Crystalline Band Energy Simulation as a Materials and Programming Project during the Covid-19 Pandemic

Syella Ayunisa Rani [1,2], Ariswan Ariswan [3], Supardi Supardi [3], Himawan Putranta [1,4], Aditya Yoga Purnama [1,5], Wipsar Sunu Brams Dwandaru [3]

[1] *Educational Sciences Department, Physics Education Concentration, Graduate School, Universitas Negeri Yogyakarta, Jl. Colombo No. 1, Sleman, Yogyakarta 55281, Indonesia*
[2] *SMA Negeri 1 Magelang, Jl. Cempaka No. 1, Kemirirejo, Magelang, Central Java 56122, Indonesia*
[3] *Physics Education Department, Faculty of Mathematics and Natural Sciences, Universitas Negeri Yogyakarta, Jl. Colombo No. 1, Sleman, Yogyakarta 55281, Indonesia*
[4] *Physics Education Department, Faculty of Tarbiyah and Teacher Training, Universitas Islam Negeri Sunan Kalijaga, Yogyakarta 55281, Indonesia*
[5] *Physics Education Department, Universitas Sarjanawiyata Tamansiswa, Jl. Kusumanegara No. 157, Umbulharjo, Yogyakarta 55165, Indonesia*

Abstract – **This study was aimed to 1) create a fun materials and programming project during the Covid-19 pandemic, 2) simulate SC, BCC, and FCC crystallines stuctures' energy bands, and 3) investigate the obtained energy bands properties. Python was used as the software. The subjects were second year undergraduate students. They were asked to simulate the crsytals' energy band using the tight-binding formulas. We concluded that 1) materials and programming can be a fun project during the Covid-19 pandemic, 2) the simulations can be done using the Python software, and 3) the larger the lattice constant, the more profiles produced.**

Keywords – **energy band simulation, crystalline structure, tight-binding formula, Python software**

1. Introduction

The Covid-19 pandemic has been going on for more than two years [1], [2], [3]. Until now, learning in higher education has not been able to be conducted normally. Several universities are still holding full online learning due to the Covid-19 pandemic [4], [5], although some of them have conducted limited offline learning or blended learning [6], [7]. Interactive face-to-face lectures turn into monotonous online learning where lecturers only taught and students listened. Consequently, many lessons are not well absorbed, one of which is at the undergraduate level [8], [9]. Laboratory experiments at universities are also still carried out on a limited basis [10], [11], [12]. Hence, to make lectures more meaningful with fun activities, we tried to combine materials and programming lectures with a project, i.e., project based learning (PjBL). So that materials courses are not only studying theory, whereas programming course is not only studying programming languages. Students can apply what they have learned from both lectures in a project.

One of the subjects learned in the materials lecture is the energy band crystals of simple cubic (SC), body-centered cubic (BCC), and face centered cubic (FCC) [13], [14], [15]. By studying the energy bands, we can find out the electronic energy levels in the crystals, so that the crystals' properties can be determined [15], [16]. In addition, the energy bands can also be used to distinguish metals,

semiconductors, and insulators [17]. Solving the Schrodinger's equation on the interacting electrons and ions is needed to determine the energy band of crystals [18]. One method that can be used is the tight-binding model. The tight-binding model is conceptually and computationally efficient for describing the electronic properties of materials [19]. It is based on the assumption that crystals are formed from isolated atoms that are slowly brought together. All wave functions obey Bloch's theorem [20], [21]. The equations and parameters for the energy bands of SC, BCC, and FCC crystals using the tight-binding method according to [15] are listed in Table 1. This method uses one electron per atom. The electron is assumed to be in the "s" state and moving due to the crystal potential of an isolated atom, while the influence of the other crystal atoms is small.

The interesting part of the study is that students are asked to make simulations of the energy bands of SC, BCC, and FCC crystals in a project. Through this activity, students can practice their programming language and investigate the characteristics of the crystals. In that way, students can understand the concepts and theories of the simulated crystal [22]. Python is used as the software in the simulation. This is because Python is learned in the programming lectures, it is a free software and no payment is required [23], [24], it is easy to apply using a computer [23], [25], contains functions that allows completing tasks without preparing the program from scratch [23], [24], contains a simple syntax that is easy for beginners to understand [24], [25], [26], and has been proven to be successfully used in learning [24], [25]. When compared with Spreadsheets [27], [28], [29], Python may be more complicated and take longer to learn, but the computational capabilities are much better [24].

