Visualization of face-centered cubic energy band using spreadsheet and javascript as innovative learning

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Constructing mathematical equations in physics often creates difficulties in students' learning process. Therefore, it is necessary to have technology-based simulations to understand physical phenomena. One technology that is easy to use for simulations in physics learning is the spreadsheet program. This study aims to use spreadsheet media to visualize the face-centered cubic (FCC) energy band using the tight-binding method and to compare the results with the JavaScript programming language. This paper succeeded in making visualization of face-centered cubic (FCC) energy band using a spreadsheet as an alternative to distance learning. The spreadsheet is easier to use because they do not use complicated programming languages like JavaScript. This paper shows the use of innovative learning media, spreadsheets, in materials courses.

Keywords: Face-centered cubic; energy band; spreadsheets; visualizations.

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1. Introduction

There are 3 types of cubic crystal structures, namely simplecubic, body-centered cubic, and face-centered cubic. The crystal structure is a group of atoms that occupy lattice points [1]. Atoms, such as calcium, aluminum, copper, and gold have a face-centered cubic (FCC) atomic structure. Each material has a different character of the energy band structure. The energy band is the energy required by electrons to move from the valence band to the conduction band [2]. This energy band determines the electrical properties of the material [3]. Energy bands can be learned using the tight-binding method. Research using the tight-binding method was already carried out, and one of which was by analyzing the energy of the ZnO nanoparticle's optical bandgap [4]. The research was able to show the maximum energy gap of ZnO nanoparticles. Another study also investigated the structure of graphene and carbon nanotube elements using the tightbinding method, by analyzing the energy bandgap variations in SWCNT (Single-walled Carbon Nanotubes) [5]. Based on previous research, constructing energy bands in the learning process is important.

Constructing mathematical equations in physics often creates difficulties in the learning process [6]. It is necessary to have a technology-based simulation that is easy to operate. A spreadsheet is a computational tool that has the advantage of not requiring a complicated programming language, especially in making physics simulations, and is suitable for general use [7]. The spreadsheet has been widely used to assist in the learning process, such as for visualizing the distribution of light intensity on optical fibers [8]. The result of this visualization can help students interpret mathematical equations and make connections between theoretical and experimental models. Modeling using another spreadsheet is carried out for student practice to build a mathematical model depicting electrons in solids [9]. The result is that students showed understanding by making models. The use of a spreadsheet has also been carried out to demonstrate the capabilities and program potency [10]. Spreadsheet programs are used to investigate important parameters in semiconductor materials. The result shows that the spreadsheet concept is proven to be a useful tool for the learning process [11]. Apart from the spreadsheet, this paper also uses JavaScript. JavaScript has been widely used to create website applications [12]. The result shows that the web application functioned to calculate various integral functions. JavaScript is used as a comparison to spreadsheet simulation.

Sheets is indeed free software. In addition, the advantage of JavaScript is that this program can interact easily with HTML [13]. JavaScript also provides convenience in the scripting process, so that through the JavaScript program which is one of the basic coding programs it becomes easy to understand. Through the JavaScript program, it is easy to use to input data such as drag and drop [14]. Meanwhile, the Spreadsheet program is one of the preferred applications for processing data, whether in finance, research, science, engineering, or education. Spreadsheets play an important role in the fields of science and education because they make it easier to calculate and process numerical data [15]. Meanwhile, the appearance of the spreadsheet program is also easier to recognize and run than other computer programs. Data storage capabilities in Spreadsheets are quite large and easy to use using formulas and logic, so many students and teachers choose Spreadsheets as a medium for representing physics equations in graphical form. Thus, visualizing the FCC energy band equation can optimize students' physical analytical abilities. This is evidenced by research that reveals that the application of computational programs such as spreadsheets in physics learning can optimize their digital literacy skills [16].

