crystal lattice model was offered by Auguste Bravais. The Bravais model is based on unit cell representation: the entire lattice can be constructed by translation of a single cell. All unit cells are divided into seven lattice systems according to edge lengths and angle values **(**Fig. 1**)** [11].

With evolving technology, the parameter identification algorithms as well as the crystal lattice comparison methods have become more relevant [4, 7-10, 12, 13].
The objective of a crystal lattice parameter identification method is to estimate unit cell parameters. There are several methods that offer a solution to the problem: NIST lattice spacing comparator [14], parameter identification methods based on estimation of atomic packing factor [15] and distances between isosurfaces [16]. However, these methods are not universal and have a number of disadvantages, such as strong dependence between the crystal lattice identification accuracy and the lattice system, high sensitivity to distortions of crystal lattice point coordinates or complexity of the sample preparation.

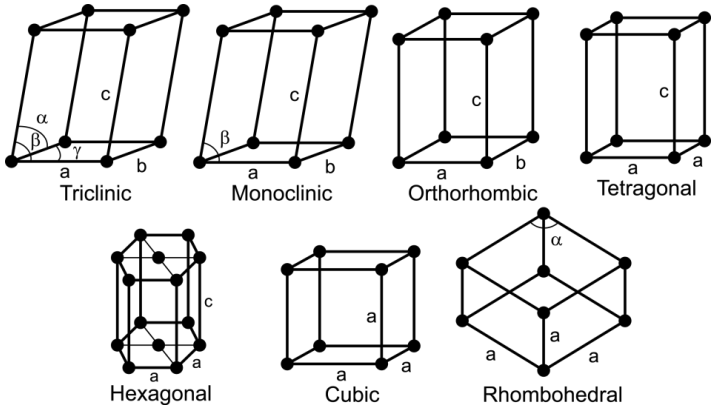

Fig. 1. Unit cells of seven lattice systems

Among the existing universal methods that provides high accuracy of crystal lattice parameter identification, we can distinguish the following ones: “The lattice identification method based on estimation of Bravais unit cell parameters” [8], “The lattice identification method based on estimation of the Wigner-Seitz cell volumes” [8]. In the experimental section, the comparison of the results obtained by these methods and the developed ones are presented.

The lattice identification method based on estimation of Bravais unit cell parameters

The method is based on calculation of six key parameters of the Bravais unit cell, i.e. three edge lengths and three included angles [6, 7, 9, 11, 19].
Initial data for the identification method based on estimation of the Bravais unit cell parameters are a finite set of radius-vectors of crystal lattice nodes.
The identification method involves a search of three non-coplanar vectors in the original set of nodes: the first vector has a minimum norm; the second vector does not lie on a straight line with a directing vector equal to the first vector; the third vector does not lie on a plane made by two found vectors.

The lattice identification method based on estimation of Bravais unit cell parameters

The method is based on calculation of six key parameters of the Bravais unit cell (Fig. 2), i.e. three edge lengths and three included angles [6, 8, 10].

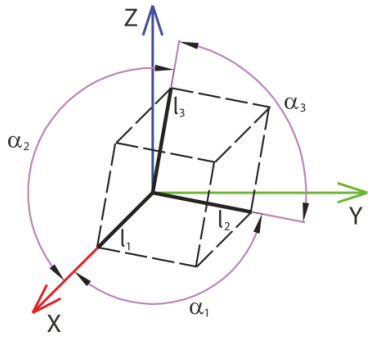

Fig. 2. Bravais unit cell

Initial data for the identification method based on estimation of the Bravais unit cell parameters are a finite set of radius-vectors of crystal lattice nodes.
The identification method involves a search of three non-coplanar vectors in the original set of nodes: the first vector has a minimum norm; the second vector does not lie on a straight line with a directing vector equal to the first vector; the third vector does not lie on a plane made by two found vectors.

The lattice identification method based on estimation of the Wigner-Seitz cell volumes

In order to find volumes of the Wigner-Seitz cells (Fig. 3), we must construct planes limiting the cell and estimate its volume using the Monte-Carlo method – a random scattering of a large number of points into a lattice area and calculation of a number of points fell into the limited area of the Wigner-Seitz cell [8].