In this study, we conducted a fun materials and programming project, i.e., simulating the energy bands of SC, BCC, and FCC crystals with lattice constant variation of 2, 4, 6, 8, 10, and 12 Å. We use Python as the software for the simulation. Finally, we investigate and discuss the energy band characteristics resulted from the three crystal structures.

Table 1. Crystal's energy band formula

Crystal	Formula	Parameters
SC	$-(\cos(k_x a) + \cos(k_y a) + \cos(k_z a))$	$a = 1$ $k_x = \pm 2\pi/a$ $k_y = \pm 2\pi/a$ $k_z = 0$
BCC	$-\cos\left(\dfrac{k_x a}{2}\right)\cos\left(\dfrac{k_y a}{2}\right)\cos\left(\dfrac{k_z a}{2}\right)$	$a = 1$ $k_x = \pm 2\pi/a$ $k_y = \pm 2\pi/a$ $k_z = \pi/2a$
FCC	$-\left(\cos\left(\dfrac{k_x a}{2}\right)\cos\left(\dfrac{k_y a}{2}\right) + \cos\left(\dfrac{k_y a}{2}\right)\cos\left(\dfrac{k_z a}{2}\right) + \cos\left(\dfrac{k_x a}{2}\right)\cos\left(\dfrac{k_z a}{2}\right)\right)$	$a = 1$ $k_x = \pm 3\pi/a$ $k_y = \pm 3\pi/a$ $k_z = \pi/2a$

2. Method

The subjects of this study were second year undergraduate students who were taking materials and programming lectures. They were asked to simulate the energy band crystals using the Phyton programming language. The crystals being studied were SC, BCC, and FCC according to the energy band equations in Table 1. Students were free to determine the wavenumber, k, on the x, y, and z axes. Note that in SC, k_z is zero. In BCC and FCC, k_z is a specific value. The selection of software and materials was based on the subjects studied in both lectures. Students were asked to investigate and discuss the energy band properties of the three types of crystals simulated.

In this study, the crystal lattice variations of 2, 4, 6, 8, 10, and 12 Å were used. Each variation was simulated twice for each type of crystal, i.e., at angles of (30, 35) and (70, 35). Angles of 30 and 70 mean that the graph was rotated upwards by 30 or 70 degrees from its original position. Angle 35 means that the graph was rotated counterclockwise by 35 degrees. The purpose of doing two simulations was to be able to observe the energy profile that was formed from two points of view.

This programming syntax involved mathematical equations. The first thing to do was to import numpy as np and matplotlib.pyplot as plt in Python. Use the variation of the lattice constant, $a = 2, 4, 6, 8, 10$, and 12 Å. Determine the intervals of k_x, k_y, and k_z. In this study, k_x and k_y were -1 to 1, with a total of 100 data. k_z was determined based on the type of crystal, that is, SC was 0, BCC and FCC were $\pi/2a$. The energy band of the crystal was expressed in the form of a function $f(x,y)$. The graph plot used 3D contours.

```
import numpy as np
import matplotlib.pyplot as plt

a = 2
phi = 3.14
x = np.linspace(-1, 1, 100)
y = np.linspace(-1, 1, 100)
z = 0

def f(x, y):
    return -np.cos(x*a)-np.cos(y*a)-np.cos(z*a)

X, Y = np.meshgrid(x, y)
E = f(X, Y)

fig = plt.figure()
ax = plt.axes(projection='3d')
ax.contour3D(X, Y, E, 50, cmap='viridis')

ax.set_xlabel('kx')
ax.set_ylabel('ky')
ax.set_zlabel('E')

#ax.view_init(30, 35)
ax.view_init(70, 35)
fig
```

Figure 1. SC energy band program using Python

```
import numpy as np
import matplotlib.pyplot as plt

a = 2
phi = 3.14
x = np.linspace(-1, 1, 100)
y = np.linspace(-1, 1, 100)
z = phi/(2*a)

def f(x, y):
    return -np.cos(x*a/2)*np.cos(y*a/2)*np.cos(z*a/2)

X, Y = np.meshgrid(x, y)
E = f(X, Y)

fig = plt.figure()
ax = plt.axes(projection='3d')
ax.contour3D(X, Y, E, 50, cmap='viridis')

ax.set_xlabel('kx')
ax.set_ylabel('ky')
ax.set_zlabel('E')

ax.view_init(30, 35)
#ax.view_init(70, 35)
fig
```

