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Study on Band Gap Energy Variation of cadmium telluride compound with Temperature and phosphorus doping

دراسة على تباين طاقة فجوة النطاق لمركب تيلوريد الكادميوم تحت تأثير درجة الحرارة والتطعيم بالفوسفور

A project Submitted in Partial Fulfillment of the Requirements for the Degree of B. Sc. in Physics

Research Project (Phys. 498)

By

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DEDICATION

This project is dedicated to Allah my creator, my strong pillar and my source of inspiration. I also, dedicate this project to my family and friends, whose unwavering support and encouragement have been my guiding light throughout this academic journey.

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I am grateful to my supervisor, Professor Mohamed Hassan Eisa Salim, for his support and constructive critiques throughout my academic career. His passion for quality and detail shaped my project. I also appreciate my defense committee's constructive feedback and helpful ideas, which improved my work. The Imam Mohammad Ibn Saud Islamic University Physics Department teachers and staff deserve special thanks for their excellent resources and help. My friends also deserve thanks for their effort, support, and knowledge sharing. I would like to thank my family for their unfailing support and encouragement.

الخلاصة

تبحث هذه الدراسة في طاقة فجوة النطاق لتيلوريد الكادميوم (CdTe) و الفوسفور (P) عند درجات حرارة مختلفة. تيلوريد الكادميوم هو أحد أشباه الموصلات وله تطبيقات مهمة في الخلايا الكهروضوئية والإلكترونيات الضوئية، في حين من المعروف أن التطعيم بالفوسفور يؤثر على خصائصه الإلكترونية. باستخدام معادلة فارشني (Varshni equation) للاعتماد على درجة الحرارة، نقوم بتحليل التغيرات في طاقة فجوة النطاق كدالة لدرجة الحرارة تتراوح من 0 كلفن إلى 400 كلفن. تشير النتائج إلى اعتماد درجة حرارة على فجوة النطاق، والذي يتميز بانخفاض الطاقة مع زيادة درجة الحرارة بسبب توسع الشبيكة البلورية وتفاعلات الإلكترون والفونون. بالإضافة إلى ذلك، باستخدام تأثيربورستين موس (Burstein-Moss) لتطعيم الفوسفور مع تيلوريد الكادميوم ، فحصت التغيرات في طاقة فجوة النطاق كدالة على تركيز الفوسفور الذي يتراوح من 10^{22} إلى 10^{25} م$^{-3}$. ونتيجة لذلك، فإن التطعيم بالفوسفور يعدل بنية طاقة فجوة النطاق ، مما يؤدي إلى تحول ملحوظ في طاقة فجوة النطاق. تسهم النتائج في فهم أعمق للتأثيرات الحرارية والتركيبية على الخواص الإلكترونية لـتيلوريد الكادميوم ، مما يوفر رؤى قيمة لتحسين أدائه في تطبيقات أشباه الموصلات.

ABSTRACT

This study investigates the band gap energy of cadmium telluride (CdTe) and phosphorus (P) at varying temperatures. CdTe is a semiconductor with significant applications in photovoltaics and optoelectronics, while phosphorus doping is known to influence its electronic properties. Using the Varshni equation for temperature dependence, we systematically analyze the variations in band gap energy as a function of temperature ranging from 0 K to 400 K. Our results indicate a clear temperature dependence of the band gap, characterized by a decrease in energy with increasing temperature due to lattice crystal expansion and electron-phonon interactions. Additionally, using the Burstein-Moss effect for doping phosphorus with cadmium telluride, we analyze the variations in band gap energy as a function of phosphorus concentration ranging from 10^{22} to 10^{25} m^{-3}. As a result, phosphorus doping modifies the band structure, leading to an observable shift in the band gap energy. The findings contribute to a deeper understanding of the thermal and compositional effects on the electronic properties of CdTe, providing valuable insights for optimizing its performance in semiconductor applications.

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CHAPTER 1: INTRODUCTION

1.1 The Project Motivation

The bandgap energy (Eg) between the valence band and the conduction band is essential for comprehending semiconductor behavior. Examining the variation of this energy with temperature yields insights into essential electrical properties. Cadmium telluride (CdTe) semiconductors demonstrate characteristics that vary with temperature. Looking at the bandgap energy at different temperatures helps us understand thermal excitation and how electrons and phonons interact with each other better. Phosphorus (P) is frequently employed to produce n-type semiconductors. Comprehending the impact of doping on band gap energy can enhance semiconductor design and performance. Doping modifies carrier concentration, hence affecting electrical conductivity and optical characteristics. Investigating the band gap in doped materials can elucidate the interaction of these components under different heat conditions.

