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Development of a vector algorithm of three-dimensional crystal lattice parametric identification based on estimation of the spacing between adjacent lattice planes

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Abstract

The analysis of a crystal nanostructure is provided by the information obtained from the electron microscopy. Mathematically, a crystal structure is described by unit cells – minimum building blocks, which form the entire crystal lattice by parallel transfer. Parametric identification is an important problem in the field of three-dimensional crystal lattice research. Application of the constant step size gradient descent method to solve this problem ensured sufficient increase of the identification accuracy. However, computational complexity of the applied algorithm significantly exceeds the computational complexity of the existing parametric identification algorithms, which has caused substantial increment of the execution time. In order to eliminate such disadvantage this work proposes vector algorithm of crystal lattice parametric identification implemented with CUDA technology.

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Keywords: Bravais lattice; unit cell; gradient descent method; parametric identification; parallel algorithm; CUDA

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1. Introduction

Currently three-dimensional reconstruction is a topical problem which is supported by a large number of publications dedicated to this issue [1-4]. Special emphasis is placed at three-dimensional reconstruction of crystal lattice [5-8]. The following methods may be singled out among the existing ways to estimate the three-dimensional crystal lattice parameters: NIST comparator [5], identification based on atomic packing factor estimation [6], isosurfaces comparison method [7]. Parametric identification methods are convenient tools to study the three-dimensional structures of crystal lattices [9-16]. The existing parametric identification algorithms for three-dimensional crystal lattices are presented in the papers [9-14]. However, the main disadvantages of the existing methods are the computational complexity and the difficulty of data decomposition.

Unlike ideal crystals, real crystal nanoscale images obtained in practice have imperfections (Fig. 1). Distortions are caused by many reasons such as dislocations, impurities, measurement errors, etc. To reduce the identification error we solve the problem by the gradient steepest descent method.

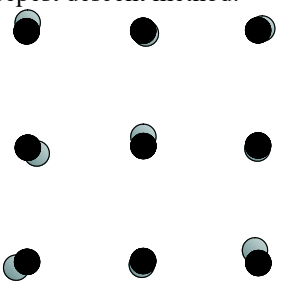

Fig. 1. Ideal (black circles) and distorted (gray circles) crystal lattices.

The crystal lattice structure can be easily described using the Bravais lattice model, i.e. with three vectors $\overline{p}_1$, $\overline{p}_2$ and $\overline{p}_3$, which can be translated into any node of a three-dimensional lattice [17] (Fig. 2). There is an algorithm of parametric identification based on the Bravais unit cell parameter estimation [12], which is the simplest as compared to algorithms based on other lattice models, e.g. based on the Wigner-Seitz cell model [9-11]. Unfortunately, the existing parametric identification problem is ill-posed in the sense of Hadamard, since the solution can be non-unique as a consequence of the Bravais lattice definition ambiguity [17] (Fig. 3).

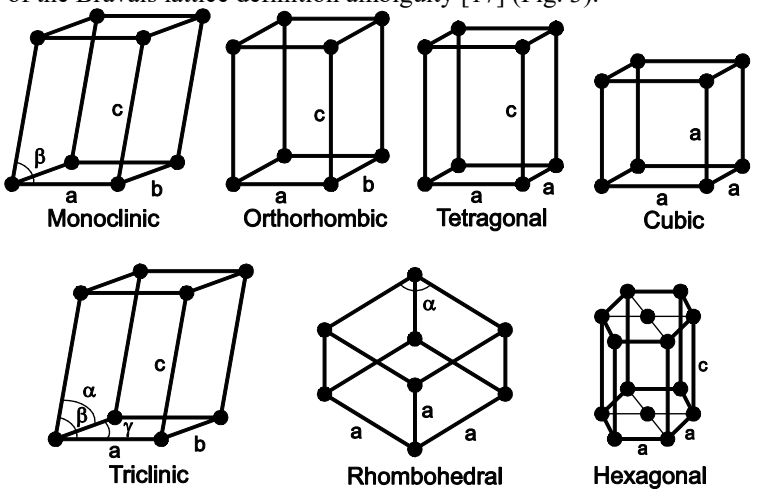

Fig. 2. Bravais unit cells of seven lattice systems.