Figure 2. BCC energy band program using Python

```
import numpy as np
import matplotlib.pyplot as plt

a = 2
phi = 3.14
x = np.linspace(-1, 1, 100)
y = np.linspace(-1, 1, 100)
z = phi/(2*a)

def f(x, y):
    return -(np.cos(x*a/2)*np.cos(y*a/2)+np.cos(y*a/2)*
            np.cos(z*a/2)+np.cos(x*a/2)*np.cos(z*a/2))

X, Y = np.meshgrid(x, y)
E = f(X, Y)

fig = plt.figure()
ax = plt.axes(projection='3d')
ax.contour3D(X, Y, E, 50, cmap='viridis')

ax.set_xlabel('kx')
ax.set_ylabel('ky')
ax.set_zlabel('E')

ax.view_init(30, 35)
#ax.view_init(70, 35)
fig
```

Figure 3. FCC energy band program using Python

3. Results and Discussion

This study aims to 1) create a fun materials and programming lecture project during the Covid-19 pandemic, 2) simulate the energy bands of SC, BCC, and FCC crystals at lattice constants of 2, 4, 6, 8, 10, and 12 Å, and 3) investigate the energy band properties of the three crystals. Second year undergraduate students who take materials and programming lectures are asked to simulate the energy band crystals. The crystals used are SC, BCC, and FCC according to the energy band equations in Table 1. Python is used as the software for the simulation. In this study, k_x and k_y are -1 to 1, with a total of 100 data. k_z is determined based on the type of crystal, i.e., SC is 0, BCC and FCC are $\pi/2a$. The variations of the lattice constant are 2, 4, 6, 8, 10, and 12 Å. Each variation was simulated twice, at angles of (30, 35) and (70, 35).

The coding using Phyton for simulating the energy bands of the SC, BCC, and FCC crystals are given in Figures 1. to 3., respectively. It may be observed that all of the codes containing equations in Table 1. are quite simple. The simplicity of the codes can make error tracking easier such that programming becomes a fun activity. Of course, the structure of the coding for all crystalline structures are the same. The difference is only on the equation used for each crsytalline structure. The results of the computations are given in Figures 4. to 9. with variation of the lattice constants, i.e., 2, 4, 6, 8, 10, and 12 Å, respectively.

Figure 4. shows the results of the computation for the lattice constant of 2 Å. At a lattice constant of 2 Å, there is no difference in the energy band profile between SC, BCC, and FCC, only the energy ranges are slightly different. The highest energy range is obtained for SC, whereas the smallest is attained for BCC. The three energy profiles are shaped like a cone, which consists of four sides. The ends of the sides are raised upwards and have a valley in the middle.
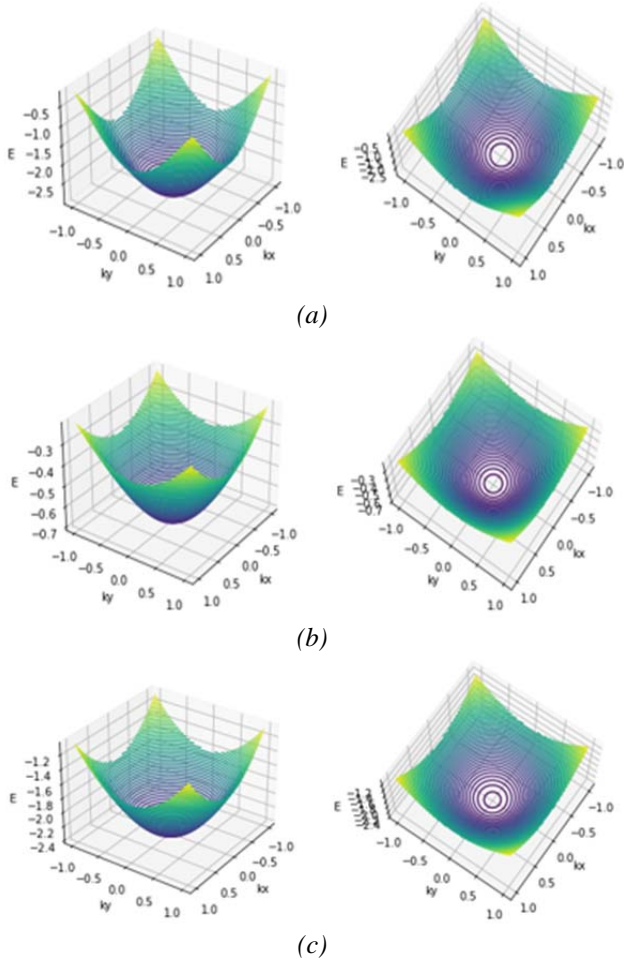