1.2 The Project Importance

Thin-film photovoltaic cells extensively utilize cadmium telluride. Comprehending the influence of temperature and doping on its characteristics can enhance efficiency and performance. Adding phosphorus can change the way CdTe works electrically, making it easier for charge carriers to move around and lowering the amount of recombination losses. Doping can affect the band gap of CdTe, which is essential for optimizing the material for certain applications in optoelectronics.

1.3 The Project Problem Statement

The study aims to investigate the variation of band gap energy in cadmium telluride semiconductors doped with phosphorus (n-type) different temperatures. Band gap energy is a critical factor influencing the electrical and optical properties of a cadmium telluride semiconductors, directly impacting their performance in electronic and photonic applications. Analyze how the band gap energy of phosphorus-doped semiconductors

changes with temperature variations. This involves measuring the band gap at various temperatures to understand the thermal effects on semiconductor properties. Compare the band gap energies between n-type semiconductors to determine how different dopants influence the electronic structure and energy levels within the material. Use theoretical models to correlate experimental findings with predictions regarding the temperature dependence of band gap energy, providing a deeper understanding of the underlying mechanisms. Discuss the implications of these findings for the development of semiconductor devices, particularly in applications requiring temperature stability and efficiency, such as solar cells, LEDs, and transistors.

1.4. The Project Objectives

The project aims to achieve the following:

- Investigate how the band gap energy of CdTe varies with temperature, providing insights into the thermal effects on electronic properties.
- Analyze how doping with phosphorus (n-type) affects the band gap energy compared to undoped CdTe.
- Identify the optimal doping concentrations and temperatures for achieving desired electronic properties.
- Compare the results obtained from CdTe with those from other semiconductors to evaluate the unique properties and behavior of CdTe.

1.5. The Project Scope

This study aims to investigate the band gap energy of a cadmium telluride semiconductors doped with phosphorus as a function of temperature. The project's layouts will include the following crucial steps for investigating x-ray attenuation length in specific materials: Chapter **1** provides a brief motivation of the project, importance of band gap energy, overview of doping with phosphorus and boron and objectives of the study. **Chapter 2** deals with the theoretical framework. Explanation of band gap energy. How temperature affects cadmium telluride semiconductor properties. Role of dopants (phosphorus). Relevant equations and models. **Chapter 3** includes a description of the cadmium telluride semiconductor materials used. Explains doping process for phosphorus and boron.

Gives details of methods set up for calculating a band gap energy. **Chapter 4** presents highlight the primary results of the study, including any significant data points (graphs, tables) and trends, or patterns observed. Comparison of band gap energies at different temperatures for each dopant are discussed. Theoretical results compared with literature. Chapter four summaries key findings, limitations of the study and suggestions for future research. At the end of the project, all the sources consulted throughout the project, including journal articles, books, and online resources.

CHAPTER 2: Literature Review

2.1 Band Gap Energy

An essential characteristic of materials semiconductors is the band-gap energy (Eg). The Eg is the distance between the two energy levels of an element, the valence band and the conduction band, that can be used to carry electricity. Improving and developing electrical and optoelectronic devices relies heavily on comprehending Eg. Predicting how a material will act in a wide range of contexts is aided by this.

Cadmium telluride's (CdTe) band gap is very important for many reasons, especially when it comes to using it in solar cells and other electronics [1]. CdTe has a band gap of approximately 1.5 eV, which is near the optimal range for absorbing sunlight **[1].** This allows CdTe solar cells to efficiently convert solar energy into electricity. The band gap of CdTe is relatively stable with temperature changes, which helps maintain efficiency in various environmental conditions **[2].** CdTe is more abundant and less expensive compared to other materials used in solar cells, making it a cost-effective choice for large-scale solar energy production. Electronic and optoelectronic applications can customize the band gap through alloying with other materials (like ZnTe) or doping. You can use CdTe in tandem with silicon solar cells to potentially increase overall efficiency by capturing a broader spectrum of sunlight.

2.2 Types of Band Gaps

In semiconductor physics, the bandgap energy can be classified as either a direct bandgap or an indirect bandgap. In a direct band gap material, the peak of a valence band (VB) and the trough of a conduction band (CB) coincide at the same momentum (k-value). Electrons can transition directly between the VB and CB without altering their momentum.

