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BAND GAP ENERGY CHARACTERISTICS IN MATERIALS

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Submiited: 02/05/2025 Accepted: 25/06/2025 Published: 30/06/2025 Vol. 3 No. 2 **Abstract-**Band gap energy is one of the most fundamental parameters in determining the electronic and optoelectronic properties of a material. The band gap value is a measure of the energy jump that electrons must make in order to actively conduct electricity. The greater the band gap value, the greater the energy required by electrons to conduct electricity.

The difference in band gap values in various materials affects the ability of the material to conduct electricity or interact with light. Therefore, understanding the characteristics of band gap energy is very important in the development of various devices such as semiconductors, photovoltaics, optical sensors, and light-emitting diodes (LEDs). This article examines the differences in band gap characteristics in three main types of materials: conductors, semiconductors, and insulators. In conductors, the band gap does not exist or is very small, allowing electrons to move freely. Insulators have a very large band gap so they do not conduct electricity. Semiconductors are in between and have high flexibility to be modified through doping, structural engineering, and external field applications. The main focus is given to semiconductors because of their very large role in modern electronic and optoelectronic devices. The fundamental differences between direct and indirect band gaps are also discussed. Materials with direct band gaps such as GaAs or InGaN are very suitable for LED applications because they allow efficient light emission without the help of phonons. Meanwhile, materials such as silicon with indirect band gaps tend to be unsuitable for LEDs because their photon emission efficiency is low. With proper understanding and engineering of band gap characteristics, the performance of devices such as LEDs can be significantly improved, both in terms of light efficiency, stability, and the range of wavelengths produced.

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Keywords: Band gap energy, semiconductor, direct band gap, indirect band gap, LED, conductor, insulator.

1 Introduction

Band gap energy is a fundamental concept in materials physics that plays an important role in determining the electronic and optoelectronic properties of a material. Band gap is the energy difference between the highest occupied electron energy level (in the valence band) and the lowest empty electron energy level (in the conduction band). The magnitude of the band gap value is the main determinant of whether a material behaves as a conductor, semiconductor, or insulator. Electrical conductivity is the intrinsic ability of a material to conduct electric current when given a potential difference. Materials are grouped into conductors, semiconductors, and insulators based on their conductivity levels. Conductors offer low resistance to current flow, while insulators offer very high resistance. (Razeghi, M. (2009). Fundamentals of Solid State Engineering (3rd Edition). Springer. nd) Semiconductor materials themselves act as insulators at very low temperatures and act as conductors at room temperature. (Madelung, O. (2012). Semiconductor Data Book (3rd Edition). Springer. nd) To explain the conductivity of a material, the concept of energy bands is often used. There are two energy bands, namely the valence band and the conduction band.

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The valence band is an energy band that may be filled by electrons from a solid until complete/full, while the conduction band is an energy band that is another place that will be filled by electrons after the valence band is full. At a temperature of 0 K, the conduction band is partially filled for conductor materials, while insulators and semiconductors have no electrons filling the conduction band. (Tilley, R.J.D. (2020). Understanding Solids: Materials Science (2nd Edition). Wiley. nd) (Yu, P.Y., & Cardona, M. (2010). Semiconductor Fundamentals: Physics and Properties of Materials (4th Edition). Springer. nd)

Band gap energy is one of the distinguishing indicators between semiconductor materials and other materials. Band gap energy is one of the typical properties of semiconductor materials that describes how much minimum energy is needed for electrons to move from the valence energy level to the conduction energy level. Information about the size of this energy gap is very useful in determining the appropriate approach or treatment of the material in various technological applications. One of the important physical characteristics to be analyzed from a material is its electron arrangement. This arrangement reflects how electrons interact with atomic nuclei in the structure of the material. (Wang, QH, Kalantar-Zadeh, K., Kis, A., Coleman, JN, & Strano, MS (2012). Electronics and Optoelectronics of Two-Dimensional Materials. Nature Nanotechnology, 7(11), 699-712. nd) For simple materials, this electron distribution can still be analyzed using a mathematical approach such as the Schrödinger equation, by considering physical parameters in the realm of quantum mechanics. However, this approach becomes increasingly difficult to apply when dealing with materials that have complex structures and involve interactions between many particles, such as those in semiconductors. Semiconductors are a type of material that plays an important role in the advancement of modern technology and various electronic devices today. Its existence is very vital in various devices such as smartphones, household appliances, and vehicles. This material has the ability to conduct electricity through the movement of electrons, with a conductivity level that is between that of conductors and insulators. (Morkoç, H. (2009). Handbook of Nitride Semiconductors and Their Devices. Wiley-VCH. nd)

