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**METHODOLOGY OF CONVERTING OF THE COORDINATES
OF THE BASIS ATOMS IN A UNIT CELL OF CRYSTALLINE β -Ga₂O₃, SPECIFIED
IN A MONOCLINIC CRYSTALLOGRAPHIC SYSTEM,
IN THE LABORATORY CARTESIAN COORDINATES
FOR COMPUTER APPLICATIONS**

One of the most important areas of modern technology is the creation of new structural materials with predetermined properties. Along with industrial methods for their preparation and technologies associated with the artificial growth of crystalline structures, various methods of computer modeling of new materials have recently become increasingly important. Such approaches can significantly reduce the number of full-scale experiments. Many applications of the computational materials science are related to the need to establish a relationship between structure and electronic characteristics, and other physical properties of crystals. This article on the example of crystalline β -Ga₂O₃ presents the algorithms used in the converting of the coordinates of the basis atoms in a unit cell of crystal, specified in a crystallographic system, in the Cartesian coordinates for the computational experiment.

1. Introduction

Gallium Oxide (β -Ga₂O₃) has recently attracted considerable interest for its unique combination of material properties, he has been recognized the perspective wide band gap semiconductor [1]. The perspectives for use of material β -Ga₂O₃ are conditioning systems, including pulsed power for avionics and electric ships, solid-state drivers for heavy electric motors, and advanced power management and control electronics. Certain classes of power electronics with capabilities beyond existing technologies due to its large bandgap, controllable doping, and the availability of large diameter, relatively inexpensive substrates In addition to having a lower electron mobility than binary alloys, high Al-AlGaN is difficult to dope controllably and selectively. The usual Si dopant ionization level becomes very deep in Al-rich AlGaN, and ion implantation activation efficiency is low. We will focus on whether Ga₂O₃ has a role in complementing SiC and GaN. Some of the key issues include the real application space of UWB semiconductors in power switching or RF power amplification, whether in realistic conditions they are capable of outperforming the mature SiC and GaN technology, and whether the material quality and cost, thermal problems, and

reliability challenges will limit their application. The biggest difficulties in implementing Ga₂O₃ relate to its high thermal resistance and the absence of p-type conductivity through doping with acceptors. This limits the type of device structures that can be realized and requires effective thermal management approaches [2].

After an unprecedented development and application of classical and compound semiconductors, that started in mid of the XX century, wide bandgap materials were a natural step in the expansion of semiconducting materials that would offer an extended functionality of both electronic and optoelectronic devices. Wide bandgap materials, such as GaN, InGaN, and SiC have been successfully industrialized in the last decade with an impact on our daily life, in particular in the case of nitrides. Nowadays, the research is directed towards ultra-wide bandgap semiconducting materials with the energy gap exceeding 4 eV. There are several that materials that attract particular research attention, including AlGaN, AlN, diamond, and β -Ga₂O₃ belonging to the class of materials called transparent semiconducting oxides. Diamond is very difficult to fabricate in a large volume and of high structural quality.

Al-based nitrides also suffer from technological difficulties in obtaining a large volume of high quality crystals. Among ultra-wide bandgap semiconducting materials only β -Ga₂O₃ can be grown in the large volume. β -Ga₂O₃ with its unique optical and electrical properties is regarded as complementary to other ultra-wide bandgap semiconducting materials in new areas of applications, as solar-blind UV photodetectors, photocatalysts, gas sensors, solar cells, phosphors, and transparent conducting films for electrodes on a variety of optoelectronic devices [3-5].

The polymorphs (i.e., different forms or crystal structures) of Ga₂O₃ and their regions of stability were identified more than 60 years ago [6]. There are five polymorphs of Ga₂O₃, labeled as corundum (α), monoclinic (β), defective spinel (γ), and orthorhombic (ϵ), with the δ phase commonly accepted as being a form of the orthorhombic phase [1, 6–10]. The β -phase (β -Ga₂O₃) is the most stable crystal structure and has been the subject of most studies [1, 6–16].

2. Methodology of converting of the coordinates of the basis atoms in a unit cell of crystal, specified in a crystallographic system, in the Cartesian coordinates

It is known that the centers of atoms of any ideal crystalline structure form, in simple cases, one or, in the general case, several regular point systems. By the correct system of points (a system of equivalent positions) we mean the set of points obtained by multiplying the starting point (nonequivalent) by all symmetry operations of a given space group [17]. Moreover, each regular point system contains only one point in an independent region.