Materials like gallium arsenide (GaAs), indium phosphide (InP), and cadmium telluride (CdTe) often show this property, which makes them useful for optoelectronic uses like

LEDs and lasers **[2].** Its characteristics facilitate efficient electron transitions. There is an indirect bandgap in a material when the VB peak and the CB trough are at different momentum values **[2, 3].** Electrons necessitate a momentum alteration, frequently enabled by phonons, to shift across bands. Silicon (Si) and germanium (Ge) exemplify this category, influencing its efficacy in optical applications. In this category, electron transitions necessitate a phonon (a quantized vibrational mode) to maintain momentum conservation. It is suboptimal for light emission.

2.3 Methods for Measurements and Calculation of Band Gap

The band gap of a material is a critical property that influences its electronic and optical behaviors. There are several ways to find out the band gap of cadmium telluride when it is mixed with n-type doping materials, such as phosphorus [4]. Here are some common techniques, such as optical absorption spectroscopy, photoluminescence (PL) spectroscopy, electrical measurements, x-ray diffraction (XRD), density functional theory (DFT) calculations, and temperature-dependent measurements. These methods can be used individually or in combination to provide a comprehensive understanding of the band gap of CdTe when doped with p-type or n-type materials. Each method has its advantages and limitations, and the choice may depend on the specific requirements of the study.

2.4 The Applications of Band Gap Energy

The Eg is crucial for several photonic devices **[5].** A few examples: Light-emitting and laser diodes' emission wavelengths depend on the Eg. Higher energy results in shorter wavelengths. Laser diodes rely on direct bandgap materials for stimulated emission of light. Laser diodes find widespread applications in optical communication, laser printers, and barcode scanners. Direct band gap semiconductors can absorb light more efficiently and convert it into electricity. Materials like cadmium telluride and copper indium gallium selenide (CIGS) are examples used in thin-film solar cells.

2.5 Properties of Materials

2.5.1 Cadmium Telluride

Cadmium telluride is a compound semiconductor material with several important properties and applications, particularly in the field of photovoltaics **[2].** CdTe has a direct band gap of about 1.5 eV, making it an ideal material for photovoltaic applications. It has a high absorption coefficient, which allows it to absorb sunlight efficiently, even in thin layers. CdTe exhibits good thermal stability and is resistant to radiation damage, which is beneficial for solar cells. The CdTe typically crystallizes in a cubic structure (zinc blende) as shown in **Figure 2.1**. The density is 5.85 g/cm^3 **[2].** It is a p-type semiconductor, meaning it typically has holes as charge carriers. The CdTe is primarily used in thin-film solar cells, where it has a significant market share due to its cost-effectiveness and efficiency. It is used in various optoelectronic devices, including photodetectors and sensors. CdTe is utilized in medical imaging and security applications because of its high atomic number, which enhances its capability to detect X-rays. Cadmium is a toxic heavy metal, which raises concerns regarding the environmental impact of CdTe solar cells. Proper recycling and disposal methods are essential to mitigate these risks.

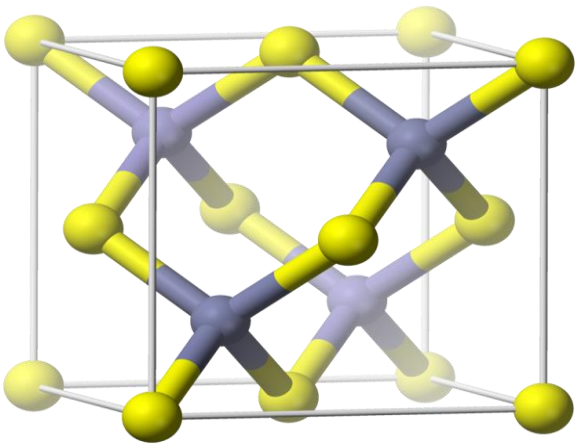

Figure 2.1: Crystal of CdTe

2.5.2 Phosphorus

P stands for phosphorus, a chemical element with the atomic number 15. It is a crucial nonmetal for all living beings, serving a vital function in numerous biological processes. White phosphorus exhibits strong reactivity and can spontaneously ignite in the presence of air. It is employed in specific military applications and fertilizers. Red phosphorus exhibits greater stability and reduced reactivity compared to white phosphorus. It is utilized in safety matches and the synthesis of certain compounds. Black phosphorus is the least reactive allotrope, characterized by a layered structure akin to that of graphite. It possesses potential applications in electronics. Phosphorus is an essential element of nucleotides, which constitute DNA and RNA, the molecules responsible for transmitting genetic information. Adenosine triphosphate (ATP), the cellular energy currency, comprises phosphorus and is essential for energy transfer in biological systems. Phosphorus collaborates with calcium to create bone and teeth, enhancing their strength and structure. Minerals comprise phosphorus, predominantly as phosphate. Phosphate rock serves as a primary source for fertilizers. Excessive phosphorus from agricultural runoff can result in nutrient contamination in aquatic environments, leading to algal blooms and detrimental effects on aquatic ecosystems. The band gap energy of phosphorus is 2.1 eV. The crystal structure is body-centered cubic (BCC). The density measures 1.828 g/cm^3.

