Enhancing student comprehension of crystal structures: The effectiveness of Vesta as a learning tool

Khoirotun Nadiyyah[1]*, Rika Aprianti[1], Zakirman[1], Widiasih[1], Fadhila Ulfa Jhora[2], Ratnawulan[2]

[1]Universitas Terbuka, Jl. Pd. Cabe Raya, Pd. Cabe Udik, Tangerang Selatan 15437, Indonesia
[2]Universitas Negeri Padang, Jl. Prof. Dr. Hamka, Air Tawar Bar., Padang 25171, Indonesia
*Corresponding author, email: khoirotun.nadiyyah@ecampus.ut.ac.id

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Abstract
The advancement of technology in education was evident in the development of digital-based learning media. It was expected to serve as a stimulus in transforming knowledge for students, particularly in abstract subjects such as crystal structures. Understanding crystal structures was crucial for studying the physical properties of materials, making it important for students to enhance their comprehension. The research objective was to determine the effectiveness of using Vesta software as a learning media to enhance students' understanding of crystal structures by employing standardized assessment instruments. This research was conducted using a quantitative approach focused on collecting numerical data and statistical analysis through an experimental method involving two groups of students taking a solid-state physics course. The research design involved a control and an experimental group. Both groups were given the same subject but using different learning media. The instrument used was a multiple-choice test that had been rigorously validated through validity, reliability, difficulty level, and discrimination index. Effectiveness was evaluated using independent sample t-test analysis with the aid of SPSS software. Instrument testing data revealed that out of 40 developed questions, 20 met the standards to be used as instruments. The results indicated a highly significant enhancement in students' understanding of crystal structures after using the Vesta software as a learning media, as represented by a sig. (2-tailed) value of 0.000. The findings indicate that Vesta can be integrated into science teaching. Further research can test the effectiveness of implementing Vesta in distance learning.

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1. Introduction

In the rapidly evolving era of digital technology, education is also transforming, particularly in teaching and learning methods (Alkan & Mertol, 2019). One critical aspect is the use of digital learning media to enhance the effectiveness of learning, especially in science and technology (Harahap et al., 2022). In physics, particularly solid-state physics, understanding the crystal structure and its relationship to the physical properties of solids is essential for solids (Hari, 2019). Digital tools and simulations play a crucial role in helping students visualize and grasp these complex structures, making the learning process more effective and engaging.

Crystals are solid materials with a regular, repeating (periodic) arrangement of atoms in three dimensions (Callister Jr & Rethwisch, 2020; Lee et al., 2019). In contrast, solid materials with irregular atomic arrangements were called amorphous (J. Kang et al., 2023). The growth of both crystals and amorphous materials was influenced by their growth processes (Lee et al., 2019). When indicated in a diffraction pattern, the crystal forms sharp peaks, while the amorphous forms wide peaks (Nadiyyah et al., 2023). Macroscopically, single crystals can be identified by their geometric shapes, consisting of surfaces with specific orientations, such as diamonds. On the other hand, inorganic solid substances are not single crystals but rather aggregates of fused crystals forming polycrystals (Callister Jr & Rethwisch, 2020; Kogan, 2018).

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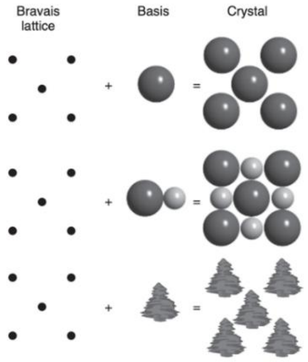


Figure 1. Illustration of Bravais lattice, base, and crystal structure in 2D (Hofmann, 2022)

The crystal was simply composed of a basis and a Bravais lattice (Figure 1). The basis could consist of atoms or molecules occupying a specific volume, known as the unit cell (Hofmann, 2022). A Bravais lattice was a set of regularly spaced points with positions defined as vector multiples (Boettcher et al., 2022). In the crystal, there are 14 Bravais lattices formed by a combination of a crystal system with a type of centering (Hoffmann, 2020). There are 7 (seven) crystal systems (triclinic, monoclinic, orthorhombic, tetragonal, rhombohedral, hexagonal, and cubic) and 4 (four) types of centering (primitive/P; Base-cantered/A, B, or C; Body-cantered/I; and Face-cantered/F) that identify the locations of lattice points in the conventional unit cell (Hofmann, 2022; Kogan, 2018).