In each spatial symmetry group, the regular point systems are subdivided into so-called Wyckoff positions. Wyckoff positions can be free (a region in three-dimensional space), or can be specified as a plane, or as a straight line, or as a point in three-dimensional space (point position). The basis atoms of the substance under study are located at specific Wyckoff positions within the framework of the topology defined by

the spatial symmetry group. In total, in 230 spatial symmetry groups, there are 1731 Wyckoff positions [18-19].

The crystalline structure means the finite set of regular systems of atoms in a given Fedorov group. The crystalline structure is described by the following characteristics:

- spatial symmetry group;
- metric parameters of a unit cell (Bravais parallelepiped), to which are the constant lattices and angles between them;
- Wyckoff 's positions of the centers of the basis atoms that make up this structure, including their indices denoting the multiplicity of positions and the numerical values of the free coordinates of these positions in the unit cell.

The coordinates of all atoms of the crystalline structure can be calculated on the basis of these data and using Fedorov symmetry groups or international crystallographic tables.

Usually, when the crystal structures are modeled, the coordinates of the basis atoms are represented in relative coordinates in an oblique system:

$x'_{1i} = \frac{x_{1i}}{a}, x'_{2i} = \frac{x_{2i}}{b}, x'_{3i} = \frac{x_{3i}}{c}$. If the origin is at the top of the unit cell, they are expressed in fractions of the elementary translations. These coordinates characterize the ratio of the lengths of the oblique projections of the radius vector coming from the origin to the lengths of the basis vectors a, b, c – elementary translations (parameters) of the Bravais lattice (unit cell). The relative coordinates of the i -th atom are positive numbers in the range from 0 to 1. Further, we will not use strokes, considering the coordinates of the atoms relative by the formula (1):

$$r_i = x_{1i}a + x_{2i}b + x_{3i}c \quad (1)$$

The point that lies in an arbitrary cell of the crystal corresponds to the vector $r + ua + vb + wc$, where u, v and w are integer numbers of translations to which this cell is separated from the origin (depending on the direction of translations,

the numbers can be either positive, and negative).

Unit cell parameters and relative atomic coordinates completely determine the crystal

$$\rho(r_i r_j) = \sqrt{\left(|a|(x_{1i} - x_{1j})\right)^2 + \left(|b|(x_{2i} - x_{2j})\right)^2 + \left(|c|(x_{3i} - x_{3j})\right)^2} \quad (2)$$

In the general case, the square of the distance between the centers of the atoms is calculated by the formula (3):

$$\begin{aligned} \rho(r_i r_j)^2 = & \left(|a|(x_{1i} - x_{1j})\right)^2 + \left(|b|(x_{2i} - x_{2j})\right)^2 + \left(|c|(x_{3i} - x_{3j})\right)^2 \\ & + 2|b||c|(x_{2i} - x_{2j}) \cdot (x_{3i} - x_{3j})\cos\alpha + |a||c|(x_{1i} - x_{1j}) \\ & \cdot (x_{3i} - x_{3j})\cos\beta + |a||b|(x_{1i} - x_{1j}) \cdot (x_{2i} - x_{2j})\cos\gamma \end{aligned} \quad (3)$$

where α , β , γ are the interplane angle. To construct the images of basis atoms, symmetry operations are applied for each Fedorov group. A symmetry operator, R , acts on a point r so that: $r'=R \cdot r$, in which R represents a 3×3 matrix by the formula (4):

$$x = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \quad (6)$$

X , Y , and Z are converted into fractional crystallographic coordinates (x,y,z) in order to perform crystallographic operations, and inversely, geometric computations are more easily performed in Cartesian space. In orthonormal systems (cubic, tetragonal, and orthorhombic) the coordinate transformation reduces to a simple division of the coordinate values by the corresponding cell constants. For example,