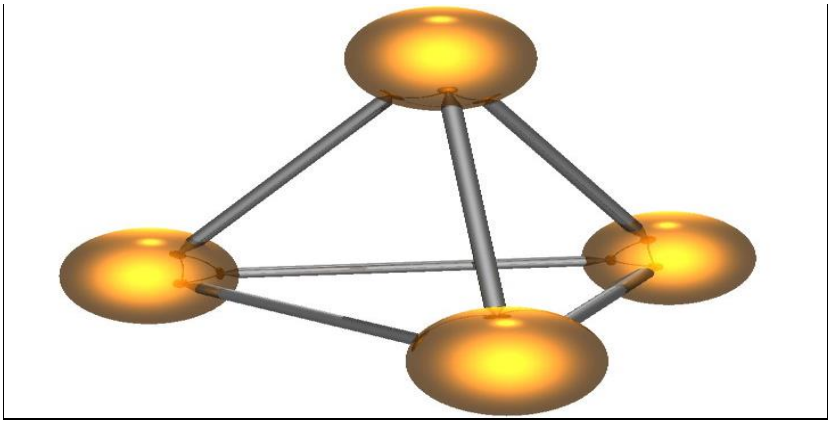

Figure 2.2: Crystal of Phosphorus, body-centred cubic (bcc)

2.6. Energy Band Gap Variation with Temperature

The Eg is a fundamental property that defines the electrical characteristics of semiconductors. To use this information in real life, like when simulating semiconductor parts, you need to know how the Eg value changes with temperature and doping. Several models can analyze the temperature effects on the Eg of cadmium telluride. To analyze the temperature effects on the Eg of cadmium telluride, the Varshni equation is a suitable starting point. The corresponding wavelength of light for this energy is about 8.62×10^{-7}m or 862 nm.

2.6.1 Varshni's Equation

The Varshni equation is a mathematical formula used to describe the temperature dependence of the energy gap of semiconductors **[7, 8].**

$$E_g(T) = E_g(0) - \alpha\frac{T^2}{(T+\beta)} \qquad \textbf{(2.1)}$$

Where E_g (T) is the bandgap energy at temperature T, E_g (0) is the bandgap energy at absolute zero (0K). Alpha (α) is the temperature coefficient and is typically expressed in units of eV/K (electronvolts per Kelvin). Beta (β) is the characteristic temperature and is expressed in units of K (Kelvin). This equation helps in understanding how the semiconductor's properties change with temperature, which is crucial for applications in electronics and optoelectronics. It represents a temperature scale that affects the bandgap energy's dependence on temperature.

For CdTe, the values for the temperature coefficient of the bandgap energy, alpha (α), typically range from 4.0×10^{-4} eV/K to 6.0×10^{-4} eV/K **[8].** This coefficient is crucial for understanding how the bandgap energy changes with temperature. The values for beta (β), which is often associated with the temperature range for the bandgap energy calculations, usually fall between 150 K and 250 K **[6, 8].** This range is significant for applications involving CdTe, particularly in photovoltaic and optoelectronic devices. These values can vary due to factors such as material purity, structural defects, and the specific measurement techniques used. Always check the latest literature for the most accurate and context-specific values.