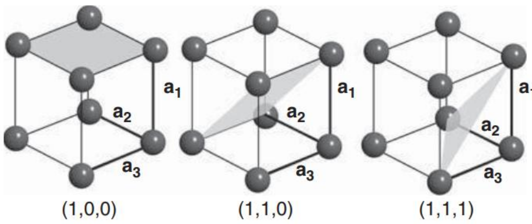


Figure 2. Crystal planes in cubic structures (Hofmann, 2022)

The most basic crystal structure was cubic, which was not commonly found in pure metals but serves as an important starting point for other structures. Based on atom arrangement, cubic structures were classified into Simple Cubic (SC), Body-cantered cubic (BCC), and Face-cantered cubic (FCC). Meanwhile, the crystal structure more prevalent in metals was Hexagonal Close-Packed (HCP) (Kogan, 2018; O'Keeffe & Hyde, 2020). Crystal planes could be formed within each unit cell, which gain significance when they contain atoms (Gault et al., 2021). To distinguish between these planes, the Miller index was commonly used, as depicted in Figure 2 (Hofmann, 2022; O'Keeffe & Hyde, 2020).

Studying crystal structures is crucial in physics as it forms the foundation for understanding material properties (Nangia & Desiraju, 2019). Physics explores how atoms and molecules are arranged in crystals and how these arrangements influence the physical properties of materials (Pham et al., 2019). Through modeling, experiments, and theory, physicists study material behavior under various conditions dependent on crystal structure, including temperature (Sun & Cava, 2019) and magnetic field (Yan et al., 2019). Furthermore, crystal structures serve as the basis for numerous practical physics applications such as crystal optics (L. Kang et al., 2020) and semiconductor materials (Egamberdiyev et al., 2020). Therefore, a deep understanding of crystal structure was essential for explaining physical phenomena and developing new technologies across various fields of physics.

In the context of physics education, understanding crystal structure was crucial as it directly relates to material properties, which form the foundation for many fields of study, including materials physics (Sani, 2021). However, this concept was often perceived as challenging for students due to its abstract nature (Pauziah & Laksanawati, 2023). In learning with image media, students still struggle to grasp material concepts due to limitations, such as presenting only two-dimensional (2D)

(Reeves et al., 2021). Therefore, there was a need for the development of more effective and engaging learning media, emphasizing digital technology-based learning (Buliali et al., 2022; Siemieniecka et al., 2017) and simulation (Yılmaz & Hebebci, 2022). This allows students to learn and understand concepts of crystal structure independently, such as atomic arrangements and crystal orientations.

Alongside technological advancements, the use of various media for studying crystal structure was becoming increasingly important in research. This is evident from the utilization of programs such as Diamond for plotting crystal structures $[CsEu(H_2O)_3(SO_4)_2]\cdot H2O$ and $CsEu(SO_4)_2$ (Denisenko et al., 2021), Mercury which not only visualizes crystal structures but also designs, analyzes, and predicts crystal materials (MacRae et al., 2020), Avogadro for depicting the structure of sodium metal (Avery et al., 2018), and Vesta for representing ZrO2 Polymorphs structures (N. Kumar et al., 2019). In their research, Nadiyyah, K., et al (2024) stated that the use of Vesta software has a positive impact on students' scientific attitudes toward learning crystal structures, particularly with high curiosity and enthusiasm toward Vesta (Nadiyyah et al., 2024). Vesta software enables three-dimensional (3D) visualization of crystal structures, making them more tangible and allowing users to engage in hands-on practice (Somveer et al., 2023).