The physics learning situation amid the COVID-19 outbreak has changed from face-to-face to online. This has been reviewed by several researchers, one of whom stated that using online methods (in a network) created a new problem, namely the transfer of knowledge to students [17]. The difficulties experienced by students are mainly in calculation materials. Teaching during the COVID-19 pandemic can be done with project-based online learning which becomes an alternative solution for learning activities [18]. Limited internet package is also one of the obstacles in implementing online learning. Project-based learning can be used to overcome it [19].

Based on the research above, the researcher suggests the use of spreadsheet media in the learning process since it has several advantages. The spreadsheet is easy to use for making simulations so that students can understand the materials deeper. The use of a spreadsheet is more cost-effective compared to online learning which requires an internet package in practice [20]. This paper aims to use spreadsheet media to visualize the face-centered cubic (FCC) energy band using the tight-binding method. The result of this paper is a simulation of the energy band and energy band diagonal slice. The energy band and diagonal slice obtained from the spreadsheet will be compared with modified JavaScript processing results from MATLAB results [21].

In this article, we propose a new approach for simulating material physics equations regarding the crystal structure of FCC using Spreadsheet and JavaScript. We use a visual representation of the FCC crystal energy band equation as a variation of distance learning physics media. By using Spreadsheet and JavaScript, students are expected to understand the theory of the FCC crystal energy band equation with a tight-binding approach easily. Interpreting the FCC crystal energy band equation with a tight-binding approach through a Spreadsheet can easily encourage teachers and students to facilitate learning activities at home during the COVID-19 pandemic.

2. Theory

The energy band is the energy needed for electrons to move. The movement of electrons in the gap between the valence and the conduction band shows the properties of a solid [22]. The energy band in the crystal structure can be studied using the tight-binding method or the interaction between the



FIGURE 1. Illustration of the tight-binding method on a simple cubic (SC) crystal structure.

closest atoms. Tight-binding calculates the first-order energy of the crystal by finding the diagonal matrix of the Hamiltonian [23]. An illustration of the tight-binding method for a simple cubic crystal structure is shown in Fig. 1.

We consider an atom in the SC system, which is shown in Fig. 1 by the yellow dot. The atom has 6 nearest neighboring atoms shown in red. Hence, it can be concluded that each atom in SC has 6 closest neighbors. We consider the tight-binding model for a Crystal system with 1 electron per atom. The electrons are assumed to occupy the "s" shell and move inside the crystal with a potential U(r) from an isolated atom having a function of $\phi(r)$.

The effect of atoms on Crystals is small. Meanwhile, the tight-binding model is a model in which electrons are tightly bound to the nucleus so that electrons tend to be around the nucleus [24]. Thus, electrons can move from one atom to another. The tight-binding model in other words can be interpreted as a model in material physics to analyze the energy band of FCC crystals [25]. Assuming that the potential of a single atom is U(r), then the Schrödinger equation can be written as in Eq. (1).

$$\left[\frac{p^2}{2m} + U(r)\right]\phi(r) = E_0\,\phi(r)\;.\tag{1}$$

We regard the effects of other atoms as disturbances. Each energy level of each atom is split into two in a two-atom hydrogen system. The degeneration of each energy level is two. For a system of n atoms, the degeneration of each energy level is n. Based on the perturbation theory, the wave function for a degenerative system can be written as a linear combination of degenerate states. If $C_{\vec{k}_j}$ in Eq. (2) is the same as on the right, the function satisfies the block theorem.

$$\psi_{\vec{k}}(\vec{r}) = \sum_{j} C_{\vec{k}_{j}} \phi(\vec{r} - \vec{r}_{j}) = \frac{1}{\sqrt{N}} \sum_{j} e^{i \, \vec{k} \cdot \vec{r}_{j}} \phi(\vec{r} - \vec{r}_{j}) \,. \tag{2}$$

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FIGURE 2. Screenshot of a spreadsheet to visualize the energy band.