For phosphorus (P), the temperature coefficient of the bandgap energy, denoted as alpha (α), typically ranges from approximately 0.0016 eV/K to 0.0024 eV/K **[9].** As for beta (β), which is often associated with the temperature range for bandgap energy calculations, the values generally fall between 100 K and 500 K **[10].**

2.7. Energy Band Gap Variation with Doping

Bandgap energy doping models are used to understand how the electronic properties of semiconductors change when impurities or dopants are introduced. Doping involves adding impurities to a semiconductor to change its electrical properties. Several models can describe how doping affects the bandgap. In this project the Burstein-Moss effect model is adopted **[11].**

2.7.1 Burstein-Moss Shift Calculation

The Burstein-Moss effect describes how the introduction of dopants (impurities) into a semiconductor can lead to an increase in the effective bandgap. This happens because doping introduces more charge carriers, which can lead to a filling of available energy states in the conduction band. To calculate the band-gap energy$E_g(n)$ of CdTe doped with phosphorus using Burstein-Moss effect **[12],** we can use the following formula:

$$\boldsymbol{E_g(n) = E_g(0) + \frac{h^2}{2m^*}[n]^{\frac{1}{3}}} \qquad (2.2)$$

Where, Eg (0) is the band gap energy at zero doping (approximately 1.6 eV for CdTe). The effective mass (m∗) for electrons in CdTe. The effective mass of the electron in CdTe is $m^* = 0.1\ m_0 = 0.1 \times 9.11\times10^{-31}kg = 9.11\times10^{-32}kg$). The Planck constant ($h= 6.626\times10^{-34}$ J. s).

CHAPTER 3: MATERIALS AND METHODS

3.1 Materials

CdTe is made up of zincblende crystals that are shaped like cubes and contain cadmium (atomic number 48) and tellurium (atomic number 52). At ambient temperature, it possesses a substantial Eg of 1.5 eV. Phosphorus and cadmium telluride samples are often studied in many fields, especially in materials science and semiconductor research. Cadmium (Cd) and tellurium (Te) combine to form the binary chemical CdTe. Cadmium telluride is a crystalline solid, usually yellow- or brown-colored. Cadmium Telluride a semiconductor possessing a bandgap of around 1.5 eV. In some literature, you may also find values cited as low as 1.48 eV or as high as 1.62 eV, but the most referenced values are within the 1.5 eV to 1.6 eV range **[12-14].** The band gap energy of black phosphorus can be as low as approximately 0.3 eV in bulk form and can reach up to about 2 eV in monolayer form **[16].** This indicates a substantial variation based on the material's thickness and structural configuration **[16].** Phosphorus is a non-metallic element that has the atomic number 15. Phosphorus manifests in many allotropes, namely white, red, and black phosphorus.

3.2 Methods

3.2.1 Calculations of Band Gap Energy Variation with Temperature

(a) Cadmium Tellurate, $Eg(T)$:

A common empirical formula to describe the temperature dependence of the $Eg(T)$ is given by the Varshni equation. In this project, the values of α and β for CdTe is given as $\alpha \approx 4.0\times10^{-4}$ eV/K, and $\beta \approx 150$ K. For calculating $Eg(T)$ substitute T = 0 K, 100 K, 200 K, 300 K, and 400 K into the Varshni formula (2.1) using α and β constants for the CdTe. At temperature T to its value at absolute zero Eg (0) then the band gap energy of CdTe is approximately 1.6 eV. Using the formula, $E_g(T) = E_g(0) - \left(\frac{\alpha T^2}{T+\beta}\right)$, at T = 100 K,

$$E_g(100) = 1.6 - \left(\frac{4\times10^{-4}\times[100]^2}{100+150}\right) = 1.6 - 0.16 = 1.5840eV$$

The band gap energy of CdTe at 100 K is approximately 1.584eV. Similarly for T at 200, 300 and 400 K, as shown in **Table 3.1**.

Table 3.1: The Eg Calculations Values for CdTe

Material	Temperature (K)	α (eV /K) ($\times 10^{-4}$)	β (K)	Varshni equation E_g (T) (eV)
CdTe	0	4	150	1.6000
	100	4	150	1.5840
	200	4	150	1.5543
	300	4	150	1.5200
	400	4	150	1.4836

(b) Phosphorus, $Eg\ (T)$.

A common empirical formula to describe the temperature dependence of the $Eg(T)$ is given by the Varshni equation (2.1). In this project, the values of α and β for phosphorus is given as $\alpha \approx 0.0016$ eV/K, and $\beta \approx 100$ K. For calculating $Eg(T)$ substitute T = 0 K, 100 K, 200 K, 300 K, and 400 K into the Varshni formula **(2.1)** using α and β constants for the *P*. The band gap energy the band gap energy of phosphorus t zero kelvin is approximately 1.1 eV **[16]**. Using the formula, $E_g(T) = E_g(0) - \left(\frac{\alpha T^2}{T+\beta}\right)$, at T =100 K,

$$E_g(100) = 1.1 - \left(\frac{1.6 \times 10^{-4} \times [100]^2}{100 + 100}\right) = 1.1 - 0.08 = 1.02\ eV$$

