CHEMISTRY AND TECHNOLOGY OF INORGANIC MATERIALS

ХИМИЯ И ТЕХНОЛОГИЯ НЕОРГАНИЧЕСКИХ МАТЕРИАЛОВ

ISSN 2686-7575 (Online)

https://doi.org/10.32362/2410-6593-2021-16-4-363-371

UDC 548.736

RESEARCH ARTICLE

Use of a 4-circle goniometer for neutron and X-ray diffractometer in the study of single crystals

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Abstract

Objectives. *This study described the 4-circle goniometer Syntex P1N and its possible applications in X-ray and neutron structure analysis of single crystals.*

Methods. *The 4-circle goniometer Syntex P1N, due to its high-precision mechanical characteristics and individual components from domestic equipment (sets of DRON type X-ray diffractometers), formed the basis for developing an instrument complex for X-ray and neutron-structure studies.*

Results. *The neutron diffractometer was upgraded based on the Syntex P1N goniometer. Therefore, the $^{10}BF_3$-based end neutron counter, included in the diffractometer kit, was replaced by the ^{3}He-based domestic side counter, SNM-16. Such a significant reduction in the linear dimensions of the detector allowed us to expand the range of measured angles of 2θ from 90° to 140° and increase the accuracy of the measured interplanar distances accordingly. The goniometer was adjusted relative to the primary neutron beam by placing it on a specially designed plate. Highly accurate measured parameters of the unit cell and the intensity of the reflexes were achieved by optimizing the installation geometry and the protection of the goniometer and detector. Based on the Syntex P1N goniometer, an instrument complex for X-ray diffraction studies has also been developed. Both the developed X-ray and the upgraded neutronography facilities were used to perform experiments to measure the unit cell parameters, the coordinates of atoms, and the parameters of their thermal vibrations on several crystals of domestic synthetic samples: diamond C, silicon Si, halite, or rock salt NaCl, and corundum a-Al_2O_3. An excellent correlation was achieved by comparing the data obtained with the corresponding chemical crystals' parameters and reference samples recommended by the International Union of Crystallographers.*

Conclusions. *This paper described a neutron installation and a Syntex P1N neutron diffractometer for the study of single crystals. Based on the latter, an instrument complex for X-ray diffraction studies has also been developed. Experiments on standard samples have shown a high level of accuracy in measuring the lattice parameters, the coordinates of atoms, and the parameters of their thermal vibrations on both the X-ray and neutron diffractometers.*
Keywords: *install neutron diffraction, neutron diffraction, crystal lattice parameters, a goniometer, standard samples, the coordinates of atoms, thermal vibrations*

For citation: Sarin V.A. Use of a 4-circle goniometer for neutron and X-ray diffractometer in the study of single crystals. *Tonk. Khim. Tekhnol. = Fine Chem. Technol.* 2021;16(4):363–371 (Russ., Eng.). https://doi.org/10.32362/2410-6593-2021-16-4-363-371

НАУЧНАЯ СТАТЬЯ

Использование 4-х кружного гониометра для нейтронного и рентгеновского дифрактометра при исследовании монокристаллов

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Аннотация

Цели. *Модернизировать нейтронный дифрактометр с помощью 4-х кружного гониометра «Синтекс P1N» и оценить особенности его применения при проведении рентгеноструктурного и нейтроноструктурного анализа монокристаллов с возможностью использования для этих целей аналогичных гониометров.*
Методы. *4-х кружный гониометр «Синтекс P1N» и отдельные узлы российского оборудования из комплектов рентгеновских дифрактометров типа ДРОН легли в основу разработки приборного комплекса для рентгеноструктурных и нейтроноструктурных исследований.*
Результаты. *На основе гониометра «Синтекс P1N» была выполнена модернизация нейтронного дифрактометра. Входивший в комплект дифрактометра торцевой нейтронный счетчик на основе $^{10}BF_3$ был заменен российским боковым счетчиком СНМ-16 на основе ^3He. Существенное уменьшение линейных размеров детектора позволило расширить диапазон измеряемых углов по 2θ с 90° до 140° и, соответственно, повысить точность измеряемых межплоскостных расстояний. Благодаря оптимизации геометрии установки и защиты гониометра и детектора, была достигнута высокая точность измеряемых параметров элементарной ячейки и интенсивностей рефлексов. На основе гониометра «Синтекс P1N» был также разработан приборный комплекс для рентгеноструктурных исследований. Как на разработанной рентгеновской, так и на модернизированной нейтронографической установках были осуществлены эксперименты по измерению параметров элементарной ячейки, координат атомов и параметров их тепловых колебаний на ряде кристаллов: алмаз C, кремний Si, галит NaCl, корунд α-Al_2O_3. Сравнение полученных данных с соответствующими параметрами кристаллов химических веществ и стандартных образцов, рекомендуемых Международным союзом кристаллографов, показало очень хорошее совпадение.*