(a)

(a)

(b)

(b)

(c)

(c)

Figure 5. Lattice constant of 4Å, (a) SC, (b) BCC, and (c) FCC

Figure 4. Lattice constant of 2Å, (a) SC, (b) BCC, and (c) FCC

At a lattice constant of 4Å (see Figure 5.), the SC has started to form like a flower petal, where the ends of each side are lifted upwards to form peaks. In the middle there is a valley. The energy band ranges tend to be the same as before. BCC shows a different profile, the ends of the sides are raised although not as high as SC. The sides are raised higher than the ends. These sides form the peaks. While the ends of the sides form a valley. On the other hand, this is less pronounced for the FCC because all four sides and ends rise simultaneously. In contrast to SC, the energy ranges of FCC and BCC change almost twice.
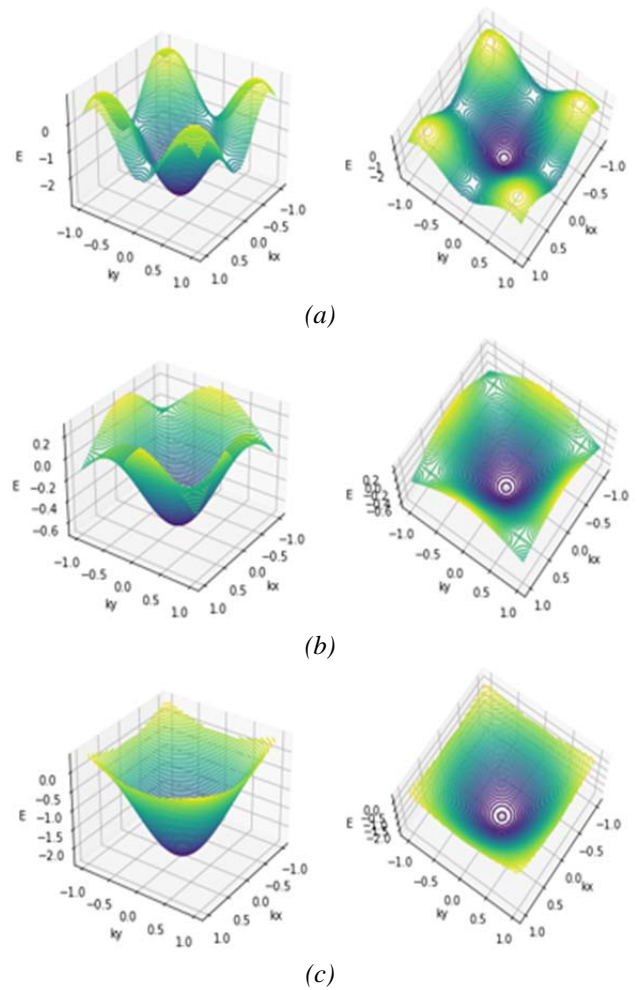
At a lattice constant of 6Å (see Figure 6.), SC forms four complete peaks with one complete valley in the middle. The energy band ranges are relatively the same. The BCC almost consists of four peaks, but not yet fully formed. In the middle there is a valley. The position of the four sides is at the top, while the sides are lower. On the other hand, the sides and ends of the FCC tend to increase and the profile on the sides seems to widen. Not a single peak is seen in this profile. Only one valley is visible in the middle and a unique profile on all four sides. When compared to the lattice constant of 4Å, the energy ranges of BCC and FCC tend to increase slightly.