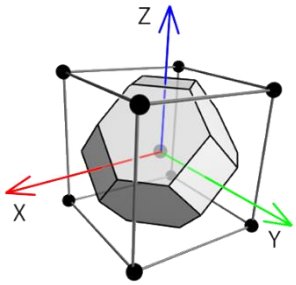

Fig. 3. Wigner-Seitz unit cell

Initial data for the identification method based on estimation of Wigner-Seitz cell volumes are the P – number of entered points and the set of radius-vectors of crystal lattice nodes as follows:

$X = \{\bar{x}_l\}_{l=1}^{L}, \bar{x}_l = (\bar{x}_{l1}, \bar{x}_{l2}, \bar{x}_{l3})^{\mathrm{T}} \in \mathbb{R}^3.$

The identification method involves calculation of Wigner-Seitz cell volumes by constructing the limiting planes: $p_{l1}x + p_{l2}y + p_{l3}z - \|\bar{p}_l\|^2 = 0,\ 1 \le l \le L-1$; generating L - values of three-dimensional random vectors which are uniformly distributed in the whole lattice volume and counting the number of vectors that hit in the region limited by planes. Calculation of the cell volume is based on the fact that the probability of hit in the Wigner-Seitz cell region is proportional to its measure (volume).
In the presented work, we use only information about limiting planes to reconstruct the whole lattice. It is necessary to compare all developed parameter identification methods uniformly.

Crystal lattice parameter identification algorithm based on optimizing translation vector search using the gradient steepest descent method

In the context of this paperwork, we have developed a crystal lattice parameter identification algorithm based on the steepest descent gradient method. The fundamental element of this algorithm is the Bravais lattice model described by three translation vectors $\bar{a}_1$, $\bar{a}_2$ and $\bar{a}_3$ [17]. The set of lattice nodes is expressed as:
$X = \{x = i\bar{a}_1 + j\bar{a}_2 + k\bar{a}_3\}: i, j, k \in \mathbb{Z}.$
In this case, both algorithms shall require initial approximation as an additional input parameter. Particularly, the result vectors of the lattice identification method based on estimation of Bravais unit cell parameters can be used as the initial approximation.
The objective function of optimization is as follows:

$$E(\bar{a}_1, \bar{a}_2, \bar{a}_3) = \sum_{l=1}^{L} \min_{i,j,k} \left\| \bar{x}_l - (i\bar{a}_1 + j\bar{a}_2 + k\bar{a}_3) \right\|^2, \quad (1)$$

where L is the number of nodes in the lattice.
Let us introduce the following notation:

$\mathrm{A} = (\bar{a}_1 \quad \bar{a}_2 \quad \bar{a}_3) \in \mathbb{R}^{3\times 3}$;

$\bar{n}_l = (i_l \quad j_l \quad k_l)^T$;

$\mathrm{N}_l = \bar{n}_l \bar{n}_l^T$;

$\bar{w}_l^s = i_l \bar{a}_1^s + j_l \bar{a}_2^s + k_l \bar{a}_3^s - \bar{x}_l$,

where *s* is the step number in the descent.
In this case a gradient (2) and a descent factor (3) are as follows:

$$\nabla E\left(\mathrm{A}\right) = 2\left[\mathrm{A}\cdot\sum_{l=1}^{L}\mathrm{N}_l - \sum_{l=1}^{L}\overline{x}_l\overline{n}_l^T\right]; \tag{2}$$

$$\lambda_s = \frac{\sum_{l=1}^{L}\left(\overline{w}_l^s, \nabla E\left(\mathrm{A}^s\right)\overline{n}_l\right)}{2\sum_{l=1}^{L}\left\|\nabla E\left(\mathrm{A}^s\right)\overline{n}_l\right\|^2}. \tag{3}$$

Expressions (2) and (3) are recorded in compact form. The desired solution is the matrix (triple translation vectors). Figure 4 shows the convergence of translation vectors to solution for a two-dimensional lattice.