Выводы. *В настоящей работе дается описание нейтронографической установки и нейтронного дифрактометра «Синтекс P1N» для исследования монокристаллов. На основе последнего разработан приборный комплекс для рентгеноструктурных исследований. Эксперименты на стандартных образцах показали высокий уровень точности измерений параметров решетки, координат атомов и параметров их тепловых колебаний как на рентгеновском, так и на нейтронном дифрактометрах.*

Ключевые слова: *нейтронографическая установка, нейтронный дифрактометр, кристалл, параметры решетки, гониометр, стандартные образцы, координаты атомов, тепловые колебания*

Для цитирования: Сарин В.А. Использование 4-х кружного гониометра для нейтронного и рентгеновского дифрактометра при исследовании монокристаллов. *Тонкие химические технологии*. 2021;16(4):363–371. https://doi.org/10.32362/2410-6593-2021-16-4-363-371

INTRODUCTION

In experimental neutron studies at pre-reactor research facilities, it is sometimes necessary to use the same equipment on different devices, including those not necessarily located in the reactor hall. Such a situation, for example, occurs during annual maintenance or prolonged reactor shutdown. The need for complex equipment usage is usually due to the uniqueness of the neutronographic installation.

EXPERIMENTAL

The neutron diffractometer Syntex P1N (*Syntex*, USA) used for carrying out neutron-structure experiments was included in the neutronography unit for the study of single crystals located on the horizontal channel of the VVR-c nuclear reactor (the water-water reactor, target, was manufactured in N.A. Dollezhal Order of Lenin Research and Design Institute of Power Engineering, Moscow, USSR) in the Branch of L.A. Karpov Research Institute of Physics and Chemistry. By design and function, the neutron diffractometer is analogous to the X-ray diffractometer.

For the diffractometer location in the reactor hall, a geometric scheme of the neutronographic installation (from the primary neutron beam to the crystal monochromator to the secondary neutron beam and finally to the sample) was implemented (Fig. 1), where the secondary neutron beam is oriented relative to the primary beam at an angle of 90° [1].

Based on the function of the diffractometer and the fact that no X-ray source was available, the X-ray detector was replaced with a neutron detector. The diffractometer's goniometer was placed in a special housing protected from the background reactor radiation. The housing walls were double-welded steel sheets, with the cavities between the walls filled with water-diluted boric acid. The selected installation geometry and the diffractometer's goniometer placement increased the area of diffraction reflections, and consequently, the experiment time, making it possible to use standard X-ray programs to clarify the diffraction reflection position in the reciprocal space.

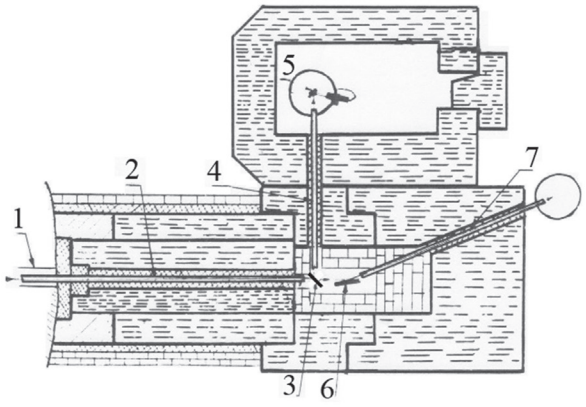

Fig. 1. Layout of the neutron diffractometric installation (cross-section at the level of the horizontal channel of the reactor) [1].
1 – reactor channel; 2, 4, 7 – collimators;
3, 6 – monochromator crystals; 5 – goniometer of the Syntex P1N diffractometer.

The reactor hall neutrons background in the "house" decreased sharply, resulting in several pulses per minute, making it possible to replace the heavy protection of the neutron detector with a thin layer of cadmium that protects the detector from gamma radiation. Later, the $^{10}BF_3$-based end neutron counter, included in the diffractometer kit, was replaced by a Russian ^3He-based side counter. The measured 2θ angles range expanded from 90° to 140° with a corrsponding increase in the accuracy of the measured interplanar distances due to significant reductions in the linear dimensions of the detector. In addition, the goniometer was aligned relative to the primary neutron beam by was placing it on a specially designed plate. In real-world applications, it is common practice to use the unit cell parameters of a crystal previously studied by X-ray diffraction in neutron diffractometers installed directly in the reactor hall with heavy detector protection from background neutrons, having a small range of measured 2θ angles, due to the low accuracy of determining interplanar distances and angles between the crystallographic axes of the crystal. However, by optimizing the installation geometry and goniometer and detector protections, accurately measured unit cell parameters and intensity of reflexes were achieved in the designed neutron diffractometer. In particular, an elementary cell's parameters were successfully determined only from neutron data by selecting a spatial group (sp. gr.), deciphering it using the "direct method," and refining the crystal structure of unknown crystals.