TABLE I. Formulas	used in a	spreadsheet.
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Cell	Variable	Formula			
A2	Value lattice constant is 1	=1			
B2	Range of k (coordinate x and y)	=3*PI()/A2			
C2	k_z fixed	=PI()/(2*A2)			
G4-G193	x-coordinate	Range (-9.4:9.4), interval 0.1			
H3-GO3	y-coordinate	Range (-9.4:9.4), interval 0.1			
H4-GO193	Energy	=-(COS(\$G4*\$A\$2/2)*COS(H\$3*\$A\$2/2) +COS(H\$3*\$A\$2/2)*COS(\$C\$2*\$A\$2/2) +COS(\$G4*\$A\$2/2)*COS(\$C\$2*\$A\$2/2))			

We can also write a first-order energy correction which is the diagonal of the Hamilton matrix. Now we consider only the integration of the atom itself and its nearest neighbors [26]. Thus, we can simplify the expression and the way we define ϕ as the atomic integration itself.

$$\alpha_0 = -\int \phi(r)\widehat{H}\phi(r) dr ,$$

and
$$\gamma_0 = -\int \phi(r-\rho_n)\widehat{H}\phi(r) dr .$$
(3)

Meanwhile, γ is the integration of its closest neighbors. The integration is determined by the overlap of the two wavefunctions and finally, we get the final dispersion relationship from the tight-binding model. A situation where the sum of all N grid points is $\vec{r_j}$ is brought to the plane waveform. If Eq. (2) experiences a displacement of \vec{T} then $\vec{r} \rightarrow \vec{r} + \vec{T}$ so that it results

$$\psi_{\vec{k}}(\vec{r}+\vec{T}) = \sum_{j} C_{\vec{k}_{j}} \phi(\vec{r}+\vec{T}-\vec{r}_{j}) e^{i\,\vec{k}\cdot\vec{T}} \psi_{\vec{k}}(\vec{r}).$$
(4)

Using Dirac notation, Eq. (2) can be written in this way

$$|\vec{k}\rangle = \frac{1}{\sqrt{N}} \sum_{j} e^{i\,\vec{k}\cdot\vec{r}_{j}} |j\rangle \,. \tag{5}$$

Where $|\vec{k}\rangle$ represents the normalized Crystal wave function $\psi_{\vec{k}}(\vec{r})$ and $|j\rangle = |\phi_j\rangle$ represents the basis of the function $\phi(\vec{r} - \vec{r_j})$. The function $|\vec{k}\rangle$ is automatically normalized because the function basis $|j\rangle$ is orthonormal. The initial calculation of the tight-binding method is to calculate the first level energy of the crystal to find the diagonal matrix elements of the Hamiltonian in Eq. (6).

$$\langle \vec{k} | \hat{H} | \vec{k} \rangle = \frac{1}{N} \sum_{j} \sum_{m} e^{i \vec{k} \cdot (\vec{r}_j - \vec{r}_m)} \langle m | \hat{H} | j \rangle .$$
 (6)

Where $\langle m|\hat{H}|j\rangle \equiv \int dV \phi(\vec{r}-\vec{r}_m)\hat{H}\phi(\vec{r}-\vec{r}_j)$. If $\vec{\rho}_m \equiv \vec{r}_m - \vec{r}_j$ and $\phi(\vec{r}-\vec{r}_m) = \phi(\vec{r}-\vec{\rho}_m-\vec{r}_j)$ so that the energy becomes Eq. (7).

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FIGURE 3. HTML coding.

$$\begin{aligned} \langle \vec{k} | \hat{H} | \vec{k} \rangle &= \sum_{m=0,nn} e^{-i \, \vec{k} \cdot \vec{\rho}_m} \int dV \phi(\vec{r} - \vec{\rho}_m) \hat{H} \phi(\vec{r}) \\ &= e^{-i \, \vec{k} \cdot \vec{\rho}_0} \int dV \phi(\vec{r} - \vec{\rho}_0) \hat{H} \phi(\vec{r}) \\ &+ \sum_{m=nn} e^{-i \, \vec{k} \cdot \vec{\rho}_m} \int dV \phi(\vec{r} - \vec{\rho}) \hat{H} \phi(\vec{r}) \\ &= -\alpha - \gamma \sum_{m=nn} e^{-i \, \vec{k} \cdot \vec{\rho}_m} \equiv \varepsilon_k . \end{aligned}$$
(7)