At a lattice constant of 8 Å (see Figure 7.), SC has four full peaks, eight incomplete peaks, one intact valley, and eight incomplete valleys. The SC energy profiles are most rapidly formed compared to other types of crystals. The BCC energy profile is almost the same as the energy profile for the 6 Å lattice constant. The difference is that this profile tends to narrow to the middle, so that a new profile is formed in the direction of the specified *x* and *y* axes, namely -1 to 1. The profile on the FCC side looks wider. The energy ranges of the FCC and BCC are relatively the same as the lattice constant of 6 Å.
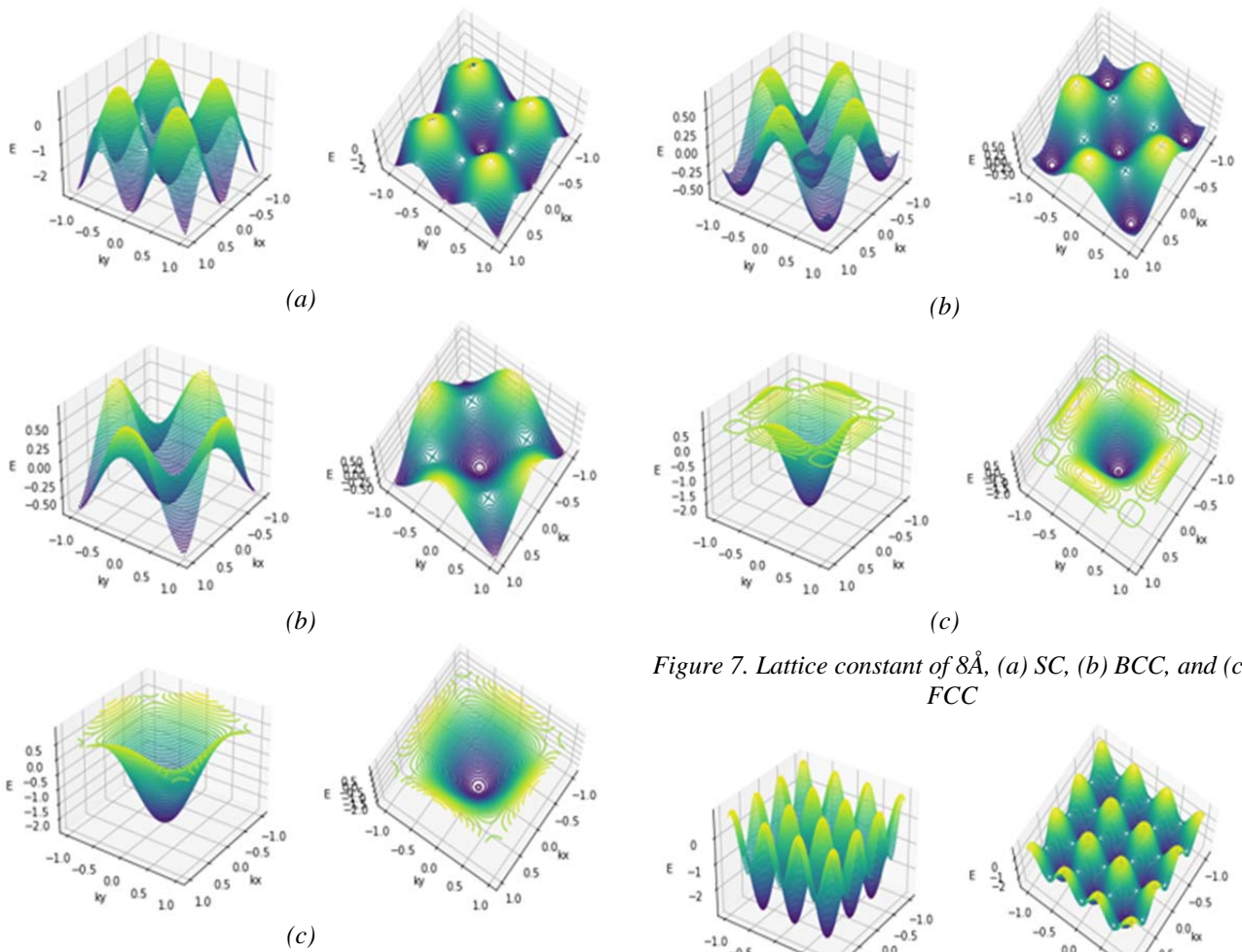
(a)

(b)

(c)