At the same time, to ensure the diffractometer's accuracy, it was required to understand its fundamental characteristics by benchmarking it against crystals recommended by the commission of the International Union of Crystallographers and used in international practice [2]. Such experiments on measuring the parameters of the unit cell were carried out on several crystals of Russian synthetic samples: diamond C, silicon Si, halite, or rock salt NaCl, and corundum α-Al_2O_3. A comparison between the obtained results and the unit cell parameters of crystals of chemicals and standard samples recommended by the International Union of Crystallographers showed an excellent correlation (Table 1).

In the experiments under consideration, the axes parameters and the angles between the axes were refined while studying highly symmetric crystals. In this case, the crystals were considered triclinic. Therefore, the symmetry relations were not superimposed, and the values of the parameters of the equivalent axes were not averaged. The results obtained in Table 1 and a comparison of the parameter values for each of the axes and the angles between the axes further confirmed the accuracy of determining these parameters using the goniometer of the Syntex P1N diffractometer. Furthermore, in the measurements taken from the same batch of quartz samples on the developed Syntex P1N neutron diffractometer and the same type of X-ray diffractometer, a very good agreement between the results of determining the structural parameters of single quartz crystals was achieved [4].

These results further justified with a crystallogfafic viewpoint the need to design a new X-ray instrument complex based on the Syntex P1N neutron diffractometer and consist of a goniometer, a counting rack, a control computer, and a Russian X-ray equipment taken from a DRON type diffractometer configuration and including a high-voltage power source, an X-ray tube with a molybdenum anode, and

Table 1. Comparison of the unit cell parameters of crystals measured on a neutron diffractometer Syntex P1N on synthetic samples with their standard values

Substance	*a*, Å	*b*, Å	*c*, Å	α, °	β, °	γ, °
Diamond, C Adopted in [3]	3.566(2) 3.568	3.568(2) = *a*	3.565(2) = *a*	89.98(4) 90.00	89.98(4) 90.00	89.98(4) 90.00
Silicon, Si Standard SRM* 640c	5.431(2) 5.4312(1)	5.430 (2) = *a*	5.431(2) = *a*	90.02(2) 90.00	89.99(2) 90.00	90.01(2) 90.00
Halite, NaCl Adopted in [3]	5.639(2) 5.640	5.638(2) = *a*	5.638(2) = *a*	89.98(3) 90.00	90.03(3) 90.00	90.02(3) 90.00
Corundum, α-Al_2O_3 Standard SRM 674	4.759(1) 4.7589(1)	4.760(1) = *a*	12.991(4) 12.9917(7)	90.02(2) 90.00	89.99(2) 90.00	119.99(2) 120.00

* SRM – standard reference material.

a desktop for a goniometer. Based on the experiment results performed using the Syntex P1N neutron diffractometer of this neutronographic installation and the X-ray instrument complex, an installation with a HUBER 511/424 goniometer was manufactured and put into operation (Fig. 2).

Fig. 2. HUBER 511/424 goniometer with vertical "side" detector in the "house."

To check the operability and stability of such an X-ray instrument complex, control X-ray diffraction experiments were also carried out on single crystals of Si, NaCl, SiO_2, etc. For comparison, the coordinates of atoms and the individual parameters of the thermal vibrations of the atoms, refining by least squares method, were taken. This was done as not only the value of *R*-factors obtained as a result of the refinement of the coordinates of atoms, but the individual factors of the thermal vibrations of atoms B_j characterize the accuracy of measurements of the intensities of the reflexes in the whole range of values of sinθ/λ. The results of refining the values of the isotropic thermal factors of the NaCl crystal atoms obtained in this study and their comparison with the data of [5] are shown in Table 2.

