Development of the crystal lattice parameter identification method based on the gradient steepest descent method

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ABSTRACT

In this paper, we propose a new method to solve a problem of crystal lattice parameter identification. The developed method is based on applying the gradient steepest descent method. The two algorithms of crystal lattice parameter identification on the basis of the developed method was proposed. The comparison of the algorithms with the existing method of lattice identification based on estimation of Bravais unit cell parameters is conducted. The experimental results show a significant increase in the crystal lattice parameter identification accuracy for all seven lattice systems.

Keywords

Crystal lattice, Bravais unit cell, translation vector, parameter identification, gradient steepest descent method.

1. INTRODUCTION

Nowadays, much attention has been concentrated on reconstruction of three-dimensional objects [Jou02a, Jou05a, Jou06a]. 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 [Con02a, Jou04a].

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 (Figure 1) [Jou07a].

With evolving technology the parameter identification algorithms, as well as the crystal lattice comparison methods become more relevant [Bra01a, Jou08a].

The objective of the 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 [Jou03a], parameter identification methods based on estimation of atomic packing factor [Smi01a] and distances between isosurfaces [Con01a]. 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.

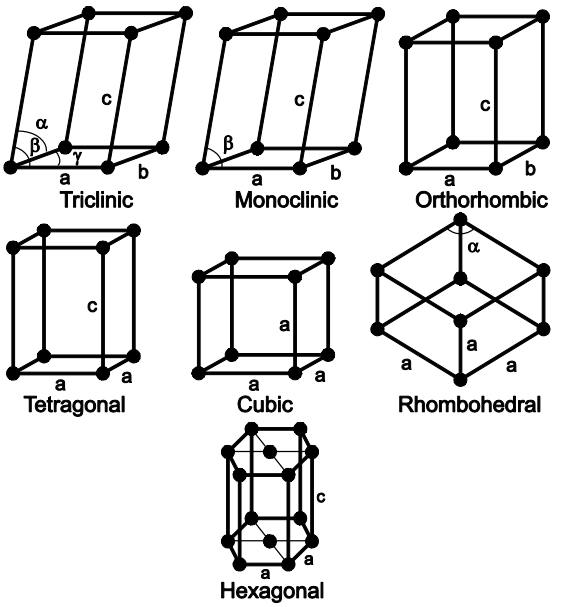

Figure 1. Unit cells of seven lattice systems.

Among the existing universal methods that provides high accuracy of crystal lattice parameter identification, we can distinguish the following one: "The lattice identification method based on estimation of Bravais unit cell parameters" [Jou01a]. In the experimental section, the comparison of the results obtained by this method and the developed one is presented.

2. 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 [Jou07a].

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.

3. DEVELOPED ALGORITHMS OF CRYSTAL LATTICE PARAMETER IDENTIFICATION BASED ON OPTIMIZATION PROBLEM SOLUTION USING THE GRADIENT STEEPEST DESCENT METHOD

Two algorithms of crystal lattice parameter identification have been developed. In both algorithms we consider the Bravais lattice represented by three translation vectors $\bar{a}_1$, $\bar{a}_2$ and $\bar{a}_3$ [Sha01a]. The set of lattice nodes is expressed as:

$$X = \left\{ \bar{x} = i\bar{a}_1 + j\bar{a}_2 + k\bar{a}_3 \right\} : \; i, j, k \in \mathbb{Z}.$$

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.

3.1. The Algorithm Based on Joint Optimization of Translation Vectors

The objective function of optimization is as follows:

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

where L is the number of nodes in the lattice.

Let us introduce the following notation:

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

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

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

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

s is the step number in the descent.

In this case a gradient (2) and a descent factor (3) are as follows:

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

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

Expressions (2) and (3) are recorded in compact form. The desired solution is the matrix (triple translation vectors). The gradient is respectively the matrix, too.

3.2. The Algorithm Based on Independent Optimization of Translation Vectors

Nodes of a crystal lattice are to be set up by translation vectors, however in this case they shall pass through recurrent planes. This property enables to break a problem of translation vector optimization, described above, into three independent problems of optimization of some vectors which describe recurrent planes. The recurrent planes shall be described by a plane normal and a plane period. Thus, the desired vector must have the same direction as the plane normal, and the vector norm should coincide with the plane period.

The objective function shall be as follows:

$$E\left(\bar{d}\right) = \sum_{l=1}^{L} \min_{i} \left[\left(\bar{x}_l, \bar{d} \right) - i \left\| \bar{d} \right\|^2 \right]^2. \qquad (4)$$

For the objective function (4) the gradient shall be determined from the equation (5), and the descent factor – from the equation of the third degree (6).

$$\nabla E = 2\sum_{l=1}^{L} \left(\left(\bar{x}_l, \bar{d} \right) - i_l \left(\bar{d}, \bar{d} \right) \right) \left[\bar{x}_l - 2 i_l \bar{d} \right]. \qquad (5)$$

$$y_0 + y_1\lambda + y_2\lambda^2 + y_3\lambda^3 = 0, \qquad (6)$$

where $y_0 = \sum_{l=1}^{L} p_l q_l$; $y_1 = \sum_{l=1}^{L} p_l r_l - \sum_{l=1}^{L} {q_l}^2$;

$y_2 = -2\sum_{l=1}^{L} q_l r_l$; $y_3 = -\sum_{l=1}^{L} {r_l}^2$;

$p_l = \left(\bar{x}_l - i_l \bar{d}^s, \bar{d}^s \right)$;

$q_l = \left(\bar{x}_l - 2 i_l \bar{d}^s, \nabla E\left(\bar{d}^s \right) \right)$;

$r_l = i_l \left\| \nabla E\left(\bar{d}^s \right) \right\|^2$.