Meanwhile, the face-centered cubic (FCC) structure has 12 interactions with the closest neighbors shown in Eq. (8).

$$\vec{\rho}_m = \left(\frac{a}{2}\right) \left((1, -1, 0), (1, 1, 0), (-1, -1, 0), (-1, 1, 0), (0, -1, 1), (0, 1, 1), (0, -1, -1), (0, 1, -1), (1, 0, 1), (-1, 0, -1), (1, 0, -1), (-1, 0, -1)\right).$$
(8)

Using Eq. (6) in the FCC, the is the energy band shown in Eq. (8).

$$\varepsilon_{\vec{k},\text{FCC}} = -\alpha - 4\gamma \left(\cos\left[\frac{k_x a}{2}\right] \cos\left[\frac{k_y a}{2}\right] + \cos\left[\frac{k_y a}{2}\right] \right) \times \cos\left[\frac{k_z a}{2}\right] + \cos\left[\frac{k_x a}{2}\right] \cos\left[\frac{k_z a}{2}\right] \right). \tag{9}$$

Based on Eq. (9) Φ is the wave function of atomic orbitals, α is the integration of the atom itself, and γ is the integration of its closest neighbors.

3. Method

This research used a spreadsheet to visualize the Energy band on the face-centered cubic (FCC) Crystal structure. Visualization was made in 3D with a surface contour graph plot and 2D with a Scatter chart plot. Plot the graph using Eq. (8). Coordinates k_x and k_y in a spreadsheet with a range of $\pm 3\pi/a$, were in a spreadsheet, for example, q and a, were lattice constants with a value of 1. The value of k_z was fixed at $k_z = \pi/2a$. The 189 × 189 matrix was obtained in a spreadsheet which was then plotted in 3 and 2 dimensions. Then, 1 energy band and a diagonal energy band slice in the FCC Crystal structure were obtained. This simulation only used 1 energy band, namely the valence band, and the results would be compared between the results of the spreadsheet and the modeling using the JavaScript programming language that had been created. The spreadsheet view is shown in Fig. 2. Meanwhile, the formulas used in the spreadsheet are shown in Table I.

Table I is the formula used in the spreadsheet. The first column is the cell in the spreadsheet, the second column is the explanation or variable in the spreadsheet, and the third column is the formula or formula used to get the calculation results. Cell A2 in the spreadsheet is filled with the value 1, which means the lattice constant is worth 1. Meanwhile, Cell B2 in the spreadsheet is filled with the formula =3*PI()/A2 which is the range in the x and y coordinates. Cell C2 is filled with a fixed value of k with the formula =PI()/(2*A2). Cells G4 to G193 are x-coordinates with a range of -9.4 to 9.4 with 0.1 intervals. Cells H3 to GO3 are y-coordinates with a range of -9.4 to 9.4 with an interval of 0.1. Cells H4 to GO193 are energy bands using equations in FCC crystal structure. The following is energy band JavaScript coding on the structure of FCC crystal. It is three dimensions of the energy band. HTML used was the plugin of https://plotly.com. HTML coding is shown in Fig. 3.

Meanwhile, the detailed explanation or information presented in Fig. 3 is as follows. The script starts with creating HTML, HTML is a framework that contains the head and body, the script is written starting with the opening tag < >and ending with the closing tag </>. The <head> section



FIGURE 4. JavaScript coding.

contains <title> which is used to give the title to the browser, then the JavaScript source code is entered in the head section by writing <script></script>. Sources for plotting graphs are taken from the plot.ly site. The head section ends with a closing tag </head>. After the head section, the core section is written with the script <body>. Furthermore, in the body section there is a script to wrap <div></div>. Inside the body section, write javascript coding by writing the script src="3D.js" and the end of the body section with the closing tag body </body> and the last closing tag </html>. Meanwhile, the code to visualize the 3D graphics using JavaScript programming language is shown in Fig. 4.