A somewhat more complex comparison was performed for single crystals of silicon and the α-SiO_2 piezoelectric. The quality of single silicon crystals considered in this study depended on the method of preparing the crystal for the experiment. Initially, the samples were taken from a batch of large crystals grown without dislocation. Cubes with rib sizes of 10 and 2 mm were then cut out of large ingots for neutron and X-ray experiments and then rolled on an air gurney to prepare spherical samples with diameters of 6 and 0.3 mm. After running in, the crystals were polished to remove the disturbed top layer. Finally, several crystals were subjected to deformation by mechanical pressure treatment under a press. In neutronographic and X-ray experiments on a Syntex P1N neutron diffractometer and the X-ray complex, the Si atom's thermal vibration parameter values depend on the method of processing the single crystal before the experiment. The corresponding data are given in Table 3. This allows us to conclude that the absolute values of thermal corrections in diffraction experiments depend on the method of crystal growth, its quality, and the types of pre-processing. Therefore, it was pretty difficult to compare the thermal vibration parameters obtained by different authors on samples with different histories.

In [4], the coordinates of quartz atoms obtained in different laboratories were compared on the different but same types of goniometers in X-ray and neutronographic experiments. However, the parameters of thermal vibrations of atoms were not considered in [4]. In this paper, an attempt was made to evaluate these parameters, given by different authors, from the point of view of the experiment's reliability on the X-ray instrument complex under consideration.

Table 2. Comparison of the parameters of individual isotropic thermal vibrations B_j for NaCl crystals obtained at $T = 296$ K in this study and [5]

Reference	Ion	*x*/*a*	*y*/*b*	*z*/*c*	B_j, Å²	R_w	N_u
This study	Na^+	0	0	0	1.77(1)	0.0088	50
This study	Cl^-	1/2	0	0	1.48(1)	0.0088	50
[5]	Na^+	0	0	0	1.689(24)	0.022	55
[5]	Cl^-	1/2	0	0	1.357(17)	0.022	55

Note: R_w is a weighted confidence factor of the specified structure; N_u is the number of independent reflexes averaged over the intensities.

Table 3. Values of the thermal parameter B_j of the Si atom depending on the type of processing of the single crystal

Si single crystal type of processing	Diffraction method	B_j, Å^2	Type of extinction	R_w-factor
Running-in	Neutronographic	0.17	Becker–Coppens (primary)	0.0165
Polishing after running-in	Neutronographic	0.10	Becker–Coppens (primary)	0.0185
Deformation	X-ray	0.52	Becker–Coppens (secondary)	0.0153
Deformation	Neutronographic	0.61	Becker–Coppens (secondary)	0.0079

The α-SiO_2 crystals belong to the space group $P3_121$ (right quartz). Samples for X-ray diffraction experiments on α-SiO_2 crystals were prepared as follows. First, small cubes with an edge of 1.5–2 mm were cut from large quartz plates. Then the cubes were ground in an air gurney into spheres with a radius of ~0.15 mm to prepare samples for the X-ray experiment. The coordinates of the atoms in the α-SiO_2 crystal structure refined after the experiment were compared with the data of [6], where the average values of the coordinates are given after analyzing the results of 18 precision works on the structure of α-SiO_2 crystals.

Data on the comparison of coordinates are shown in Table 4. Plates of natural and synthetic single crystals of α-SiO_2 for further processing and preparation for the experiment were provided by B.N. Kodess, Doctor of Sciences in Physics and Mathematics.

To analyze the values and compare thermal vibrations parameters of the atoms (Table 5), data from [7, 8] were used, in which the most reliable values of thermal vibrations parameters of atoms in the α-SiO_2 crystal structure are given. The * means that the isotropic parameters, B_j were calculated in this study from the root-mean-square displacements of U_{ij} atoms provided in the publication [9]. The ** means that the values of the isotropic root-mean-square displacements of U_j atoms, provided in the publication [10], have been recalculated in this study and incorporated into the parameters of isotropic thermal vibrations B_j (Table 6).

Discrepancies in the parameters of thermal vibrations of atoms (Table 5), obtained by different authors, exceeded 3σ. Nevertheless, similar anisotropic thermal parameters of the ion oscillations were obtained for silicon as a heavier ion. The values for oxygen ions also correctly reflected the relations

Table 4. Comparing the refined coordinates of atoms in the α-SiO_2 crystal structure in this study and those recommended in [6]. Sp. gr. No. 152, $P3_121$, right quartz

Reference	*a*, Å	*c*, Å	Ion	*x*/*a*	*y*/*b*	*z*/*c*
[6]	4.9130(1)	5.4047(1)	Si^{4+}	0.5301(2)	0	1/3
[6]	4.9130(1)	5.4047(1)	O^{2-}	0.4139(5)	0.1466(4)	0.1188(3)
This study^n	4.913(1)	5.404(1)	Si^{4+}	0.5302(2)	0	1/3
This study^n	4.913(1)	5.404(1)	O^{2-}	0.4131(4)	0.1458(4)	0.1192(3)
This study^s	4.913(1)	5.404(1)	Si^{4+}	0.5304(1)	0	1/3
This study^s	4.913(1)	5.404(1)	O^{2-}	0.4131(3)	0.1463(3)	0.1189(2)

Note: The upper index "s" means the results obtained from synthetic crystals, and the upper index "n"—on natural crystals.