The purpose of this article is to provide a deep understanding of the concept of band gap energy in materials and its role in determining the electrical properties of a substance, whether it is a conductor, semiconductor, or insulator. This article also aims to identify various types of materials based on their band gap energy values and relate them to real applications in technology, such as solar cells, light-emitting diodes (LEDs), and other semiconductor devices. In addition, the discussion will cover how the size of the band gap energy affects the performance of a material in a particular application, as well as the latest developments in engineering and manipulation of band gaps to produce materials with desired characteristics for current and future technological needs. (Chhowalla, M., Shin, H.S., Eda, G., Li, L.J., Loh, K.P., & Zhang, H. (2013). Chemistry of Two-Dimensional Transition Metal Dichalcogenide Sheet Materials. Nature Chemistry, 5(4), 263–275. nd)

2 Research methodology

The research method of this article uses a literature study method, namely by reviewing, evaluating, collecting, studying in depth from various relevant scientific sources, and analyzing them to understand the concept of band gap energy in materials. The sources used include physics and materials textbooks, scientific journal articles, conference publications, and recent research reports obtained through academic databases such as Google Scholar, ScienceDirect, and IEEE Xplore. With the main focus of literature searches on the basic concept of band gap energy, types of materials based on their band gap values (conductors, semiconductors, and insulators), and practical applications of these materials in everyday life and modern technology. The author also examines how experts explain the energy band structure, the mechanism of band gap formation, and its effect on the electrical and optical properties of a material. The author also compares the band gap energy values of various materials and relates them to their use in various technological devices, such as solar cells, LEDs (light emitting diodes), sensors, and transistors. The

collected data and information are analyzed qualitatively to understand the relationship between band gap energy values and the physical and applicative properties of the material, as well as to identify the latest technological developments in band gap control.

2.1 Discussion

To determine the energy band gap of a thin layer of amorphous silicon that has been deposited, the common method used is the Tauc Plot method. (Tauc 1972)

$$(ahv)^n = (hv - E_9)....(1.1)$$

In this context, the absorption coefficient is calculated for a thin film using the transmittance data obtained from UV-Vis measurements. The variable 'd' represents the thickness of the deposited film, 'hv' is the photon energy, 'A' is a constant, 'r' is ½ for indirect band gap materials, and 'Eg' is the band gap energy. The band gap energy of a thin film can be determined by finding the linear portion of the Tauc Plot curve, extrapolating it until it intersects the X-axis; the intersection point represents the band gap energy value. Figure 2.5 illustrates an example of measuring the band gap energy of amorphous silicon thin films using the Tauc Plot method. (Tauc 1972) Through the linear line drawn so that the band gap energy of a film draws a straight line on the graph and sees where it intersects the X-axis with a range of 1.5 eV. The smaller the band gap energy number, the more light can be absorbed by the film. This film can only absorb light with an energy greater than its band gap energy. If the energy is smaller, the light will be reflected. So, the band gap energy is important because it determines how well the coating absorbs light and how much light can pass through. This has a big impact on how efficiently a solar cell can convert solar energy into electricity.