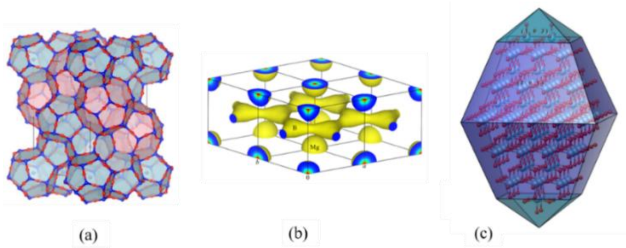


Figure 3. Visualization of 3D crystal systems with vesta in (a) structural, (b) volumetric, and (c) morphological aspects (Momma & Izumi, 2014)

During the period from 2001 to 2006, Koichi Momma and Fujio Izumi developed Vesta in the C++ programming language with OpenGL technology for electronic and structural analysis (Rini, 2019). Vesta was capable of modeling not only structural data but also volumetric and morphological data (Figure 3) (Momma & Izumi, 2014). Within the Vesta software, crystal constituents such as atoms, bond types, coordination polyhedra, and isosurfaces can be rapidly rotated, scaled, and translated for 3D visualization (Constant, 2019). Structural models were represented in various forms, including ball-and-stick, space-filling, polyhedral, stick, wireframe, and ellipsoid models (Lorchirachoonkul, 2019). The algorithm implemented in Vesta is highly sophisticated, ensuring high scalability and enabling the simulation of molecular dynamics with a large number of atoms (Momma & Izumi, 2014). Through the use of Vesta, students could explore and study fundamental concepts related to crystal structure, such as Bragg's law and Miller indices, and facilitate 3D visualization of crystal structures, bonds, lattice planes, and X-ray diffraction patterns (Beekman, 2022).

Given its potential as a learning tool, Vesta warrants further exploration regarding its effectiveness as a technology-based learning media in enhancing students' understanding of crystal structure concepts. Therefore, the objective of this research was to empirically measure the impact of using Vesta in improving students' understanding of the material and their engagement in the crystal structure learning process, assessed through validated instruments.

2. Method

This research was conducted using a quantitative approach, focusing on the collection of numerical data and statistical analysis to answer research questions and test hypotheses (Basias & Pollalis, 2018). The research involved a structured design (Figure 4) utilizing instruments that have been quantitatively validated (Table 2). The research was conducted in three stages preparation of research instruments, subjects, and effectiveness (Figure 5).

	Initial Value	Treatment	Test
Experiments (A)	T_1	*Software Vesta*	T_2
Control (B)	T_1	-	T_2

Figure 4. Effectiveness Data Collection Design

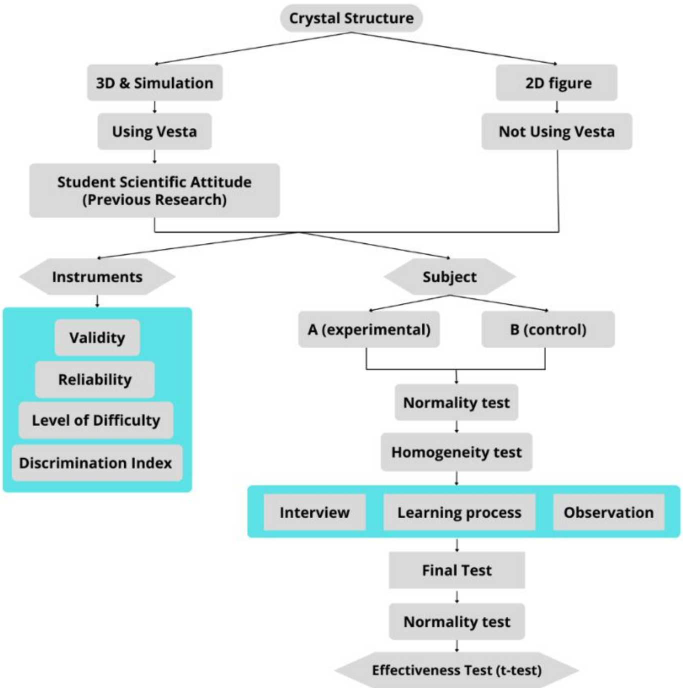


Figure 5. Research Scheme

2.1. Instruments and Subject

The research instruments were analyzed four test types, 1) the validity was used the Corrected Item Total Correlation analysis (Santoso, 2020), 2) the reliability was used in the Kuder Richardson 20 (KR.20) analysis (Sürücü & Maslakçi, 2020). 3) The level of difficulty (P) was analyzed using Equation 1 and 4) The discrimination index (D) was analyzed using Equation 2.

$$P = \frac{B}{n} \tag{1}$$

$$D = P_A - P_B = \frac{BA}{JA} - \frac{BB}{JB} \tag{2}$$

Where B (the number of respondents who answered correctly), n (the number of all respondents), P_A (the proportion of upper-group respondents who answered correctly), P_B (the proportion of lower-group respondents who answered correctly), BA (the number of correct answers in the upper group), BB (the number of correct answers in the lower group), JA (the number of respondents in the upper group), and JB (the number of respondents in the lower group) (Alika et al., 2018). The classification of the tests were shown in Table 1.

