

**Oriental Journal of Education****NUMERICAL SIMULATION OF X-RAY DIFFRACTION IN CRYSTALS IN THE STUDY OF OPTICS IN HIGHER EDUCATION INSTITUTIONS****B.A. Abdikamalov***Karakalpak State University named after Berdakh, Professor**Candidate of Physical and Mathematical Sciences*[bakh.abdik@gmail.com](mailto:bakh.abdik@gmail.com)*Nukus, Uzbekistan***R.M. Khojanazarova***Karakalpak State University named after Berdakh, Senior Lecturer**Doctor of philosophy (PhD) pedagogical sciences*[rai.khozha@mail.ru](mailto:rai.khozha@mail.ru)*Nukus, Uzbekistan***G.Z. Babaxova***Nukus State Pedagogical Institute named after Ajiniyaz**Doctoral student of the Department of Methods of Teaching Physics*[bgulziba@bk.ru](mailto:bgulziba@bk.ru)*Nukus, Uzbekistan***ABOUT ARTICLE**

**Key words:** computer demonstration, demonstration experiment, optics, interference and diffraction of light, X-ray diffraction, crystal lattice, structural factor, modeling of radiographs, lauegram, swing radiogram, efficiency, CrystalDiffract, PowderCell, phase transformations.

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**Abstract:** The article presents the results of pedagogical research on the application of numerical simulation of X-ray diffraction in crystals and computer experiments in the study of optics in higher educational institutions. It is shown that the transition to the study of diffraction of X-rays of different spectra in monocrystalline and polydomain crystals significantly increases the efficiency of the educational process in forming a deeper knowledge of the physical foundations of interference and diffraction waves. It is shown that depending on the spectrum of used X-ray wave, the geometry of shooting should be chosen polychromatic Laue method, rocking method (or rotation) for computer demonstration of formation of X-ray diffraction pictures during lectures and during students' independent works. On the basis of the fact that for all methods of X-ray diffraction of crystals diffraction maxima are obtained only in the directions satisfying diffraction and geometric conditions, the

necessary information about the features of diffraction patterns formation and calculation formulas for determining the coordinates of reflexes on the X-ray diffraction pattern and their intensities are given. Mathematica computer algebra, the high-level programming language Delphi, and the universal programming language Python were used to visualize the obtained data. Calculated Lauegrams of a hexagonal crystal and rotation radiographs for polysynthetic and polydomain ZnS crystals are presented. It is noted that similar computer demonstrations can be performed for electron and neutron diffraction. As a conclusion, it is shown that computer simulations provide a visual representation of X-ray diffraction in crystals, which can help students better understand the basis of diffraction physics of different wave nature.

## OLIY TA'LIM MUASSASALARIDA OPTIKANI O'RGANISHDA KRISTALLARDA RENTGEN NURLARINING DIFRAKSIYASINI SONLI MODELLASHTIRISH

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## MAQOLA HAQIDA

**Kalit so'zlar:** kompyuter namoyishi, namoyish tajribasi, optika, yorug'lik interferensiyasi va difraksiyasi, rentgen nurlari difraksiyasi, kristall panjara, struktura faktori, rentgenogrammalarni modelashtirish, Lauegramma, tebranish rentgenogrammasi, samaradorlik, CrystalDiffraction, PowderCell, fazaviy o'zgarishlar.

**Annotatsiya:** Maqolada oliy ta'lim muassasalarida optikani o'rganishda kristallarda rentgen nurlari difraksiyasini sonli modelashtirish va kompyuter tajribalarini qo'llash bo'yicha olib borilgan pedagogik tadqiqot natijalari bayon etilgan. Turli spektral tarkibga ega rentgen nurlarining monokristall va ko'p domenli kristallardagi difraksiyasini o'rganishga o'tish interferensiya va difraksiya hodisalarining fizik asoslari haqidagi bilimlarni chuqurroq shakllantirish orqali ta'lim jarayoni