Figure 4 starts with initialization or input variables can be written with var. Creates an empty matrix place for the data. Next use for looping data. In the for command, write the equation for the energy band of the FCC crystal structure as Eq. (9). After obtaining the energy band for each point, a graph is made by setting the naming of the x, y, z axes and the title of the graph using a 3D layout script in which there is a title, text, font type, and size. Then naming the x-axis, y-axis, and z-axis. After naming the 3D graph plotted using the plot command.

4. Results and Discussion

Learning using a spreadsheet could ease students in understanding the energy band in the crystal structure. Energy bands determine the electrical properties of materials such as conductors, semiconductors, and insulators. Therefore, this simulation needs to be done by creating learning innovations using a spreadsheet. In the case of the FCC Crystal structure, a spreadsheet can be used in understanding metals' structure.

Metals are known as heat conductors. They are conductors because materials do not show any gap [26]. This paper can visualize energy bands in FCC crystal structure with a spreadsheet or JavaScript software. The energy band of the FCC crystal structure is shown in Fig. 5.

So far, the mastery of physics concepts is still lacking due to the difficulty of visualizing complex physics equations [27]. Therefore, innovations are needed in carrying out the learning process, such as spreadsheets, especially in material courses. This paper shows a simulation of the energy band using the spreadsheet shown in Fig. 5a). Meanwhile, Fig. 5b) simulates the energy band using JavaScript. The two simulations show compatibility. It shows that the use of a spreadsheet has the advantage of being easy to use in making simulations without requiring a complicated programming language. Figure 5 illustrates 1 energy band in the FCC Crystal structure with an energy value range of -2.5 to 1. The x and y coordinates have a range of -9 to 9 with an interval of 0.1 so that a 189×189 matrix is obtained and the lattice constant is 1.

This spreadsheet learning media is used as a visual aid, such as a picture or model which can provide concrete experiences for students so that they can improve their learning



FIGURE 5. Energy band simulation in the FCC Crystal structure using a) a spreadsheet, b) JavaScript.



FIGURE 6. The diagonal slice of the energy band is normalized using a) a spreadsheet, b) JavaScript.

outcomes, especially during the COVID-19 pandemic which requires distance learning. In addition to the 3-dimensional simulation, this paper also used a simulation in a 2dimensional model obtained by making a diagonal slice in the 3-dimensional energy band image shown in Fig. 6. This paper shows that a spreadsheet is a tool that can be used for innovative learning. This technology-based learning is suitable for use during the COVID-19 pandemic in distance learning.

Spreadsheet and JavaScript have their respective strengths and weaknesses. When viewed in terms of making, JavaScript graphics are superior to the spreadsheet as they can make 3-dimensional graph plots more freely. However, the limitation is that JavaScript is relatively difficult to be used since it employs a programming language. The advantage of using a spreadsheet can be found in the calculation process and they do not use complicated programming languages such as JavaScript [28]. The weakness of spreadsheets exists in creating graphics, especially 3-dimensional, which cannot be as flexible as JavaScript.

Meanwhile, currently, the whole world is being hit by a coronavirus outbreak. As a result, the education process in Indonesia uses distance learning as an effort to tackle the transmission of the coronavirus. The distance learning method is sought to be effective because of the importance of transferring knowledge to students. The effectiveness of distance learning can be made using easy to use and effective media, namely spreadsheets. This paper has successfully used a spreadsheet in simulating the band energy in the crystal structure of the FCC. An understanding of the energy band is important in materials courses in physics majors. The spreadsheet helps in improving critical thinking skills, data analysis, mathematical skills, problem-solving, creativity, and innovation [29]. This ability is urgently needed in this era. The visualization simulated shows that difficult physics equations can be easily simulated using a spreadsheet when compared to complex JavaScript programming language. This paper suggests that a spreadsheet is a suitable medium for distance learning.