Table 1. Classification of Reliability (Sağlam et al., 2021), Difficulty Levels, and Discrimination Index (Belmar Garrido, 2023)

Item	Score	Interpretation
Reliability (r_{20})	< 0.40	Unreliable
	0.60 – 0.90	Reliable
	> 0.90	Highly reliable
Level of Difficulty (P)	< 0.40	Difficult
	0.40 – 0.60	Moderate
	0.61 – 0.89	Easy

	> 0.90	Very Easy
Discrimination Indeks (D)	0.00 – 0.19	Does not discriminate
	0.20 – 0.29	Discriminates poorly
	0.30 – 0.39	Discriminates well
	> 0.40	Discriminates very well

The crystal data used in operating Vesta were sourced from *the Crystallography Database* (http://www.crystallography.net/cod/) or the *Inorganic Crystal Structure Database* (ICSD) (http://icsd.kisti.re.kr/icsd/icsd_chemistry.jsp). The Vesta software can be downloaded for free at https://jp-minerals.org/vesta/en/ for educational and research purposes.

Table 2. Indicators of the Research Instrument

No.	Indicators	Cognitive Level	Number of Questions	Question Number
01	Identify the lattice of a crystal	C2	1	1
02	Identify the basis of a crystal	C2	2	2, 3
03	Determine the crystal system	C3	1	4
04	Determine the crystal structure	C3	1	5
05	Determine the image of the crystal structure	C3	1	6
06	Determine the lattice parameters (a, b, c) of a crystal	C3	2	7, 8
07	Determine the angle parameters (α, β, γ) of a crystal	C3	2	9, 10
08	Determine the interatomic distance in a crystal	C3	2	11, 12
09	Determine the coordinates of atoms in a crystal	C3	2	13, 14
10	Determine the angle formed by three atoms in a crystal	C3	2	15, 16
11	Determine crystal planes	C3	1	17
12	Determine the Miller index of a crystal	C3	2	18, 19
13	Determine the coordination number of a crystal	C3	1	20
Total		20		

For subject research, the normality test was using the Shapiro-Wilk and the homogeneity test using the Levene Statistic with a significance level (α) of 5% (Arifin & Aunillah, 2022). According to Mascha & Vetter, the α was a probability used in statistical tests to determine the error limit that could be tolerated and could reject the hypothesis (Mascha & Vetter, 2018). The hypotheses were h_o (data not normally distributed/ inhomogeneous) and h_1 (data normally distributed/ homogeneous). If $\alpha < 0.05$ (h_o was accepted, h_1 was rejected), but if $\alpha > 0.05$ (h_1 was accepted, h_o was rejected) (Arifin & Aunillah, 2022).

2.2. Effectiveness

For normally distributed research data, hypothesis testing was conducted using t-test analysis, a statistical method used to determine differences between two sample means (Sugiyono, 2022). The effectiveness was analyzed using the *independent sample t-test* because it involved a single variable - students' learning outcomes regarding the understanding of crystal structure - and compared the average learning outcomes of A and B groups, which were separate and unrelated research subjects (Sirakaya & Ozdemir, 2018). The α was based on *2-tailed significance* data because the use of the Vesta software was expected to encompass or represent all levels of intelligence among the student subjects, whether their intelligence level was below the lower threshold or above the upper threshold (Ben Ouahi et al., 2021). The hypothesis was h_o (no significant difference) and h_1 (significant differences). If $\alpha > 0.05$ (h_o was accepted, h_1 was rejected), but if $\alpha < 0.05$ (h_1 was accepted, h_o was rejected).

3. Results and Discussion

In the previous section, it was stated that this research involved a series of instrument tests before employing them as tools to measure the effectiveness of the Vesta learning media in enhancing students' understanding of crystal structures. The series of instrument tests consisted of four types of item tests. To measure effectiveness, the initial crucial step was to ensure that the research instruments used were valid and reliable. Firstly, the validity test uses *corrected item-total correlation* analysis on 40 questions, with the results presented in Table 3.