samaradorligini sezilarli darajada oshirishi ko'rsatilgan. Foydalaniladigan rentgen nurlari spektriga qarab, ma'ruzalarda va talabalarning mustaqil ishlarida rentgen difraksion tasvirlarining hosil bo'lishini kompyuter yordamida namoyish etish uchun suratga olish geometriyasini, ya'ni polixromatik Laue usulini yoki tebranish (yoxud aylantirish) usulini tanlash lozimligi asoslab berilgan. Kristallarda rentgen nurlari difraksiyasining barcha usullarida difraksion maksimumlar faqat difraksion va geometrik shartlarni qanoatlantiruvchi yo'nalishlarda hosil bo'lishiga asoslanib, difraksion tasvirlarning shakllanish xususiyatlari, rentgen difraktogrammasidagi reflekslar koordinatalarini hamda ularning intensivliklarini aniqlash uchun zarur ma'lumotlar va hisoblash formulalari keltirilgan. Olingan ma'lumotlarni vizuallashtirish uchun Mathematica kompyuter algebra tizimi, Delphi yuqori darajali dasturlash tili va Python universal dasturlash tilidan foydalanilgan. Geksagonal kristall uchun hisoblangan Lauegrammalar, shuningdek, polisintetik va ko'p domenli ZnS kristallari uchun aylantirish rentgenogrammalari taqdim etilgan. Shunga o'xshash kompyuter namoyishlarini elektronlar va neytronlar difraksiyasi uchun ham amalga oshirish mumkinligi ta'kidlangan. Xulosa sifatida, kompyuter modellashtirish kristallarda rentgen nurlari difraksiyasini yaqqol tasvirlash imkonini berishi va talabalarga turli fizik tabiatga ega to'lqinlar difraksiyasining fizik asoslarini yaxshiroq tushunishda yordam berishi ko'rsatilgan.

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## ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ ДИФРАКЦИИ РЕНТГЕНОВСКИХ ЛУЧЕЙ В КРИСТАЛЛАХ ПРИ ИЗУЧЕНИИ ОПТИКИ В ВЫСШИХ УЧЕБНЫХ ЗАВЕДЕНИЯХ

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## О СТАТЬЕ

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**Ключевые слова:** компьютерная демонстрация, демонстрационный эксперимент, оптика, интерференция и дифракция света, дифракция рентгеновских лучей, кристаллическая решётка, структурный фактор, моделирование рентгенограмм, лауэграмма, качательная рентгенограмма, эффективность, CrystalDiffract, PowderCell, фазовые превращения.

**Аннотация:** В статье представлены результаты педагогического исследования, посвящённого применению численного моделирования дифракции рентгеновских лучей в кристаллах и компьютерных экспериментов при изучении оптики в высших учебных заведениях. Показано, что переход к изучению дифракции рентгеновских лучей различного спектрального состава на монокристаллах и многодоменных кристаллах значительно повышает эффективность образовательного процесса, способствуя формированию более глубоких знаний о физических основах интерференции и дифракции волн. Обосновано, что в зависимости от спектра используемого рентгеновского излучения для компьютерной демонстрации формирования рентгенодифракционных картин во время лекций и самостоятельной работы студентов следует выбирать соответствующую геометрию съёмки: полихроматический метод Лауэ или метод качания (либо вращения). Исходя из того, что при всех методах рентгеновской дифракции в кристаллах дифракционные максимумы возникают только в направлениях, удовлетворяющих дифракционным и геометрическим условиям, приведены необходимые сведения об особенностях формирования дифракционных картин, а также расчётные формулы для определения координат рефлексов на рентгенограмме и их интенсивностей. Для визуализации полученных данных использовались система компьютерной алгебры Mathematica, язык программирования высокого уровня Delphi и универсальный язык программирования Python. Представлены расчётные лауэграммы гексагонального кристалла и вращательные рентгенограммы полисинтетических и многодоменных кристаллов ZnS. Отмечается, что аналогичные компьютерные демонстрации могут быть выполнены и для дифракции электронов и нейтронов. В заключение показано, что компьютерное моделирование обеспечивает наглядное

представление дифракции рентгеновских лучей в кристаллах и помогает студентам лучше понять физические основы дифракции волн различной природы.