The iterative process of this algorithm may be controlled. A vector of an individual problem does not correlate with vectors of two remaining problems at all. If the first developed algorithm carries out S iterations for all three vectors (matrix), then in the case of the latest algorithm each desired vector shall

be found only for the required number of iterations. The case when one vector can result in an incorrect solution shall be also excluded due to dependence on other vectors.

The algorithm suggests the connection between a basis of translation vectors and a new basis of "independent" vectors. The transition from the basis of translation vectors to the basis of independent vectors shall be carried out by simultaneous linear algebraic equations (7). The reverse transition is performed using the following expressions (8).

$$\left(\bar{d}_1 \quad \bar{d}_2 \quad \bar{d}_3\right)^T \bar{a}_i = \left\|\bar{d}_i\right\|^2 \bar{e}_i, \quad i = \overline{1,3}, \tag{7}$$

where $\bar{e}_i$ is a unit vector in the i-direction;

$$\bar{d}_i = \frac{\left(\left[\bar{a}_k \times \bar{a}_j\right], \bar{a}_i\right)}{\left\|\left[\bar{a}_k \times \bar{a}_j\right]\right\|^2}, \quad i \neq j \neq k = \overline{1,3}. \tag{8}$$

4. ANALYSIS OF THE DEVELOPED ALGORITHMS OF CRYSTAL LATTICE PARAMETER IDENTIFICATION

The criterion of accuracy of the results obtained by applying the parameter identification algorithm is a solution error. Let us select the function used in the first developed algorithm as the solution error (1).

To calculate this function, the radius-vectors of the original lattice nodes and the parameters obtained by some algorithm shall be required.

For the experiments, crystal lattices have been modeled using the unit cell parameters of the seven existing materials. Each lattice consisted of 125 nodes. Then modeled 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.

Parameters of the Bravais unit cell were estimated for each modeled lattice, and the solution error was calculated. Figure 2 gives the research findings as values of the objective function. Both developed algorithms have considerably reduced an error obtained as the result of performing the identification algorithm based on estimation of parameters of the Bravais cell.

The accuracy of the parameter identification algorithm based on independent optimization of translation vectors depends crucially on the selection of the stop criteria. In case of the standard stop criteria, the iteration process continues until the objective function begins to grow or the optimizing vector stops changing. However, the experimental data showed that the second algorithm with the standard stop criteria returns bad results.

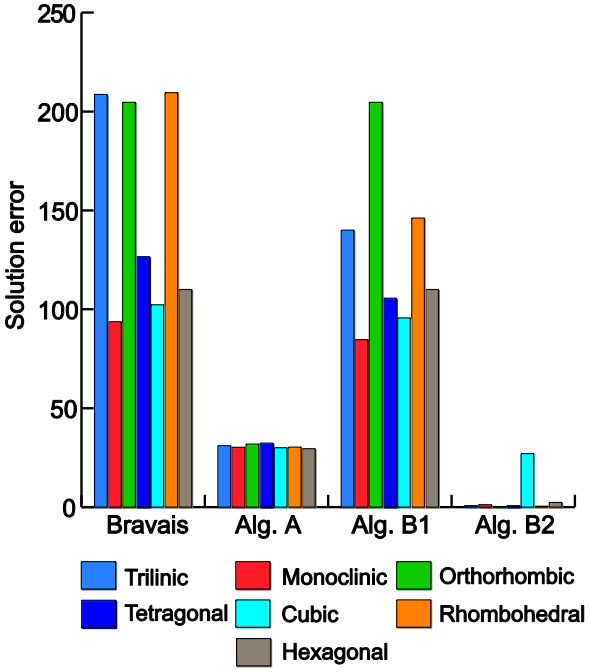

Figure 2. Accuracy of parameter identification:
A – algorithm from Section 3.1;
B1 – algorithm from Section 3.2 (standard stop criteria);
B2 – algorithm from Section 3.2 (weakened stop criteria).

To improve the accuracy, we proposed to weaken the stop criteria by excluding the first condition (non-increasing objective function). The data in Figure 2 indicate that the weakened stop criteria allow to substantially reduce the error.

5. CONCLUSION

In the course of the present work we have developed two algorithms of parameter identification based on the gradient steepest descent method. In both algorithms, the result vectors of the lattice identification method based on estimation of Bravais unit cell parameters is used as the initial approximation.

The research showed that in most cases the developed algorithms can provide better results than the Bravais unit cell parameter estimation algorithm. Moreover, the second algorithm with the weakened stop criteria demonstrates the minimum errors of parameter identification for all seven lattice systems.

6. ACKNOWLEDGMENTS

This work was partially supported by the Ministry of education and science of the Russian Federation in the framework of the implementation of the Program of increasing the competitiveness of SSAU among the world's leading scientific and educational centers for 2013-2020 years; by the Russian Foundation for Basic Research grants (# 14-01-00369-a, # 14-07-97040-p_povolzh'e_a, # 15-29-03823, # 15-29-07077); by

the ONIT RAS program # 6 “Bioinformatics, modern information technologies and mathematical methods in medicine” 2015.

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