Table 3. Validity Test Results for Each Item Indicator

Classification	Item indicator number													Number of items
	01	02	03	04	05	06	07	08	09	10	11	12	13	
Valid	2	2	1	1	1	2	2	3	4	3	2	2	1	26
Invalid	1	1	2	2	2	0	0	1	0	0	2	2	1	14

Through the validity test, we could determine and ensure that the instrument accurately measures the intended construct, which was the effectiveness of using the Vesta learning media in understanding crystal structures. Table 3 shows that not all the 40 items were found to be valid. This data was taken based on the results of data processing by comparing the values between r and r_{table}. Only 26 items had r values greater than r_{table} (r_{table} = 0.361 for n = 30, and significance level 5%), indicating validity (Radeswandri et al., 2021). Meanwhile, the other 14 items had r values less than r_{table} and were thus considered invalid, necessitating revision or removal. The existence of invalid items indicates that these items lack accuracy and precision, and therefore cannot be used as instruments for the effectiveness test. However, when evaluated by item indicators, it was found that each indicator contained valid items, suggesting that the thirteen-item indicators (Table 2) developed have the potential to be used as instruments for testing the effectiveness of the Vesta learning media.

Secondly, the reliability test measured how consistently the instrument provided measurement results. This reliability test was conducted using the Kuder Richardson 20 (KR.20) analysis and produced an r_{20} value of 0.875, indicating that all items (question items) were reliable (Sağlam et al., 2021). This showed that the developed instrument was consistent in measuring the effectiveness of the Vesta learning media. This test was crucial to ensure that the results were not influenced by unwanted external factors.

Thirdly, the level of difficulty test was conducted to determine the difficulty level of each question item. It measures how challenging each item is, helping to determine how well the items could differentiate between respondents with varying levels of knowledge (Belmar Garrido, 2023). Using Equation 1 and analysis based on classification by Garrido & Hector (2023), the difficulty test results for the 26 valid items were presented in Figure 6a. The item difficulty data in Figure 6a was divided into four categories: very easy, easy, moderate, and difficult. The difficulty level analysis showed that the distribution predominantly consisted of items with a "moderate" difficulty level, but there were some items in the other three categories in smaller quantities. These results indicated that the instrument was well-balanced in terms of difficulty, as it was neither too easy nor too difficult overall (D. Kumar et al., 2021). This balance provided an appropriate level of challenge for students, allowing them to accurately interpret their understanding of crystal structures using Vesta.