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**Introduction.** It is known that in the course of optics special attention is paid to the study of interference and diffraction of visible radiation in mainly one-dimensional (diffraction lattice), two-dimensional (fog, other turbid media) and three-dimensional (crystal structure) structures [1-2]. Special attention is paid to the creation of numerous developments on computer demonstration of diffraction phenomena including Fresnel and Fraunhofer diffraction [3-7]. Demonstration of optical phenomena is devoted to a separate section of Wolfram Demonstrations Project [8]. As a rule, interference and diffraction phenomena occurring in one-dimensional structures are taken as the basis for study. However, as daily observations show, we witness the influence of two-dimensional and three-dimensional periodic structures on the propagation of light. At the same time, from the point of view of practical applicability of such phenomena, the transition to the study of propagation of other types of radiation, such as poly- and monochromatic X-rays, flows of monoenergetic electrons and neutrons, is important especially for studying the structure of crystal materials, structural processes occurring in them under various external influences, and from the pedagogical point of view for better understanding the physical nature of the phenomenon being studied. Therefore, the transition to the study of general laws of diffraction phenomena in three-dimensional crystal structures is an urgent task in teaching the course of optics in higher educational institutions. Note that the theory of three-dimensional lattices is of great practical interest because such lattices are formed in crystals due to the proper arrangement of atoms. The crystal lattice constant coincides in order of magnitude with the wavelength of X-rays. As a result, when X-rays pass through a poly- or monocrystal, they form a diffraction pattern, by analyzing which we can obtain useful information regarding its atomic-crystalline structure.

Note that depending on the spectrum of the X-ray wave used, the shooting geometry should be considered in teaching optics classes the polychromatic Laue method, the swing (or rotation) method, as well as the Debye-Scherer method, which is notable for its clarity and simplicity [9-11]. These methods are widely used in radiography of crystals to determine the Laue class of symmetry, lattice constants, and to determine both point and spatial symmetry groups. Therefore, they should be selected for computer demonstration of X-ray diffraction pattern formation.

It should be noted that currently there are various programs designed to simulate X-ray diffraction patterns of crystals (software package for the analysis of X-ray and neutron diffraction data, CrystalDiffRACT - a convenient software designed for the simulation and analysis of X-ray and neutron powder diffractograms, VESTA, PowderCell, etc.) [12-19]. However, they are not intended

for demonstration of physical phenomena underlying formation of diffraction patterns and, therefore, they should be used for independent work of students or for teaching subjects related mainly to solid state physics or physical materials science.

Statement of the Question. As a rule, when teaching a course of optics, special attention is paid to practical importance of diffraction on spatial inhomogeneities. In [1] it is noted that in this case a wave does not propagate in a homogeneous medium, but in a medium that includes areas where the velocity of the wave differs from the velocity in the rest of the medium. However, if the medium is quite optically homogeneous, naturally, a light wave will propagate in the medium without changing direction and, in particular, a plane wave propagating in such a medium will remain flat. This important circumstance allows us to consider Fresnel diffraction in crystalline substances of different symmetry and physical properties. In this case, electromagnetic wave falling on crystal will lead to appearance of elementary spherical waves scattered by each element of substance volume. Periodic distribution of atoms or molecules in space will lead to certain phase relations between these waves, respectively, a diffraction pattern. Thus, a more detailed study of the phenomenon of X-ray diffraction in crystals leads to a deeper understanding of the physical essence of the phenomenon under study.

It is usually proved in the optics course that in the case of diffraction on a spatial structure with periods  $d_1$ ,  $d_2$  and  $d_3$  one can obtain maximum waves only in directions satisfying three diffraction conditions and one geometrical condition.

The geometric conditions for the formation of the diffraction pattern look like this:

$$d_1 \cos \alpha = m_1 \lambda, d_2 \cos \alpha = m_2 \lambda, d_3 \cos \alpha = m_3 \lambda. \quad (1)$$

Here  $m_1$ ,  $m_2$  and  $m_3$  are integers.

To consider the diffraction of X-rays in crystals, we introduce the direction of the incident radiation by means of the vector  $\vec{t}_0$ . Here we use the vector  $\vec{t}$ , which is related to the wave vector accepted in optics as  $\vec{k} = \vec{t} \lambda$ , to denote the direction of the diffracted radiation. The relation between the principal lattice vectors  $\vec{a}$ ,  $\vec{b}$  and  $\vec{c}$  and the direction of the diffracted beam  $\vec{k}$  is then determined by the equations:

$$\left. \begin{aligned} \vec{a}(\vec{k} - \vec{k}_0) &= h, \\ \vec{b}(\vec{k} - \vec{k}_0) &= k, \\ \vec{c}(\vec{k} - \vec{k}_0) &= l, \end{aligned} \right\} \quad (2)$$

where  $h, k, l$  are integers. Now the desired direction  $\vec{k}$  is determined using the following single equation:

$$\vec{k} - \vec{k}_0 = (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*) = \vec{H}_{hkl}. \quad (3)$$