Figure 6. Lattice constant of 6Å, (a) SC, (b) BCC, and (c) FCC

At a lattice constant of 10 Å (see Figure 8.), the number of peaks and valleys of the SC energy increase. There are four intact peaks, twelve incomplete peaks, and nine complete valleys. This means that the larger the lattice constant over a certain range of *x* and *y* axes produced more peaks and valleys. The BCC forms four full peaks and five full valleys. The FCC begins to form a profile like flower petals. The energy profile in this petal has different characteristics compared to SC and BCC. The energy ranges of the BCC and FCC are relatively the same compared to the lattice constants of 6 Å and 8 Å. Meanwhile, the SC energy range does not change much from the initial variation of the lattice constant.
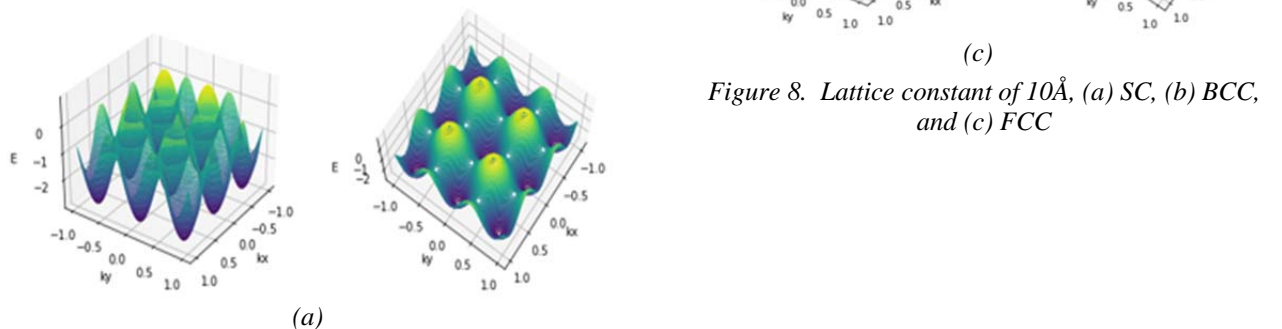

(a)

(b)

(c)

Figure 7. Lattice constant of 8Å, (a) SC, (b) BCC, and (c) FCC

(a)

(b)

(c)

Figure 8. Lattice constant of 10Å, (a) SC, (b) BCC, and (c) FCC
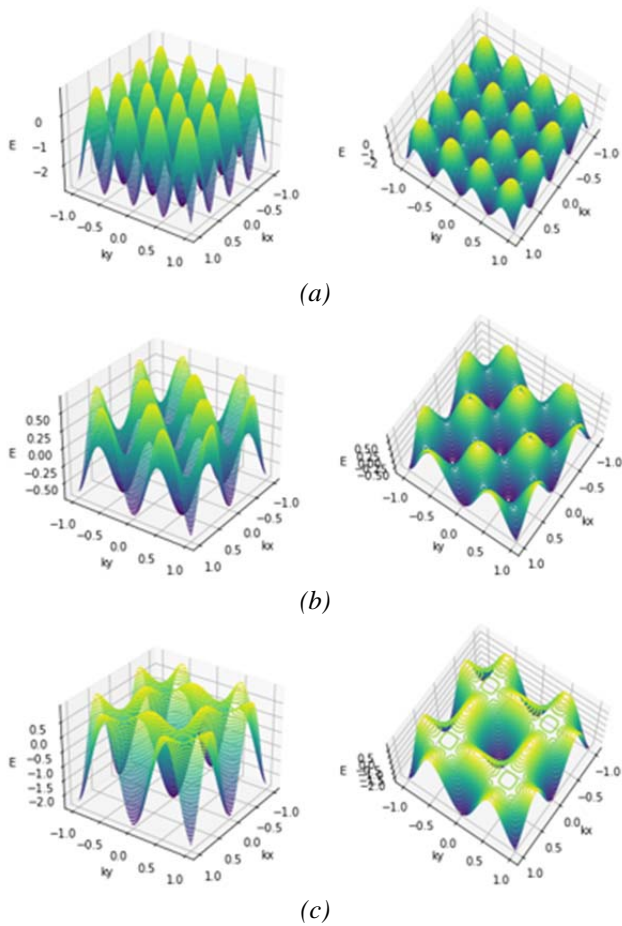
(a)

(b)

(c)