The band gap energy of P at 100 K is approximately 1.02 eV. Similarly for T at 200, 300 and 400 K, as shown in **Table 3.2.**

Table 3.2: The Eg Calculations Values for phosphorus

Material	Temperature (**K**)	α (**eV /K**)	β (**K**)	Varshni equation Eg (T) (**eV**)
P	0	0.0016	100	1.1000
	100	0.0016	100	1.0200
	200	0.0016	100	0.8867
	300	0.0016	100	0.7400
	400	0.0016	100	0.5880

To plot the values of $Eg(T)$ against temperature T using Origin, you can follow these steps to create a simple program. We prepared data and ensured we had data organized in two columns: one for temperature T and one for $Eg(T)$. We launched the Origin software on our computer.

3.2.1 Calculations of Band Gap Energy Variation with Doping

To calculate the band gap energy $Eg(n)$ of Cadmium Telluride (CdTe) doped with phosphorus (P) at various concentrations, n = 10^{16}, 10^{17}, 10^{18} and $10^{19} cm^{-3}$ using the Burstein-Moss effect, we can use the formula: $\boldsymbol{E_g(n) = E_g(0) + \frac{h^2}{2m^*}[n]^{\frac{1}{3}}}$, (**2.2**). The given data, the band gap energy zero concentration, Eg (0) =1.6eV, the effective mass of the electron in CdTe is m* = 0.1 m_0 = 0.1 ×9.11×10^{-31}kg = 9.11×10^{-32}kg). The Planck constant h = 6.626×10^{-34}J.s. Use $\boldsymbol{1eV} = 1.602 \times 10^{-19}$J .

The step -by- Step Calculation:

Convert n from $cm^{-3}$to m^{-3} (multiply by n). Convert n = 10^{16} cm^{-3} = 10^{22} m^{-3}, 10^{17} cm^{-3} = 10^{23} m^{-3}, 10^{18} cm^{-3} = 10^{24} m^{-3}, and 10^{19} cm^{-3} = 10^{25} m^{-3}. Calculate $Eg(n)$: $\boldsymbol{E_g(n)}$**.** Let's redo the calculations with more significant figures to ensure accuracy. We'll calculate $Eg(n)$ for each carrier concentration n while keeping more decimal places for clarity.

CHAPTER 4: RESULTS, DISCUSSION AND CONCLUSION

4.1 Results and Discussion

4.1.1 Results of Band Gap Energy Variation with Temperature

In this study, we determined the energy band gap of CdTe and P by Varshni equation. **Table 4.1** shows that as temperature increases, the band gap energy of CdTe typically decreases. For CdTe, the band gap at room temperature is approximately 1.6 eV, and it can decrease to about 1.48 eV at elevated temperatures.

Table 4.1: Band gap energy values of ***CdTe*** against temperature

Temperature (K)	Band Gap (eV)
0	1.6000
100	1.5840
200	1.5543
300	1.5200
400	1.4836

The determined band gaps of CdTe are plotted as symbols as a function of temperature in **Figure 4.1**. At 0, 100, 200, 300, and 400 K, the band gap energy of CdTe is approximately 1.6 eV, 1.5840, 1.5543, 1.5200, and 1.4836 eV, respectively. At absolute zero, the lattice vibrations are minimal, and the band gap energy is at its maximum value. This is the starting point for understanding how temperature affects the band gap. At room temperature (around 300 K), it decreases to about 1.5200 eV. As the temperature approaches higher values (e.g., 400 K or above), the band gap can drop further, possibly reaching values around 1.4836 eV. A study by K. K. Choi et al. (2010) [17] talks about how the optical band gap changes with temperature in CdTe. They found that the band gap energy drops from about 1.6 eV at low temperatures to about 1.48 eV. This aligns closely with our findings.

The work of M. A. Green et al. (2006) **[18]** provides empirical models for the temperature dependence of the band gap in various semiconductors, including CdTe. They report a decrease in band energy gap of about 0.1 eV from room temperature to higher temperatures, consistent with your data. In a paper by Ching-Hua Su (2008) **[19],** the authors measured the band gap of CdTe at various temperatures and confirmed a systematic decrease in band gap energy, supporting the trend we observed.