In equation (3) the vector  $\vec{H}_{hkl}$  is called the inverse vector of the crystallographic (hkl) or radius-vector of the inverse lattice node. The diffraction condition for the inverse space is written as  $\vec{k} - \vec{k}_0 = \vec{H}_{hkl}$ . It is important to note that the diffraction condition is satisfied for those nodes of the inverse lattice that are inside a sphere of radius  $1/\lambda$  (the Ewald sphere).

Experience has shown that in a lecture class it is advisable to give specific information about Laue's interference function, which determines the conditions for observing diffraction maxima when radiation is scattered by a crystal lattice consisting of nodes of the same kind.

Two questions naturally arise here, the illumination of which is of important methodological importance in the study of both optics and other branches of physics.

a) It is known that the modulus of the wave vector as  $|\vec{k}| = 2\pi/\lambda$  or  $|\vec{k}| = 1/\lambda$ . Here both notations represent the modulus of the wave vector, but they differ in the units used to express it.

The notation  $2\pi/\lambda$  represents the modulus of the wave vector in units of radians per unit length (often called reciprocal meters or inverse meters). This notation is widely used in physics, especially in the context of Fourier analysis and wave phenomena, where the wave vector is often used to describe the spatial frequency of a wave. In this context, wavelength ( $\lambda$ ) represents the distance between two consecutive peaks (or troughs) of the wave, and  $2\pi/\lambda$  is the number of radians of phase change per unit wavelength.

On the other hand, the notation  $1/\lambda$  represents the modulus of the wave vector in inverse length units (often called inverse centimeters or inverse nanometers). This notation is widely used in spectroscopy and other fields where the wavelength of electromagnetic radiation is an important parameter. In this context, wavelength ( $\lambda$ ) represents the distance between two consecutive ridges of an electromagnetic wave, and  $1/\lambda$  is the number of wave cycles per unit length. Therefore, in general, these two designations represent the same physical quantity, but are expressed in different units depending on the context in which they are used. We will not use  $2\pi$  in our presentation.

(b) The second side of the question is closely related to the notion of an inverse grating and interference function in inverse space. It is a mathematical construction that is a fundamental concept in crystallography, and it is closely related to the diffraction of X-rays, electrons or neutrons in a crystal. As shown above, the diffraction pattern is related to the periodicity of the crystal, which is described by the inverse lattice. Therefore, the notion of inverse lattice is among the fundamental concepts that are crucial for understanding the diffraction of X-rays, electrons or neutrons in a crystal. Therefore, a presentation on the relationship between forward and backward lattices of crystals of different syngonies or systems is very important from the point of view of teaching methodology in various sections of physics.

Another important question is related to the intensity of the so-called X-ray reflexes. As it is known, it depends mainly on the geometric features of the radiographs, the spectrum of the used

radiation, the square of the structural factor, and also on the repeatability factor, which in its numerical value is equal to the number of families of planes having the same interplanar distance and the same structural factor [6]. Here the question of the kinematic theory of X-ray scattering comes up, which is based on the assumption that the scattering process takes place without any interaction between the scattered X-rays and the crystal lattice. In other words, the kinematic theory assumes that X-rays are scattered from the crystal elastically, without energy or momentum change as in the case of light diffraction. This theory is useful for describing diffraction patterns produced by perfect crystals, where the positions of the atoms are clearly defined and the crystal lattice is homogeneous.

Practical implementation of computer modeling of X-ray diagrams of crystals. Naturally, the initial information required for the simulation of any type of X-ray radiographs are the lattice constants, the used radiation (usually wavelength for K<sub>α</sub> radiation for monochromatic wavelengths or wavelength interval in the polychromatic Laue method), and the dimensions of diffraction patterns [20-22]. For all calculations, a laboratory coordinate system with the z-axis directed along the X-ray beam is taken [20]. Special attention should be paid to the relation between the directions of the radiation incident on the crystal and the z-axis (parallel or antiparallel), since it determines the condition for the reflex to hit the diffraction pattern.