Figure 9. Lattice constant of 12Å, (a) SC, (b) BCC, and (c) FCC

At a lattice constant of 12 Å (see Figure 9.), there are sixteen full peaks, nine full valleys, and twelve incomplete valleys in the SC energy profile. However, the SC does not experience any significant change in the energy range during the variation of the lattice constants of 2, 4, 6, 8, 10, and 12 Å. The BCC forms four full peaks, eight incomplete peaks, five full valleys, and eight incomplete valleys. Moreover, the formation of FCC energy profiles is slower than SC and BCC. The FCC has one full valley in the center and eight surrounding incomplete valleys. This FCC energy profile has no peak. The flat profile part form a unique energy profile. The energy ranges of the BCC and FCC are relatively the same compared to the lattice constants of 6, 8, 10, and 12 Å.

4. Conclusion

Based on this study, we can conclude that the materials and programming lectures can be combined in a fun lecture project during the Covid-19 pandemic. The energy band simulations using the tight-binding method on various lattice constants can be done using the Python program language. From the simulation, we can find that the larger the lattice constant over a certain range of *x* and *y*-axes, the more energy profiles produced. The profile formation is fastest and slowest for the SC and FCC crystalline structures, respectively. There is no difference in the profiles of SC, BCC, and FCC at a lattice constant of 2 Å. The difference is only on the energy range where the largest and smallest energy ranges are obtained for SC and BCC crystalline structures, respectively. The SC and BCC have peak and valley profiles, while FCC does not have any peak profiles. The SC does not experience a significant change in the energy range during the constant lattice variation. The BCC and FCC have increasing energy range at lattice constants of 4 Å and 6 Å. The highest increase is found for the lattice constant of 4 Å. The energy ranges of the BCC and FCC do not change for the lattice constants from 6 Å to 12 Å.

References

[1]. Daniel, S. J. (2020). Education and the COVID-19 pandemic. *Prospects*, *49*(1), 91-96.

[2]. Klein, P., Ivanjek, L., Dahlkemper, M. N., Jeličić, K., Geyer, M. A., Küchemann, S., & Susac, A. (2021). Studying physics during the COVID-19 pandemic: Student assessments of learning achievement, perceived effectiveness of online recitations, and online laboratories. *Physical review physics education research*, *17*(1), 010117.

[3]. Szopiński, T., & Bachnik, K. (2022). Student evaluation of online learning during the COVID-19 pandemic. *Technological Forecasting and Social Change*, *174*, 121203.

[4]. Sarpong, S. A., Dwomoh, G., Boakye, E. K., & Ofosua-Adjei, I. (2021). Online teaching and learning under COVID-19 pandemic; perception of university students in Ghana. *Eur J Interact Multimedia Educ*, *3*(1), e02203.

[5]. Adeyeye, B., Ojih, S. E., Bello, D., Adesina, E., Yartey, D., Ben-Enukora, C., & Adeyeye, Q. (2022). Online Learning Platforms and Covenant University Students' Academic Performance in Practical Related Courses during COVID-19 Pandemic. *Sustainability*, *14*(2), 878.

[6]. McLure, F. I., Koul, R. B., & Fraser, B. J. (2022). University Students' Classroom Emotional Climate and Attitudes during and after COVID-19 Lockdown. *Education Sciences*, *12*(1), 31.

[7]. Finlay, M. J., Tinnion, D. J., & Simpson, T. (2022). A virtual versus blended learning approach to higher education during the COVID-19 pandemic: The experiences of a sport and exercise science student cohort. *Journal of Hospitality, Leisure, Sport & Tourism Education*, *30*, 100363.

[8]. Xin, M., Luo, S., She, R., Yu, Y., Li, L., Wang, S., ... & Lau, J. T. F. (2020). Negative cognitive and psychological correlates of mandatory quarantine during the initial COVID-19 outbreak in China. *The American psychologist*, *75*(5), 607-617.

[9]. Tan, C. (2021). The impact of COVID-19 pandemic on student learning performance from the perspectives of community of inquiry. *Corporate Governance*, 1215-1228.

[10]. Mukhtar, K., Javed, K., Arooj, M., & Sethi, A. (2020). Advantages, Limitations and Recommendations for online learning during COVID-19 pandemic era. *Pakistan journal of medical sciences*, *36*(COVID19-S4), S27.