$x=X/a$, and $X=ax$. In the case of a generic oblique crystallographic system, the transformation is described by a matrix operation: let the atomic positions be described by a Cartesian coordinate vector X by the formula(5):

$$X = \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} \quad (5)$$

and the fractional coordinate vector in the crystallographic system be x by the formula (6):

$$M^{-1} = \begin{pmatrix} a & ab \cos\gamma & \frac{c \cos\beta}{\sin\gamma} \\ 0 & b \sin\gamma & \frac{c(\cos\alpha - \cos\beta \cos\gamma)}{\sin\gamma} \\ 0 & 0 & \frac{V}{ab \sin\gamma} \end{pmatrix} \quad (7)$$

structure. If we consider the orthogonal basis a , b , c , then the distance between the atoms i and j will be calculated by the formula (2):

With the systems having the same origin the operation reduces to $x = MX$ and its

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \quad (4)$$

inversion to $X = M^{-1}x$, with M the de-orthogonalization matrix, and its inverse M^{-1} the orthogonalization matrix. There are multiple choices of M depending on the order and selection of the axis rotations. The following convention is followed by most crystallographic programs:

- Cartesian axis A is collinear with crystallographic axis a ;
- B is collinear with $(a \times b) \times A$;
- C is collinear with $(a \times b)$.

Using the above convention and we get the formula (7):

with

$$V = \sqrt[2]{abc(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha \cos\beta \cos\gamma)}$$

or

$$V = \det(M^{-1})$$

$$M = \frac{\text{adj}(M^{-1})}{\det(M^{-1})} \quad (8)$$

The deorthogonalization matrix M , can be obtained by inversion of M^{-1} following Cramer's rule get by the formula (8):

and reduces to (9):

$$M^{-1} = \begin{pmatrix} a & b \cos\gamma & \left(\frac{b \cos\gamma c (\cos\alpha - \cos\beta \cos\gamma)}{\sin\gamma} \right) \frac{1}{V} \\ 0 & b \sin\gamma & - \frac{ac(\cos\alpha - \cos\beta \cos\gamma)}{V \sin\gamma} \\ 0 & 0 & \frac{ab \sin\gamma}{V} \end{pmatrix} \quad (9)$$

3. Converting of the coordinates of the basis atoms in a unit cell of crystalline β -Ga₂O₃, specified in a monoclinic crystallographic system, in the laboratory Cartesian coordinates

The above techniques will be applied to crystalline β -Ga₂O₃ for construction in the laboratory Cartesian coordinate system associated with a computer-generated author program of an atomic environment within a unit cell β -Ga₂O₃.

The monoclinic β -Ga₂O₃ [20] with space group C2/m has two nonequivalent Ga sites: Ga1 is the sixfold-coordinated site, while Ga2 is the fourfold. In addition, there are three nonequivalent O sites, which are threefold-coordinated O1 and O3 sites, while O2 is the four-fold. The lattice parameters at

room temperature are measured to be $a = 12.23 \text{ \AA}$, $b = 3.04 \text{ \AA}$, $c = 5.80 \text{ \AA}$

and the unique axis $\beta=103.7^\circ$ (angle between a and c axes) unit cell. The unit cell contains four formula units, eight Ga atoms and twelve O atoms are evenly distributed into two Ga and three O nonequivalent sites

at positions $4i: (000, \frac{1}{2}, 0) \pm (x0z)$ [20-23] (Table 1).

Table 2 contains selected geometric parameters.

Table 1.
Nonequivalent atomic fractional positions of β -Ga₂O₃ [20]

Atom	x	y	z	Coordination
Ga1	0.09050 (2)	0	0.79460 (5)	fourfold
Ga2	0.15866 (2)	1/2	0.31402 (5)	sixfold
O1	0.1645 (2)	0	0.1098 (3)	threefold
O2	0.1733 (2)	0	0.5632 (4)	fourfold
O3	0.0041 (2)	1/2	0.2566 (3)	threefold

Table 2.

Selected geometric parameters (\AA , $^\circ$) [20]

Ga1-O1	1.835 (2)	Ga2-O1	1.937 (1)
Ga1-O2	1.863 (2)	Ga2-O2	2.074 (1)
Ga1-O3	1.833 (1)	Ga2-O2	2.005 (2)
O1-Ga1-O2	119.59 (9)	Ga2-O3	1.935 (2)

O1-Ga1-O3	106.79 (7)	O1-Ga2-O2	91.87 (7)
O2-Ga1-O3	105.92 (7)	O1-Ga2-O3	94.66 (7)
O3-Ga1-O3	111.9 (1)	O2-Ga2-O2	94.14 (6)
O1-Ga2-O1	103.22 (9)	O2-Ga2-O2	80.91 (6)
O1-Ga2-O2	80.91 (6)	O2-Ga2-O3	91.95 (7)

The fractional crystallographic coordinates of the atoms shown in Table 1 were converted to Cartesian coordinates using the algorithm described in paragraph 2. Their values are shown in Fig. 1, which is a screen shot of an authoring computer program cre-

ated in the Delphi programming environment [24-28]. Two nonequivalent Ga atoms [Ga1 and Ga2] and three nonequivalent O atoms [O1, O2 and O3] are showed on Fig. 2.