The spreadsheet used in interpreting the FCC equation with a tight-binding approach certainly has benefits in learning at home during the COVID-19 pandemic. This is done by teaching FCC material with a tight-binding approach to students through tutorials or project activities by providing an understanding of the operation of spreadsheets [30]. In addition, students are also given examples of the process of interpreting some physics equations through a Spreadsheet which is then visualized in a graph through a Spreadsheet. Through these activities, spreadsheets can certainly be used as one of the useful learning media in supporting distance learning of physics [31]. In addition, through a spreadsheet, students are asked to understand the physics equation first and then convert the physics equation into coding in the Spreadsheet. Thus, students can optimize their theoretical understanding of the FCC equations with their tight-binding approach and analytical skills.

6

In this study, FCC crystal energy bands were visualized through Spreadsheet and JavaScript programs to know the differences in the ease of the visualization process and the results produced by the two programs. Based on the results of the visualization of the FCC crystal energy bands from the two programs, the results of the graphical visualization are better in a smoother sense through JavaScript. The use of programming languages in this study can assist students in solving problems logically through propositional algorithms [32]. This research does not use other computational programs such as Mathematica because it emphasizes the novelty of the research. The novelty of this research is to create scripts using the JavaScript programming language which can later be inserted into a website. In addition, learning physics combined with the application of physics concepts in spreadsheet computing programs and JavaScript can optimize students' computational thinking skills.

It is true that the use of Spreadsheets in lectures for distance undergraduate students provides variety in learning and makes it easier for students to understand and apply physics equations independently [33]. This is because the visualization of physics equations such as the FCC energy band through the Spreadsheet can be done independently by each student by transferring the existing physics equations into the Spreadsheet workspace without writing complicated coding. Students just write down the existing physics equations [34]. While the use of JavaScript must be done with expert guidance considering that compiling a JavaScript program requires quite complicated coding [35]. However, the graphical visualization results generated by JavaScript are smoother than the graphical visualization results generated by sheets. With the advantages and disadvantages of the two computational programs used in this study, it can provide more varied choices of learning media according to learning conditions and needs. In addition, with the current conditions that are still being affected by the COVID-19 pandemic, it is more realistic to use spreadsheets [36]. This is because visualizing physical equations, especially FCC energy bands, does not require the help of others to teach the coding process. This can also be used as a step to break the chain of the spread of the COVID-19 pandemic.

Meanwhile, the ways that can be done in using the Spreadsheet program to motivate students in learning are as follows. The spreadsheet program can be used as one of the learning media that makes it easier for students to understand and apply simple physics equations. Optimizing students' motivation to learn physics using Spreadsheets is done by the teacher providing explanations about physics concepts which are sometimes realized in the laboratory. Especially with the current conditions affected by the COVID-19 pandemic, it is possible that learning in the laboratory cannot be carried out. After the teacher gave an example of using Spreadsheets to visualize physics equations by generating graphs without complex coding like other computational programs, students were asked to visualize similar graphs. Through these activities, students' motivation in studying physics material that tends to be abstract is increased [37]. Moreover, learning physics represented in graphic visualization can increase student interest in participating in learning [38]. This is due to variations in the delivery of material by the teacher in the form of verbal, narrative, or visual. Furthermore, the implementation of spreadsheets in physics learning, especially material physics lectures, also has a positive impact on students' abilities. This is because spreadsheets are easy to operate, so the integration of spreadsheets in material physics lectures is more attractive to students to take the lectures [39, 40].

5. Conclusion

This paper shows the use of a spreadsheet that can be implemented in learning, especially physics. Difficult equations can be easily simulated using a spreadsheet when compared to JavaScript. Spreadsheet as a learning medium can be used to visualize the face-centered cubic (FCC) energy band using the tight-binding method. This paper demonstrates the use of innovative learning media using a spreadsheet. However, the spreadsheet also has some disadvantages when compared to JavaScript, that it is less suitable to use in 3-dimensional graph plots if the equation using the *z*-axis changes.

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