[11]. Gamage, K. A., Wijesuriya, D. I., Ekanayake, S. Y., Rennie, A. E., Lambert, C. G., & Gunawardhana, N. (2020). Online delivery of teaching and laboratory practices: continuity of university programmes during COVID-19 pandemic. *Education Sciences*, *10*(10), 291.

[12]. Andrews, J. L., de Los Rios, J. P., Rayaluru, M., Lee, S., Mai, L., Schusser, A., & Mak, C. H. (2020). Experimenting with at-home general chemistry laboratories during the covid-19 pandemic. *Journal of chemical education*, *97*(7), 1887-1894.

[13]. Mitchell, B. S. (2004). An Introduction to Materials Engineering and Science for Chemical and Materials Engineers. *Hoboken, NJ: John Wiley & Sons, Inc.*

[14]. Kittel, C. (2005). Introduction to solid state physics, John Wiley & Sons. *Inc., Sixth edition,(New York, 1986).*

[15]. Hasbun, J. E., & Datta, T. (2019). *Introductory Solid State Physics with MATLAB® Applications*. CRC Press.

[16]. Pamungkas, M. A., Setyowati, D. A., & Abdurrouf. (2018, October). Optical properties of Ga-doped silicene and as-doped silicene: First principle calculations. In *AIP Conference Proceedings* (Vol. 2021, No. 1, p. 050014). AIP Publishing LLC.

[17]. Han, T., Ruan, H., Cao, S., Guan, Y., Tang, D., & Yang, X. (2021). *Photoelectric Materials and Devices*. World Scientific.

[18]. Abdurrouf, M., Nurhuda, & Wiyono. (2019, July). Modelling one-dimensional crystal by using harmonic oscillator potential. In *IOP Conference Series: Materials Science and Engineering* (Vol. 546, No. 5, p. 052001). IOP Publishing.

[19]. Supka, A. R., Lyons, T. E., Liyanage, L., D'Amico, P., Al Orabi, R. A. R., Mahatara, S., ... & Fornari, M. (2017). AFLOWπ: A minimalist approach to high-throughput ab initio calculations including the generation of tight-binding hamiltonians. *Computational Materials Science*, *136*, 76-84.

[20]. Watanabe, H. (2019). A proof of the Bloch theorem for lattice models. *Journal of Statistical Physics*, *177*(4), 717-726.

[21]. Agustino, R., & Rosyid, M. F. (2013). Bentuk Fungsional Energi Elektron Bloch Pada Potensial Periodik Semikonduktor. *Jurnal Fisika Indonesia*, *17*(51), 31-34.

[22]. Rani, S. A., Mundilarto, W., & Dwandaru, W. S. B. (2019). Physics virtual laboratory: an innovative media in 21st century learning. In *Journal of Physics: Conference Series* (Vol. 1321, p. 022026).

[23]. Rivas, D., Alvarez, M., Velasco, P., Mamarandi, J., Carrillo-Medina, J. L., Bautista, V., ... & Huerta, M. (2015, February). BRACON: Control system for a robotic arm with 6 degrees of freedom for education systems. In *2015 6th International Conference on Automation, Robotics and Applications (ICARA)* (pp. 358-363). IEEE.

[24]. Ozgur, C., Colliau, T., Rogers, G., & Hughes, Z. (2017). MatLab vs. Python vs. R. *Journal of Data Science*, *15*(3), 355-371.

[25]. Marowka, A. (2018). On parallel software engineering education using python. *Education and Information Technologies*, *23*(1), 357-372.

[26]. Gabdrakhmanova, K. F., Izmaylova, G. R., & Samigullina, L. Z. (2021, October). Python-provided algorithm for calculating oil field operation parameters for expansion drive reservoirs. In *Journal of Physics: Conference Series* (Vol. 2032, No. 1, p. 012038). IOP Publishing.

[27]. Singh, I., & Kaur, B. (2018). Teaching graphical simulations of Fourier series expansion of some periodic waves using spreadsheets. *Physics Education*, *53*(3), 035031.

[28]. Uddin, Z., & Hani Zaheer, M. (2019). Simulating Physics Experiments in Spreadsheets–Experimenting with Ohm's Law. *The Physics Teacher*, *57*(3), 182-183.

[29]. Pratidhina, E., Kuswanto, H., & Dwandaru, W. S. B. (2020). Visualising Spatial Light Intensity Distribution on Optical Fibre Core with Spreadsheet. *Revista Brasileira de Ensino de Física*, *42*.