Nº	x	y	z	sort
1	0,00980027299030384	3,49024519729932E-16	4,47755899835075	1 Ga1
2	1,50905469516035	1,52	1,76949795703763	2 Ga2
3	1,86100699505957	4,82291621776322E-17	0,618721341579301	3 O1
4	1,34581298558789	2,47383097800023E-16	3,17362349341951	4 O2
5	-1,02117977115405	1,52	4,18904777167625	5 O3

Fig. 1. Laboratory Cartesian coordinates of five atoms in nonequivalent atomic positions

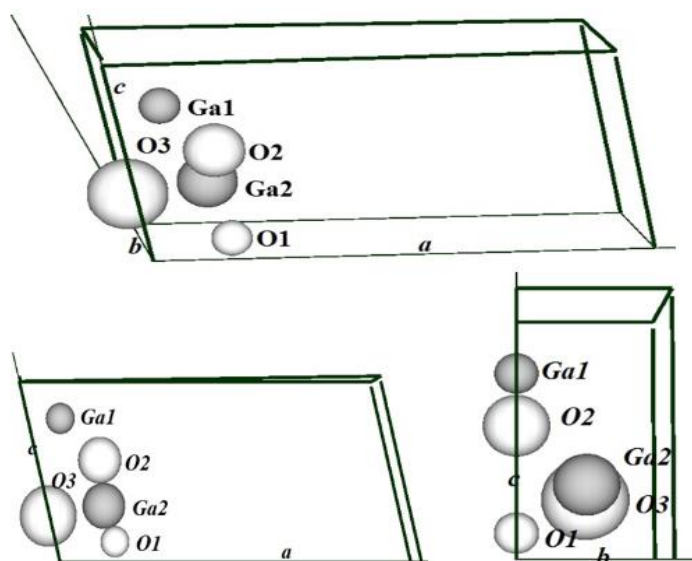


Fig. 2. Unit cell of β -Ga₂O₃, which possesses two nonequivalent Ga sites: Ga1, Ga2 (gray spheres) and three nonequivalent O-sites: O1, O2 and O3 (white spheres) in different angles of observation. The image is built in a laboratory Cartesian coordinate system using an author's computer program

To construct the images of basis (nonequivalent) atoms, symmetry operations are applied for $C2/m$ Fedorov group:

$$\begin{array}{ll}
 1 & x, y, z & 1 \\
 2 & \bar{x}, y, \bar{z} & 2 (0, y, 0) \\
 3 & \bar{x}, \bar{y}, \bar{z} & \bar{1} (0, 0, 0) \\
 4 & x, \bar{y}, z & m (x, 0, z)
 \end{array}$$

$C2/m$ Symmetry Operators

$$\begin{array}{l}
 5 \quad \frac{1}{2} + x, \frac{1}{2} + y, z \quad t_c \left[\frac{1}{2}, \frac{1}{2}, 0 \right] \\
 6 \quad \frac{1}{2} - x, \frac{1}{2} + y, \bar{z} \quad 2_1 \left(\frac{1}{4}, y, 0 \right) \left[0, \frac{1}{2}, 0 \right]
 \end{array}$$

$$7 \frac{1}{2} - x, \frac{1}{2} - y, z \quad \bar{1} \left(\frac{1}{4}, \frac{1}{4}, 0 \right)$$

$$8 \frac{1}{2} + x, \frac{1}{2} - y, z \quad a \left(x, \frac{1}{2}, z \right) \left[\frac{1}{2}, 0, 0 \right]$$

$$T = \begin{pmatrix} -a & 0 & c \cos\beta \\ 0 & b & 0 \\ 0 & 0 & c \sin\beta \end{pmatrix} \quad (10)$$