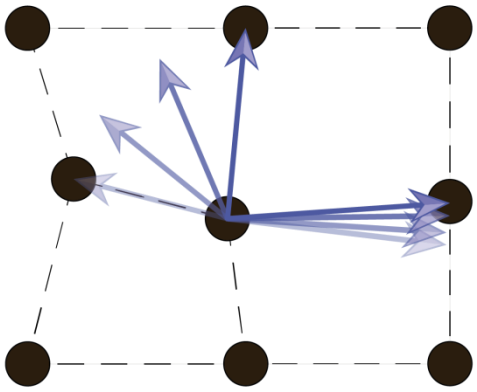

Fig. 4. Convergence of translation vectors to the solution

Analysis of parameter identification accuracy of the developed algorithms

The aim of the crystal lattice parameter identification algorithm based on the steepest descent gradient method is finding the vectors $\overline{a}_1$, $\overline{a}_2$ and $\overline{a}_3$, minimizing the objective function (1). In addition, the objective function (1) determines the error of the obtained solution in relation to the source set of nodes.
Using computational experiments, we studied the dependence between the reduction of the objective function (1) and the lattice systems. For the experiments, 20 lattices were generated for each crystal system. All modeled lattice consisted of 125 nodes (5 translations in each direction). Then the lattices was distorted through a random offset of each node from its ideal position in a random direction at a distance no more

than 0.5 Å. The solution error (1) between the original lattice and the lattice reconstructed by estimated parameters determined the accuracy of parameter identification methods. Figure 5 shows the obtained results as values of the averaged objective function.

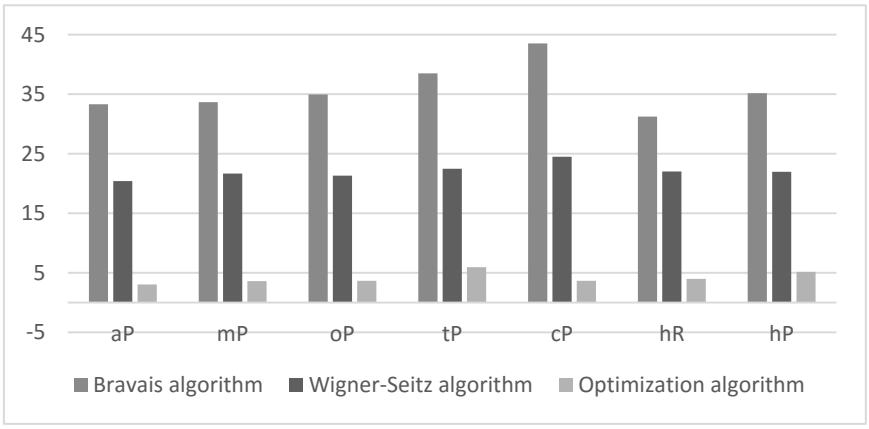

Fig. 4. Results of study of dependence of solution error from syngony when running parameter identification algorithms being tested

According to experiment results, the Bravais unit cell parameter estimation algorithm is highly sensitive to the distortion of lattice structure. It is obvious, since the method analyze only 4 nearest lattice nodes but not the whole lattice structure. On the contrary, a Wigner-Seitz cell of three-dimensional lattice are described by 27 lattice nodes. As a result, the Wigner-Seitz cell volume estimation algorithm demonstrated significantly better results than the previous one. The error decreased on average by 47 %. However, the Wigner-Seitz cell volume estimation algorithm has a crucial disadvantage – an extremely high computational complexity.

The best result was obtained using the developed parameter identification algorithm based on the gradient steepest descent method. It greatly improved the results obtained by the Bravais unit cell parameter estimation algorithm and reduced almost sixfold the solution error.

Conclusion

In the presented work, we have developed algorithm of parameter identification based on the gradient steepest descent method. The algorithm uses the result vectors of the lattice identification method based on estimation of Bravais unit cell parameters is used as the initial approximation.

The experiments proved that the parameter identification algorithm based on the gradient steepest descent method is stable to lattice distortion and allows to reduce six-

fold the solution error compared to the Bravais unit cell parameter estimation algorithm and threefold compared to the Wigner-Seitz cell volumes estimation algorithm.

Acknowledgments

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