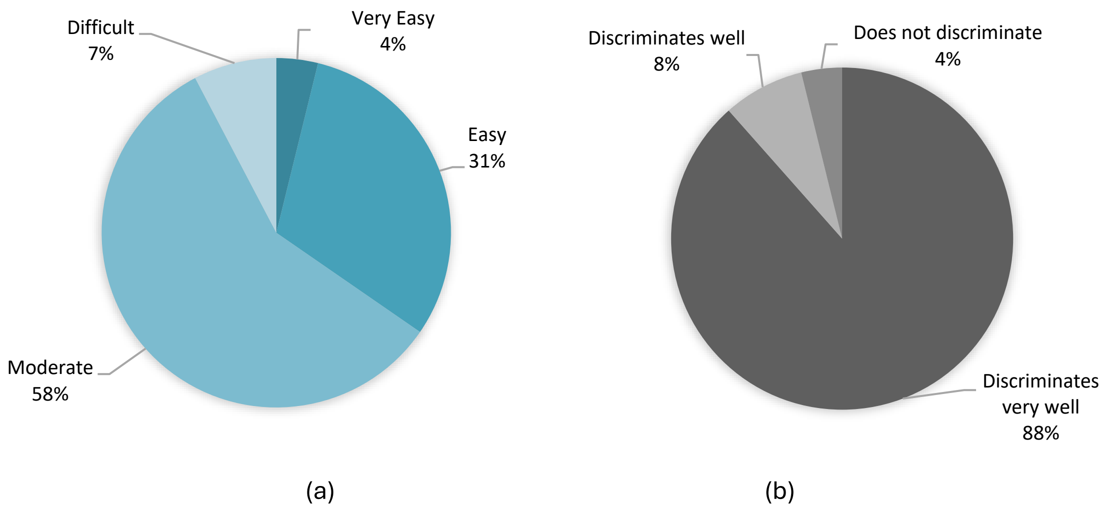


Figure 6. Analysis of (a) Level of Difficulty (b) Discrimination Index

Lastly, the discrimination index test was conducted to identify each item's ability to distinguish between groups of respondents with different levels of ability. The discrimination index was obtained from data processing using Equation 2. Based on Garrido & Hector's (2023) classification of the discrimination index, the data for the 26 valid items are shown in Figure 6b. There were three categories, with the "discriminates very well" type (D > 0.40) being predominant. These results indicated that most of the instrument items had an excellent ability to distinguish between students with high and low levels of understanding. However, three items (4%) with "does not discriminate" needed to be improved to enhance the instrument's discriminative capability. Subsequently, by correlating the overall results of the instrument tests and considering the item indicators related to understanding crystal structures, items that did not meet the criteria were eliminated. Consequently, out of the 40 tested items, 20 items that met the criteria (validity, reliability, level of difficulty, and good discrimination) were selected to be used as the research instrument for the effectiveness test.

Before conducting the effectiveness test, it was necessary to ensure that the data from both groups were homogeneous, which was done through a homogeneity test. However, before performing this test, it was essential to start with a normality test. In this research, the normality test was conducted using the Shapiro-Wilk analysis, and the results are presented in Table 4.

Table 4. Normality test results before treatment

Group	*df*	*Sig.*
A	16	.261
B	15	.262

Table 4 shows that the data was normally distributed for both groups of students before receiving any special treatment. This was evidenced by the significance level (α) value obtained from both groups. With significance values greater than 0.05, specifically 0.261 and 0.262, it could be said that the data was normally distributed. Table 4 also presents the value of ***df*** (*degrees of freedom*), which in this context refers to the number of samples used in the normality test. According to Kim (2019), the degree of freedom is the amount of free value in statistical calculations that can vary (Kim, 2019). After confirming the normal distribution of the data, a homogeneity test was conducted using Levene Statistical analysis, and the results are shown in Table 5.

Table 5. Homogeneity Test Results

Methods	df1	df2	Sig.
Based on Mean	1	29	.223
Based on Median	1	29	.389
Based on the Median and with adjusted df	1	28.85	.391
Based on trimmed mean	1	29	.227

Like the normality test, Table 5 also shows the significance level value, where α value greater than 0.05 was obtained for all methods. *Based on the mean* (α = 0.223) indicated that there was no significant difference in variance between groups based on the average values, thus the variances are considered homogeneous. The other methods—*based on median*; *based on median, and with adjusted df;* and *based on trimmed mean* also consistently showed results indicating homogeneous variance between the data groups, allowing for the effectiveness test of using the Vesta learning media. In the homogeneity test, the data provided two degrees of freedom (Table 5), ***df1*** represented the degrees of freedom between groups. In this research, ***df1*** had a value of 1 which was obtained because there were two compared groups (experimental group/A and control group/B), thus ***df1*** = k - 1 = 2 - 1 = 1. Meanwhile, ***df2*** represented the degrees of freedom within groups, which in this case was 29, obtained from the total number of observations minus the number of groups (N - k = 31 - 2 = 29).

The crystal structure is fundamental knowledge that every physics student, especially those taking courses in solid-state physics. In these courses, all physical properties were further analyzed within crystalline materials composed of atoms, crystal planes, and their constituent bonds. The physical properties analyzed include electrical, magnetic, thermal, etc. Therefore, there was a need for media that could stimulate students to understand them, particularly through visual aids and simulations. To quantitatively assess this hypothesis, an effectiveness test was necessary.

This independent sample t-test required that the data for each variable to be tested must be normally distributed (Sugiyono, 2022). Therefore, before conducting the effectiveness test, a normality test was performed using Shapiro-Wilk analysis, and the results are presented in Table 6.