It is also known that for all nodes present in the selected region of the inverse grating, the coordinates of reflexes X and Y in the monitor coordinate system are calculated by the following formulas [20]:

$$\begin{aligned} X &= R \cos \delta, \delta = \arccos \left[ H_x / \sqrt{H_x^2 + H_y^2} \right] \operatorname{sign} H_y, \\ Y &= R \sin \delta, \\ R &= -L \operatorname{tg} (2\alpha), \alpha = \arccos(H_z/H), 2\theta = \pi - 2\alpha. \end{aligned} \quad (4)$$

Here, H stands for the modulus of vector  $\vec{H}_{hkl}$ ,  $\theta$  is the so-called diffraction angle,  $H_x$ ,  $H_y$  and  $H_z$  are the components of vector  $\vec{H}_{hkl}$ ,  $\alpha$  is the angle between the Z axis and vector  $\vec{H}_{hkl}$ .

Computer algebra Mathematica, the high-level programming language Delphi, and the universal programming language Phyton were used to calculate the diffraction pattern, depending on the level of relevant training of students.

Fig. 1 shows the calculated lauegram obtained for a hexagonal crystal when the z-axis is directed along the crystallographic axis [0001].

Very interesting results can be obtained by construction of sway (or rotation) radiographs. Here one can clearly demonstrate the X-ray diffraction pattern not only of single crystals, but also

of polydomain crystals formed at phase transitions proceeding by the martensitic mechanism. For example, in zinc sulfide ZnS crystals grown from melt, the transition from the high-temperature wurtzite (hexagonal) modification to the low-temperature sphalerite (cubic modification) one of  $\sim 150$  polytypes, more often an unconjugated polysynthetic structure, is usually completed [23-24]. In the presence of structural domains, the back space of the crystal becomes a superposition of the back spaces of all structural domains present in a given crystal sample and analysis of the resulting X-ray diffraction pattern provides unambiguous information on the orientation relationships between the crystal lattices.

Figure 2 shows fragments of calculated X-ray rotation patterns of polysynthetic and monocrystalline ZnS samples. The rotation axis of the crystal corresponds to the [0001] axis of the original hexagonal modification (a) and the [111] axis of the cubic sphalerite modification of the crystal. It is immediately obvious that in case of cubic modification of the crystal the symmetry with respect to the [111] plane disappears and all signs of cubic symmetry are restored.

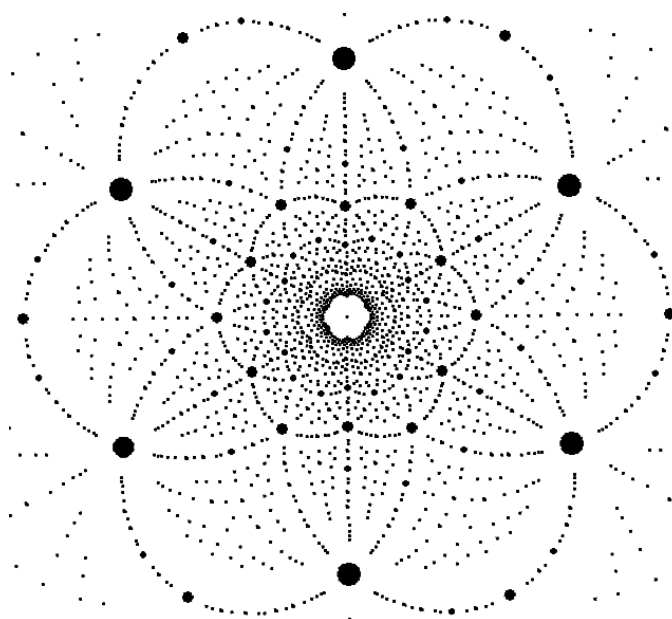


**Fig. 1. Calculated lauegram constructed for a hexagonal crystal when imaging along the [0001] axis.**

During the demonstration of the calculated X-ray diffraction patterns obtained from polydomain and monodomain crystals of lead orthovanadate  $[\text{Pb}]_3 [(\text{VO}_4)]_2$ , where the polydomain state is formed during a phase transition resulting from a change in structure from rhombohedral to monoclinic [25].