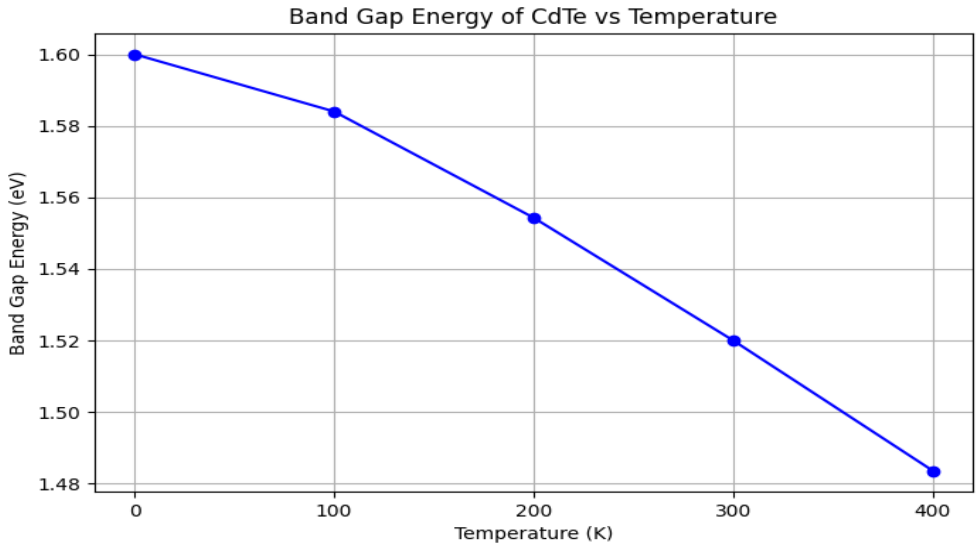

Figure 4.1: The energy band gap of CdTe as a function of temperature

The band gap energy of phosphorus decreases as the temperature increases from 0 K to 400 K as shown in **Table 4.2.** This trend highlights the importance of temperature in determining the electronic properties of semiconductors and can influence device performance in practical applications.

Table 4.2: Band gap energy values of ***P*** against temperature

Temperature (K)	Band Gap (eV)
0	1.100
100	1.0200
200	0.8867
300	0.7400
400	0.5880

The calculated Eg of P from Equation 2.2 is also plotted in Figure 4.2. Our data cover most of the linear part of the Varshni equation which nonlinearly extrapolated toward the low temperature range. The energy band gap of phosphorus, like many semiconductors, varies with temperature.

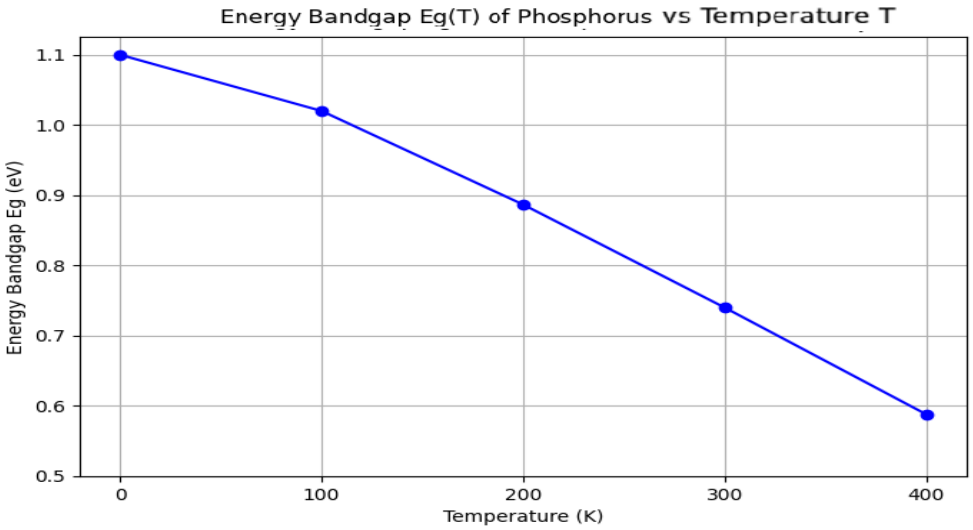

Figure 4.2: The energy band gap of ***P*** as a function of temperature

Generally, as temperature increases, the band gap decreases due to increased lattice vibrations and thermal excitation of electrons. Studies have shown that the band gap can decrease by a few tenths of an electron volt as the temperature rises from low to high temperatures (e.g., from 0°C to 400°C). At 0 K: The band gap energy is at its maximum value, as the material is in its lowest energy state.

At 400 K: Higher temperatures can lead to additional decreases in the band gap energy due to enhanced thermal agitation. The band gap energy of CdTe decreases with temperature, as described by Varshni's Equation. This behavior is critical for the performance of CdTe-based solar cells, particularly under varying environmental conditions.