The lattice vectors of the unit cell are given in the (x, y, z) -system as:

$$a_1 = T(1, 0, 0)$$

$$a_2 = T(0, 1, 0)$$

$$a_3 = T(0, 0, 1)$$

As a result, the elementary cell is filled with thirty atoms, which are shown in fig.3. Their values are shown in Fig. 4, which is a screen shot of an authoring computer program

with the transformation matrix given by the formula (10):

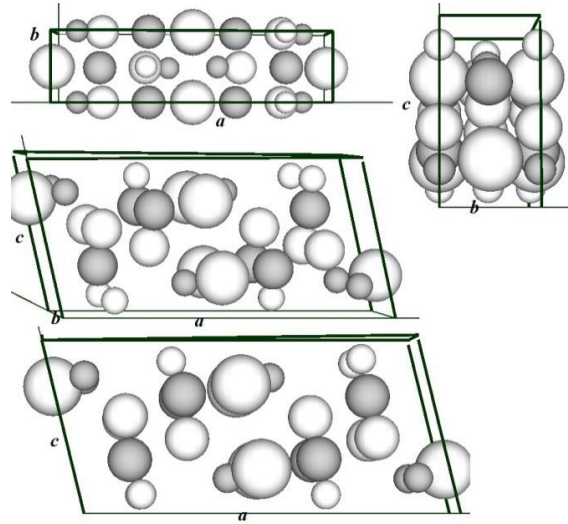


Fig. 3. Unit cell of β -Ga₂O₃ in different angles of observation.

The image is built in a laboratory Cartesian coordinate system using an author's computer program

Table 3.

Geometric parameters (Å, °) that are calculated using laboratory Cartesian coordinates

Ga1-O1	1.835
Ga1-O2	1.867
Ga1-O3	1.859
O1-Ga1-O2	119.59
O1-Ga1-O3	106.79
O2-Ga1-O3	106.77
O3-Ga1-O3	114.72
O1-Ga2-O1	103.26
O1-Ga2-O2	80.89
Ga2-O1	1.939
Ga2-O2	2.076

Ga2-O2	2.009
Ga2-O3	1.889
O1-Ga2-O2	91.95
O1-Ga2-O3	94.43
O2-Ga2-O2	94.15
O2-Ga2-O3	80.85
O2-Ga2-O3	92.20

We have transformed the coordinate from the crystallographic monoclinic system to Cartesian, and the geometry of the crystal does not distort (Tabl. 3). So, our actions were correct and the obtained set of atomic coordinates can be used to calculate the characteristics of the electronic subsystem of the crystal.

Nº	x	y	z	sort
1	0,00980027299030384	3,49024519729932E-16	4,47755899835075	1
2	1,50905469516035	1,52	1,76949795703763	2
3	1,86100699505957	4,82291621776322E-17	0,618721341579301	3
4	1,34581298558789	2,47383097800023E-16	3,17362349341951	4
5	-1,02117977115405	1,52	4,18904777167625	5
6	4,73153847982911	1,52	1,1574258976356	1
7	3,23228405765906	3,01313667309765E-16	3,86548693894871	2
8	2,88033175775984	1,52	5,01626355440705	3
9	3,39552576723152	1,52	2,46136140256684	4
10	5,09382022884595	3,26535147202658E-16	4,18904777167625	5
11	11,8775185239735	1,52	1,4459371243101	5
12	0,00980027299030403	3,04	4,47755899835075	1
13	1,86100699505957	3,04	0,618721341579301	3
14	1,34581298558789	3,04	3,17362349341951	4
15	10,8465384798291	3,04	1,1574258976356	1
16	9,34728405765906	1,52	3,86548693894871	2
17	8,99533175775984	3,04	5,01626355440705	3
18	9,51052576723152	3,04	2,46136140256684	4
19	6,1248002729903	1,52	4,47755899835075	1
20	7,62405469516035	3,04	1,76949795703763	2
21	7,97600699505957	1,52	0,618721341579301	3
22	7,46081298558789	1,52	3,17362349341951	4
23	5,76251852397346	3,04	1,4459371243101	5
24	10,8465384798291	9,02210374434031E-17	1,1574258976356	1
25	8,99533175775984	3,91016394995703E-16	5,01626355440705	3
26	9,51052576723152	1,91862459373313E-16	2,46136140256684	4
27	5,09382022884595	3,04	4,18904777167625	5
28	5,76251852397346	1,12710409970678E-16	1,4459371243101	5
29	3,23228405765906	3,04	3,86548693894871	2
30	7,62405469516035	1,37931889863571E-16	1,76949795703763	2