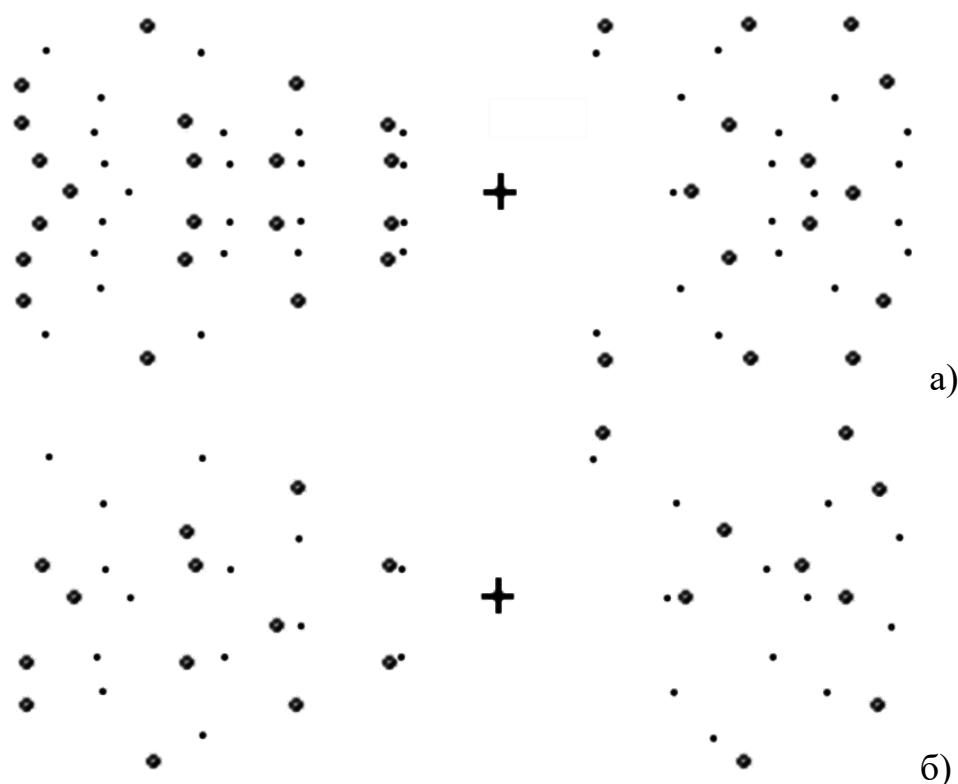


**Fig. 2. Calculated X-ray bobs obtained for polysynthetic (a) and monodomain ZnS crystals. the calculation was performed for K $\alpha$ - (circles) and K $\beta$ -radiation of the copper anode.**

As the studies show, similar computer experiments can be performed for the case of electron and neutron diffraction. The peculiarities of their interaction with matter, their quantum properties, and the range of wavelengths used in both crystal electronography and neutronography are particularly evident. Note that the use of computer programs such as CrystalDiffract is sufficient to study the X-ray diffraction pattern formation of polycrystalline or powdered samples.

Thus, the computer simulation of X-ray diffraction of various crystalline samples can give visual representations of the formation of diffraction patterns of light and X-rays on the basis of unified representations.

**Conclusions.** As our research has shown, the demonstration of X-ray diffraction in crystals using computer simulation has proven to be a useful and effective teaching tool in teaching optics courses at institutions of higher education. First, computer simulations provide a visual representation of X-ray diffraction in crystals, which can help students better understand the basic physics of diffraction of different wave natures. Simulations can show how X-rays interact with the crystal lattice and how the resulting diffraction pattern is formed. Second, computer experiments can be interactive, allowing students to adjust the shooting geometry of different radiographs and observe how the diffraction pattern changes. Third, X-ray diffraction experiments are usually conducted in specialized laboratories that may not be available to all students. Computer experiments allow the concept to be demonstrated in the classroom or independently, making it

more accessible to a wide range of students. Cost effectiveness should also be added, as X-ray diffraction experiments can be expensive, requiring specialized equipment and materials. Computer simulations can be a cost-effective alternative that can be used repeatedly without the need for additional resources.

In conclusion, computer simulations can be a valuable teaching tool to demonstrate X-ray diffraction in crystals and should be used in conjunction with other teaching methods, especially for students' independent work.

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