The decrease in the energy band gap will be accompanied by an increase in the absorption level of the layer. Thin films can only absorb photons with higher energy than their energy gap, while photons with lower energy are reflected. Therefore, the energy band gap of the layer is an important parameter in the absorption and transmittance aspects that can affect the efficiency of solar cells from the sunlight energy entering the layer. (Green, MA (2019). Third Generation Photovoltaics: Advanced Solar Energy Conversion. Springer. nd)

Bandgap is an important concept in semiconductor materials, referring to the minimum energy required for an electron to jump to a higher energy level. It is similar to a child needing enough force to jump to the next square in a jump rope game. The size of the bandgap determines the range of photon wavelengths that the material can absorb, which is important for generating current in solar panels by efficiently absorbing photons across the solar spectrum. (Bhattacharya, P., et al. (2017). Band Gap Engineering and Its Applications in Optoelectronic Devices. Progress in Quantum Electronics, 54, 1–25. nd) Varying the size of the bandgap allows the material to optimize photon absorption in the high- or low-energy light regions, adapting to different environmental and application needs. For conductors, there is no gap between the conduction band and the valence band, so the conduction band is filled with electrons, making the material highly conductive. Insulators, on the other hand, have a large gap between the valence band, making the material nonconductive. Semiconductors have a band gap that lies between these two extremes, making them normally nonconductive. However, when energy is added (via light, heat, etc.), electrons in the valence band can move to the conduction band, making the material conduct electricity. (Geim, A. K., & Grigorieva, I. V. (2013). Van der Waals Heterostructures. Nature, 499(7459), 419–425. nd)



Figure 1.1Semiconductor band gap

Amorphous silicon is a semiconductor material that is widely studied and used in various thin-film technologies. One of its main applications is in solar panels (photovoltaic or PV). However, the efficiency of solar panels using amorphous silicon is still relatively low. Currently, PV modules based on amorphous silicon with a single-pin structure can only achieve efficiencies of around 6-8%. This means that only a small portion of the solar energy that hits the panel is successfully converted into electrical energy. (Shockley, W., & Queisser, H.J. (1961). Efficiency Limits of pn Junction Solar Cells. Journal of Applied Physics, 32(3), 510–519. nd) One way to make solar cells better is to improve the performance of amorphous silicon (a-Si) solar panels. Amorphous silicon has an energy band gap of around 1.8 eV, which is ideal for absorbing energy from sunlight. The graph shows that the highest efficiency can be achieved with an energy band gap around this value. Theoretically, ideal amorphous silicon solar cells can achieve efficiencies approaching 30%, making it a very promising material for solar cell manufacturing. (Sari, DP, & Nugraha, ART (2022). Band Gap Study of Semiconductor Materials for Solar Cell Applications. Indonesian Journal of Physics, 26(2), 155–162. nd)



Figure 1.2 This schematic diagram, as described by Yuan et al. (2014)

Figure 1.2 is an example of one of the measurements of the energy gap of amorphous silicon thin films using the Tauc Plot method. Through a linear line drawn to intersect the x-axis, it can be determined that the energy band gap of the film is around 1.5 eV. A decrease in the energy band gap will be accompanied by an increase in the absorption level of the film. Thin films can only absorb photons with higher energy than their energy gap, while photons with lower energy are reflected. Therefore, the energy band gap of the

film is an important parameter in the absorption and transmittance aspects that can affect the efficiency of solar cells from the sunlight energy entering the film. (Saha, S., et al. (2018). Recent Advances in Semiconductor Band Gap Engineering for Solar Cell Applications. Materials Today: Proceedings, 5(9), 18548–18554. nd)

2.2 Material Classification Based on Band Gap Energy

In general, materials are classified based on the size of their band gap energy as follows: (Dutta, AK, et al. (2020). Band Gap Tuning in Perovskite Materials for Optoelectronic Applications. Journal of Materials Chemistry C, 8(3), 670–686. nd)

1. Conductor

It does not have a significant band gap; the valence and conduction energy bands meet. Electrons can move freely without any additional external energy. Therefore, conductors such as copper (Cu) and aluminum (Al) are very efficient in conducting electricity.