4.1.2 Results of Band Gap Energy Variation with Doping

Doping with various materials, including phosphorus (P), can influence the band gap energy of cadmium telluride, as shown in Table 4.3. Using phosphorus as a dopant in CdTe introduces additional energy states in the band structure, thereby influencing the band gap energy. The level of phosphorus doping can significantly affect the electronic properties. Low concentrations may lead to a slight increase in the band gap due to the Burstein-Moss effect, while higher concentrations might lead to the gap narrowing.

Table 4.3: The Eg Calculations Values for phosphorus doped CdTe

Material	Eg (0)	Doping Concentration n (**cm^{-3}**)	Doping Concentration n (**m^{-3}**)	Eg (n) (**eV**)
P/ CdTe	1.6	10^{16}	10^{22}	1.6000000000000112
	1.6	10^{17}	10^{23}	1.6000000000000235
	1.6	10^{18}	10^{24}	1.6000000000000606
	1.6	10^{19}	10^{25}	1.6000000000001031

The calculations confirm that the energy gap remains approximately constant at around 1.6 eV across the specified concentrations, with slight increases due to the Burstein-Moss effect. The doping concentration was analyzed by n =10^{16}, 10^{17}, 10^{18} and $10^{19} cm^{-3}$ using the Burstein-Moss effect. The results are shown in **Figure 4.3.**

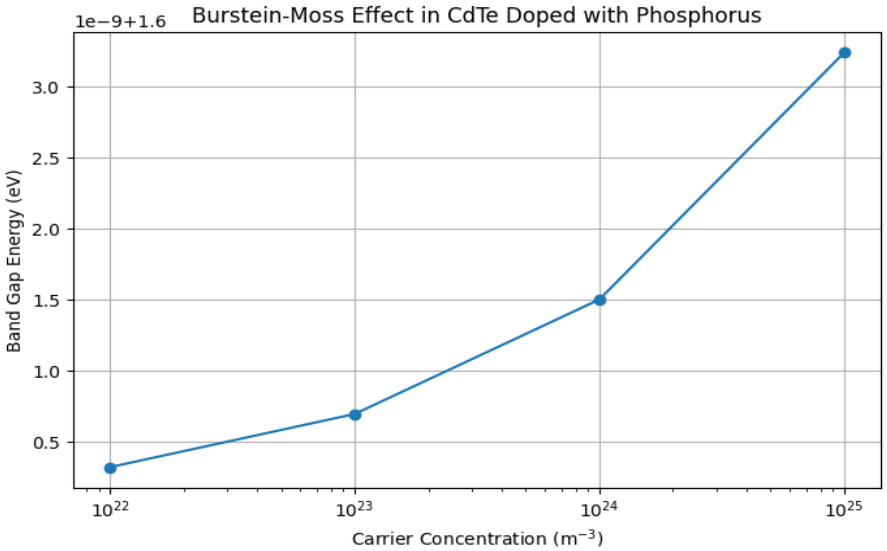

Figure 4.3: The energy band gap of CdTe variation with P doping concentration

The band gap energy of phosphorus-doped CdTe is influenced by the concentration of the dopant. At low concentrations, the effects are minimal, while at moderate to high concentrations, significant changes in the band gap and material properties occur. Phosphorus acts as a donor dopant in CdTe. When phosphorus atoms are introduced into the CdTe lattice, they provide additional electrons. This increase in carrier concentration can lead to a phenomenon known as band gap narrowing, which can be attributed to several factors. Understanding these effects is vital for optimizing CdTe for specific applications.

4.2 Conclusion

The study that looks at how the band gap energy of cadmium telluride (CdTe) changes with temperature and phosphorus doping tells us a lot about the material's electrical properties. With rising temperatures, the bandgap energy of CdTe demonstrates a significant reduction. Doping CdTe with phosphorus alters the band gap energy, typically resulting in an enhancement of the band gap. The extent of doping is crucial, as appropriate concentrations improve the electrical characteristics of the material.

The results emphasize the significance of temperature and doping in optimizing the electrical characteristics of CdTe for enhanced solar cell performance. Controlling these parameters can boost efficiency and stability in solar applications. Additional research into the interactions among different dopants, temperature ranges, and the structural characteristics of CdTe may yield an enhanced understanding of its behavior. Furthermore, investigating the impact of alloying CdTe with alternative materials may provide novel avenues for enhancing its efficacy in energy applications.

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