Fig. 4. Laboratory Cartesian coordinates of thirty atoms in unit cell

Conclusions

The technique of converting of the coordinates of the basis atoms in a unit cell of crystal, specified in a crystallographic system, in the Cartesian coordinates is described. This technique is applied to crystalline β -Ga₂O₃ for construction in the laboratory Cartesian coordinate system associated with a computer-generated author program of an atomic environment within a unit cell β -Ga₂O₃. Conversion of the coordinates from the crystallographic monoclinic system to Cartesian did not distort the geometry of the crystal.

References

1. Stepanov, S.I., Nikolaev, V.I., Bourgov, V.E., Romanov, A.E. Gallium Oxide: properties and applications – a review. *Rev. Adv. Mater. Sci.* **2016**, *44*, 63-86.
2. Pearton S.J., Ren Fan, Tadjer Marko, Kim Jihyun Perspective: Ga₂O₃ for ultra-high power rectifiers and MOSFETS. *J. Appl. Phys.* **2018**, *124*(22), 220901.
3. Galazka Z. β -Ga₂O₃ for wide-bandgap electronics and optoelectronics. *Semicond. Sci. Technol.* **2018**, *33*(11), 113001.
4. Park J., McClintock R., Razeghi M. Ga₂O₃ metal-oxide-semiconductor field effect transistors on sapphire substrate

- by MOCVD. *Semicond. Sci. Technol.* **2019**, *34*(8), 08LT01.
5. K.D. Chabak et.al. Lateral β -Ga₂O₃ field effect transistors. *Semicond. Sci. Technol.* **2020**, *35*, 013002.
 6. He H., Orlando R., Blanco M.A., Pandey R., Amzallag E., Baraille I., Rerat M. First-principles study of the structural, electronic, and optical properties of Ga₂O₃ in its monoclinic and hexagonal phases. *Phys. Rev.* **2006**, *B74*, 195123.
 7. He H., Blanco M.A., Pandey R. Electronic and thermodynamic properties of β -Ga₂O₃. *Appl. Phys. Lett.* **2006**, *88*(26), 261904.
 8. Higashiwaki M., Sasaki K., Murakami H., Kumagai Y., Koukitu A., Kuramata A., Masui T., Yamakoshi S. Recent progress in Ga₂O₃ power devices. *Semicond. Sci. Technol.* **2016**, *31*, 034001.
 9. Mastro M.A., Kuramata A., Calkins J., Kim J., Ren F., Pearton S.J. Opportunities and future directions for Ga₂O₃. *ECS J. Solid State Sci. Technol.* **2017**, *6*, P356-P359.
 10. Higashiwaki M., Murakami H., Kumagai Y., Kuramata A. Current status of Ga₂O₃ power devices. *Jpn. J. Appl. Phys.* **2016**, *55*, 1202A1.
 11. Higashiwaki H., Kuramata A., Murakami H., Kumagai Y. State-of-the-art technologies of gallium oxide power devices. *J. Phys. D Appl. Phys.* **2017**, *50*, 333002.
 12. Peelaers H., Van de Walle C.G. Brillouin zone and band structure of β -Ga₂O₃. *Phys. Stat. Solidi* **2015**, *B252*, 828–832.
 13. Varley J. B., Janotti A., Franchini C., Van de Walle C.G. Role of self-trapping in luminescence and p-type conductivity of wide-band-gap oxides. *Phys. Rev.* **2012**, *B85*, 081109(R).
 14. Furthmüller J., Bechstedt F. Quasiparticle bands and spectra of Ga₂O₃ polymorphs. *Phys. Rev.* **2016**, *B93*, 115204.
 15. Mohamed M., Janowitz C., Unger I., Manzke R., Galazka Z., Uecker R., Fornari R., Weber J.R., Varley J.B., Van de Walle C. G. The electronic structure of β -Ga₂O₃. *Appl. Phys. Lett.*, **2010**, *97*, 211903.
 16. Dong L., Jia R., Xin B., Peng B., Zhang Y. et al. Effects of oxygen vacancies on the structural and optical properties of β -Ga₂O₃. *Sci. Rep.* **2017**, *7*, 40160.
 17. Shaskolskaya M.P. Crystallography / M.P. Shaskolskaya. - M.: Higher school, **1996**. - 459 p.
 18. Henry N., Lonsdale K. *International tables for X-ray crystallography* / N. Henry, K. Lonsdale Symmetry Groups The Kynoch Press, Birmingham, **1999**; Vol. 1, p. 372.