2. Insulator

Having a large band gap (>5 eV). Electrons are tightly bound in the valence band and require large energy to move to the conduction band, making them almost incapable of conducting electricity. Examples of insulators are glass, ceramics, and mica. (Novoselov, KS, Mishchenko, A., Carvalho, A., & Castro Neto, AH (2016). 2D Materials and Van der Waals Heterostructures. Science, 353(6298), aac9439. nd)

3. Semiconductor

Having a medium band gap (around 0.5 - 3 eV). At room temperature, some electrons are able to move to the conduction band and provide medium conductivity properties. (Pearton, SJ, et al. (2018). Wide Band Gap Semiconductor Materials for Power Electronics. Materials Science and Engineering: R: Reports, 125, 1–36. nd) Examples of semiconductors:

- Silicon (Si): 1.1 eV (indirect band gap)
- ➤ Gallium Arsenide (GaAs): 1.42 eV (direct band gap)
- Gallium Nitride (GaN): 3.4 eV (direct band gap)(Mak, K. F., Lee, C., Hone, J., Shan, J., & Heinz, T. F. (2010). Ultrathin MoS2: A New Direct Band Gap Semiconductor. Physical Review Letters, 105(13), 136805. nd)

2.3 Band Structure: Direct vs Indirect Band Gap

The fundamental difference between direct and indirect band gap semiconductors lies in the energy band structure and electron transition mechanism.

1. Direct Band Gap

In direct band gap semiconductors, the minimum position of the conduction band and the maximum of the valence band are in the same momentum (k-space). This means that electrons can move directly from the conduction band to the valence band by emitting photons, without the help of momentum changes. This makes it very efficient in the process of light emission.

Examples: GaAs, GaN, InP.

2. Indirect Band Gap

In indirect band gap semiconductors, the conduction band minimum and valence band maximum are not at the same momentum. Electron transitions require additional interactions with phonons (lattice vibrations) to change momentum. This process is inefficient in emitting light, making it unsuitable for optoelectronic applications. (Singh, J. (2007). Semiconductor Optoelectronics: Physics and Technology. McGraw-Hill. n.d.)

Example: Si, Ge.

2.4 Implications for LED Applications

LED (Light Emitting Diode) utilizes the recombination of electrons and holes in semiconductor materials to produce light. Materials with a direct band gap are ideal because they are efficient in converting electrical energy into light. This process is called radiative recombination. (Li, L., Yu, Y., Ye, G.J., Ge, Q., Ou, X., Wu, H., Feng, D., Chen, X.H., & Zhang, Y. (2014). Black Phosphorus Field Effect Transistors. Nature Nanotechnology, 9(5), 372–377. nd)

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Material	Band Gap (eV)	Color of Light	Wavelength (nm)	Band Gap Type
GaAs	1.42	Infrared	~870	Direct
InGaP	1.9 – 2.1	Red	~650	Direct
GaN	3.4	Blue	~450	Direct
AlGaN	4.0 - 6.0	UV	~280	Direct

Here are examples of LED materials based on wavelength and light color:

Table 1.1LED materials

In contrast, materials such as silicon that have an indirect band gap are not used in making LEDs because the light produced is very weak or almost nonexistent. This is why even though silicon dominates the microelectronics industry, it is not used in light-emitting applications. (Fiori, G., et al. (2014). Two-Dimensional Material-Based Electronics. Nature Nanotechnology, 9(10), 768–779. nd)

2.5 External Factors Affecting Band Gap

In addition to intrinsic properties, the band gap can be influenced by:

- 1. Temperature: The band gap tends to narrow at high temperatures due to expansion of the crystal lattice and increased atomic vibrations.
- 2. Doping: The addition of foreign atoms can modify the energy levels in the valence and conduction bands (example: n and p doping in semiconductors).
- 3. Pressure and stress: Can cause changes in crystal structure and affect the bandgap energy.
- Particle size: In the nanoscale (quantum dot), the band gap can be increased due to the energy quantization effect (quantum confinement). (O'Donnell, K.P., & Chen, X. (2015). Semiconductor Luminescence Spectroscopy. Taylor & Francis. n.d.)