Table 5. Comparing the parameters of isotropic thermal vibrations of atoms in α-SiO_2 crystal structure

Reference	Si^{4+}, B_j, Å²	B_j, O^{2-}, Å²	R_w	N_a /N_u
[7][c]	0.50*	1.03*	0.020	383/369
[8][c]	0.36**	0.80**	0.023	1324/279
This study[n]	0.45(1)	0.85(4)	0.0205	1411/318
This study[s]	0.47(1)	0.88(2)	0.0180	1903/439

Note: see Note to Table 4.

Table 6. Comparing the parameters of anisotropic thermal vibrations of atoms in the structure of α-SiO_2 crystal

Reference	Ion	B11	B22	B33	B12	B13	B23
[7][c]	Si^{4+}	0.549	0.428	0.485	1/2B22	0.006	2B13
[7][c]	O^{2-}	1.219	0.873	0.892	0.693	0.238	0.362
This study[n]	Si^{4+}	0.536(9)	0.40(1)	0.439(9)	1/2B22	0.009(6)	2B13
This study[s]	O^{2-}	1.15(3)	0.66(3)	0.88(2)	0.49(2)	0.24(2)	0.12(2)

Note: see Note to Table 4.

of the thermal parameters for both ions. The crystal structure of α-SiO_2 is shown in Fig. 3. It is not trivial to compare the parameters of thermal vibrations for structures obtained by different authors; since the quality of the studied single crystals may be different, the results of studies that are sensitive to the refinement of structural parameters will be different. Such work requires high experimental accuracy and appropriate data processing programs [9]. However, the thermal parameters obtained in this work for natural and synthetic quartz were similar, which may be due to experiments performed with sufficiently high accuracy, good quality of the initial, well prepared single-crystal samples for diffraction study, as well as the same tactics of parameter refinement in the crystallographic calculations.

The close agreements between the specified structural parameters obtained in the control experiments in this work compared to the generally accepted data published in the literature have validated the developed instrument complex for conducting X-ray experiments in the future within the framework of actual problems.

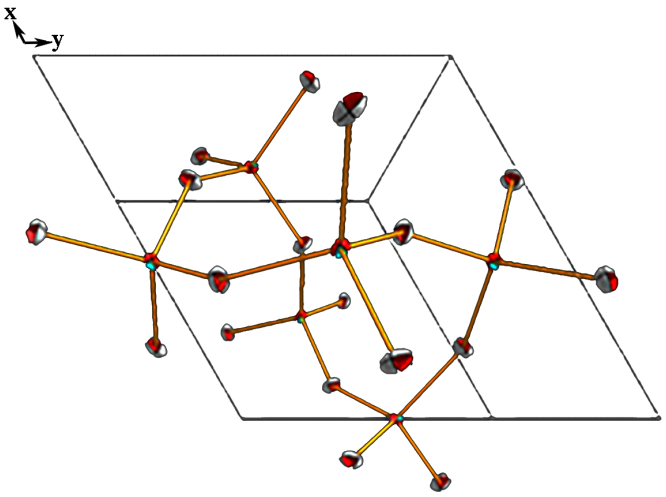

Fig. 3. The crystal structure of α-SiO_2. Viewed along the "c" axis. The image is constructed according to the data of this study[s] (Tables 3–6) using the Diamond graphic program.

CONCLUSIONS

Based on the Syntex P1N goniometer, the neutron diffractometer was upgraded, and an instrument complex for X-ray diffraction studies was developed. Experiments on standard samples have shown a high level of accuracy in measuring the lattice parameters, coordinates of atoms, and parameters of their thermal vibrations on both X-ray and neutron diffractometers.

Acknowledgments

The author is grateful to the leading engineers N.N. Bydanov and E.E. Reader and the adjuster of the instrumentation and control system V.P. Chubykin for the engineering support of all mechanical and electronic work within the framework of this project.

Author's contribution

V.A. Sarin – conducting X-ray and neutron structural experiments, processing results, and writing the text of the article.

The author declares no conflicts of interest.

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The article was submitted: February 11, 2021; approved after reviewing: April 13, 2021; accepted for publication: July 27, 2021.

Translated from Russian into English by N. Isaeva
Edited for English language and spelling by Enago, an editing brand of Crimson Interactive Inc.