Table 6. Normality Test Results After Treatment

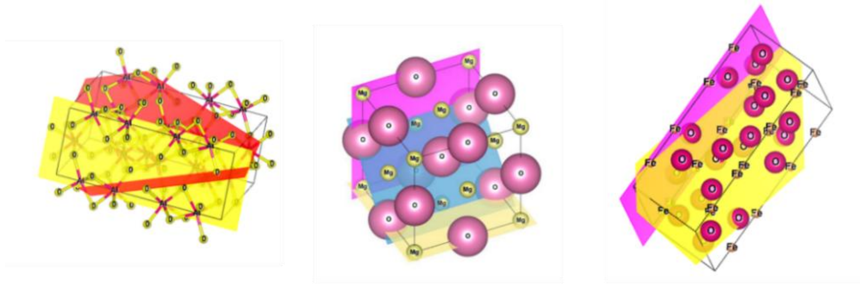
Group	df	Sig.
A	16	.190
B	15	.364

One of the aims of this normality test was to determine the next step in testing. If the data was not normally distributed, subsequent testing would require non-parametric methods (Mishra et al., 2019). Based on Table 6, the data of the A and B groups were normally distributed as indicated by significance values exceeding 0.05. These results showed that by giving different treatments, the A group used Vesta software as a learning media for crystal structure, while the B group did not use Vesta, and the data remained normally distributed. Therefore, an effectiveness test could proceed using the *independent sample t-test*, with results detailed in Table 7.

Table 7. Result of Independent Sample t-test

t value		df	Sig. (2-tailed)
t_{table}	t		
2,045	4,336	29	.000

In the effectiveness analysis using the *independent sample t-test*, the significance level value was determined based on *2-tailed significance* data. Based on the data in Table 7, the sig. (*2-tailed*) value of 0.000 was obtained, which was less than 0.05. This value indicated a highly significant improvement in students' understanding of crystal structure when using Vesta as a learning medium compared to conventional learning without Vesta. In addition to the sig. (*2-tailed*) value, *independent sample t-test* data also showed the existence of *t* and *df* values. When comparing the *t* and t_{table} *values* obtained $t > t_{table}$ (t_{table} = 2.045), indicating that Vesta was effective as a learning medium for crystal structure. (Oktarina et al., 2021).



(a) (b) (c)

Figure 7. Results of Vesta Operations on the (a) Al_2O_3, (b) MgO, and (c) Fe_2O_3 Crystal Structures by Students

The high effectiveness of Vesta in this research stems from its capability to allow students not only to visualize crystal structures in three dimensions (3D) but also to simulate the assembly process of crystal structures. This includes determining the types and sizes of atoms, crystal lattice structures, and even the bonds between constituent atoms within a crystal. In their research, Lv, et al (2024) used Vesta to visualize the crystal structure tetragonal of H_2O_2, analyzing its electronic and bonding properties (Lv et al., 2024). This was relevant to research conducted by Zakirman, et al (2023), where the use of technology-based learning media with visuals and simulations could enhance understanding of specific concepts, such as augmented reality for earthquake topics (Zakirman et al., 2023). These findings were also consistent with previous research on Vesta-based media, which explored students' scientific attitudes toward its application. According to Nadiyyah, K., et al. (2024), the seven scientific attitudes in using Vesta media were categorized as very good, particularly in terms of *curiosity*, which reached 88.03% (Nadiyyah et al., 2024). This attitude was evident during the observation process conducted by researchers. When using Vesta for learning, students are enthusiastic and have the desire to explore other features available in Vesta software so that they can construct crystal structures of various molecules in various orientations (Figure 7). It made the learning process more enjoyable and easier to comprehend crystal structure for the students. Across various disciplines, the current use of media, particularly those leveraging digital technology, has positively impacted student interest and learning outcomes. In addition to the many advantages of implementing Vesta software in education, research, science, and technology, it's important to acknowledge some weaknesses in this research. This research was limited to a relatively small number of samples and it did not fully consider external factors such as technological skills or students' previous experiences with crystallography concepts, which can impact learning outcomes. Further research is needed to address these limitations.

4. Conclusion

Based on the data processing and analysis in this research, it was concluded that there was a reduction in the number of test items used as standardized effectiveness instruments, decreasing from 40 items to 20 items. Furthermore, the results of the independent sample t-test analysis indicated a highly significant improvement in students' understanding of crystal structure concepts when using the Vesta software as a learning media. However, due to the limitations of this research which only involved a small number of samples, the results are less generalizable. Therefore, suggestions for further research include expanding the sample number to improve the understanding of the crystal structure and conducting effectiveness tests of the Vesta software in distance learning.

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All authors have equal contributions to the paper. All the authors have read and approved the final manuscript.

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Declaration of Conflicting Interests

The author declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

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