2.6 Band Gap Contribution to the Technological Revolution

The development of modern technology is highly dependent on band gap engineering, for example: (Jain, M. (2017). Band Gap Engineering in Semiconductors. Journal of Materials Science, 52(10), 6001–6016. nd)

- 1. Energy-efficient LEDs and full-color displays based on materials such as GaN and InGaN.
- 2. A new generation of solar cells that combine direct band gap materials and multi-junction structures to capture a wider spectrum of light.
- 3. Semiconductor lasers for optical communications.
- 4. Direct band gap semiconductor based photonic sensors and devices. (Chuang, S.L. (2012). Physics of Photonic Devices (2nd Edition). Wiley. nd)

3 Conclusion

Based on this article, it can be concluded that the band gap energy is a key parameter that defines the electronic and optoelectronic properties of materials. Materials are classified into conductors, semiconductors, and insulators based on the size of their band gap energy, where conductors have small or no band gap, insulators have large band gaps (>5 eV), and semiconductors are in between with band gaps of around 0.5 to 3 eV. (Zhang, Y., et al. (2019). Band Gap Tuning in Two-Dimensional Materials: Methods and Applications. Nano Today, 25, 104–119. nd) The energy band structure is also an important factor, especially in determining the efficiency of devices such as LEDs, where materials with direct band gaps are ideal because they can emit light efficiently, while indirect band gaps tend to be less suitable for this application. Current technological developments concentrate on engineering and manipulating band gaps through doping, structural engineering, and other techniques to improve the performance of electronic and optoelectronic devices. With a deep understanding of the band gap energy characteristics, material innovations can continue to be developed to meet the needs of future technologies, such as more efficient and diverse solar cells, optical sensors, and LEDs (Nelson, J. (2003). Physics of Solar Cells. Imperial College Press. nd)

In the context of band gap measurement, the Tauc Plot method has proven to be effective, especially for the characterization of thin film materials such as amorphous silicon (a-Si). By analyzing the relationship curve between photon energy and optical absorption, the band gap value can be estimated accurately. For example, a-Si is known to have a band gap of around 1.5–1.8 eV, which makes it a suitable material for photovoltaic applications due to its ability to absorb photons in a wide spectrum of solar energy. A decrease in the band gap value correlates with an increase in the absorption of the layer to light, and this is a key factor in the design of the active layer of solar cells. (Fox, M. (2019). Optical Properties of Solids (3rd Edition). Oxford University Press. n.d.)

In addition to intrinsic material factors, external factors such as temperature, pressure, doping, and particle size also greatly affect the size of the band gap of a material. Increasing the temperature can reduce the band gap, while engineering pressure or strain can change the crystal structure and thus shift the position of the energy band. The energy quantization effect, especially in nanometer-scale materials such as quantum dots, allows precise manipulation of the band gap by changing the particle size. Doping with foreign elements can also open new energy levels that modify the electrical and optical properties of the material. (Streetman, B. G., & Banerjee, S. (2016). Solid State Electronic Devices (7th Edition). Pearson. nd)

Understanding and controlling the energy characteristics of the band gap are at the heart of many recent technological innovations, including the development of efficient, broad-spectrum LEDs, multijunction solar cells with optimal absorption across a wide range of wavelengths, high-power semiconductor lasers for optical communications, and semiconductor-based sensors for industrial and medical applications. Indeed, in emerging materials such as perovskites and 2D materials (such as MoS₂ or graphene), band gap engineering is a key strategy for tailoring materials to specific applications. (Ashcroft, N. W., & Mermin, N. D. (2011). Solid State Physics. Cengage Learning. n.d.)

Thus, it can be concluded that band gap energy is not just a theoretical concept in materials physics, but is the practical foundation of many technologies that shape the modern world. The study and engineering of band gaps will continue to play a central role in the creation of smarter, more efficient, and more environmentally friendly devices ranging from renewable energy to flexible electronics and next-generation optoelectronics. A deep understanding of these characteristics will be key to unlocking the full potential of future materials. (Kittel, C. (2018). Introduction to Solid State Physics (8th Edition). Wiley. nd)

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