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Summary. One of the most important areas of modern technology is the creation of new structural materials with predetermined properties. Along with industrial methods for their preparation and technologies associated with the artificial growth of crystalline structures, various methods of computer modeling of new materials have recently become increasingly important. Such approaches can significantly reduce the number of full-scale experiments. Many applications of the computational materials science are related to the need to establish a relationship between structure and electronic characteristics, and other physical properties of crystals. This article on the example of crystalline β -Ga₂O₃ presents the algorithms used in the converting of the coordinates of the basis atoms in a unit cell of crystal, specified in a crystallographic system, in the Cartesian coordinates for the computational experiment.

Key words: crystalline β -Ga₂O₃, unit cell, basis atoms, monoclinic crystallographic system, Cartesian coordinates

МЕТОДОЛОГІЯ ПЕРЕРАХУНКУ КООРДИНАТ АТОМІВ БАЗИСУ В ЕЛЕМЕНТАРНІЙ КОМІРЦІ КРИСТАЛІЧНОГО β -Ga₂O₃, ЩО ЗАДАНІ В МОНОКЛІННІЙ КРИСТАЛОГРАФІЧНІЙ СИСТЕМІ, В ЛАБОРАТОРНІ ДЕКАРТОВІ КООРДИНАТИ ДЛЯ КОМП'ЮТЕРНОГО ЗАСТОСУВАННЯ

Резюме. Одним із найважливіших напрямків сучасних технологій є створення нових конструкційних матеріалів з наперед заданими властивостями. Поряд з промисловими способами їх отримання і технологіями, пов'язаними з штучним вирощуванням кристалічних структур, останнім часом все більшого значення набувають різні методи комп'ютерного моделювання нових матеріалів. Такі підходи дозволяють істотно скоротити число натурних експериментів. Багато задач прикладного обчислювального матеріалознавства пов'язані з необхідністю встановлення взаємозв'язку між структурою та електронними характеристиками, іншими фізичними властивостями кристалів. У статті на прикладі кристалічного β -Ga₂O₃ представлені алгоритми, використовувані при проектуванні кристалічних структур, що дозволяють досліджувати їх властивості в обчислювальному експерименті.

Ключові слова: кристалічний β -Ga₂O₃, елементарна комірка, атомні базиси, моноклінна кристалографічна система, декартові координати

МЕТОДОЛОГИЯ ПЕРЕРАСЧЕТА КООРДИНАТ АТОМОВ БАЗИСА В ЭЛЕМЕНТАРНОЙ ЯЧЕЙКЕ КРИСТАЛЛИЧЕСКОЙ β -Ga₂O₃, ЗАДАНИЕ В МОНОКЛИННОЙ КРИСТАЛЛОГРАФИЧЕСКОЙ СИСТЕМЕ, В ЛАБОРАТОРНЫЕ ДЕКАРТОВЫЕ КООРДИНАТЫ ДЛЯ КОМПЬЮТЕРНОГО ПРИМЕНЕНИЯ.

Резюме. Одним из важнейших направлений современных технологий является создание новых конструкционных материалов с заранее заданными свойствами. Наряду с промышленными способами их получения и технологиями, связанными с искусственным выращиванием кристаллических структур, в последнее время все большее значение приобретают различные методы компьютерного моделирования новых материалов. Такие подходы позволяют существенно сократить число натурных экспериментов. Многие задачи прикладного вычислительного материаловедения связанные с необходимостью установления взаимосвязи между структурой и электронными характеристиками, другими физическими свойствами кристаллов. В статье на примере кристаллического β -Ga₂O₃ представлены алгоритмы, используемые при проектировании кристаллических структур, позволяющие исследовать их свойства в вычислительном эксперименте.

Ключевые слова: кристаллический β -Ga₂O₃, элементарная ячейка, атомные базисы, моноклинная кристаллографическая система, декартовы координаты