JEL Classification: O32, O38, D85, Q42, Q55
UOT: 539.2:537.226.1

THEORETICAL ANALYSIS OF THE VARIATION OF REFRACTIVE INDEX WITH BAND GAP IN SEMICONDUCTOR MATERIALS USING DIFFERENT MODELS

Mammadova V.
PhD in Physics,
lecturer at Baku State University
https://doi.org/10.5281/zenodo.17121604

Abstract

This study investigates the variation of the refractive index (n) as a function of the band gap energy (Eg) in semiconductor materials using several theoretical models, including Moss, Ravindra, Herve–Vandamme, Reddy, and Kumar–Singh. The results obtained from these models were systematically compared through tables and graphical representations to identify their consistencies and deviations. All models demonstrated a general trend of decreasing refractive index with increasing band gap, which is attributed to optical dispersion. The Herve–Vandamme model exhibited no intersection with the other models, reflecting its strong theoretical and physical foundation. In contrast, the Reddy and Kumar–Singh models showed closer agreement with experimental data, indicating their practical

Keywords: Semiconductors, Refractive index, Band gap, Optical dispersion, Moss, Ravindra, Herve–Vandamme, Reddy, Kumar–Singh

1. Introduction

The efficiency of modern optoelectronic technologies— including solar cells, photodetectors, smart windows, advanced optical sensors, and transparent conducting electrodes— is largely determined by the optical properties of the materials employed [1–3]. Among these properties, the relationship between the refractive index (n) and the band gap energy (Eg) is of particular importance, as these two parameters govern a material's ability to absorb, transmit, and reflect light [4, 5].

The refractive index (n) defines the propagation and phase velocity of electromagnetic waves within a material, directly influencing the refraction, propagation, and reflection of light. On the other hand, the band gap energy (Eg) determines whether a material can absorb photons within a specific energy range, thereby defining its sensitivity spectrum with respect to photon energy. The correlation between these two parameters is crucial not only from the perspective of fundamental semiconductor physics but also for the optimal selection of materials in optoelectronic device applications [1, 6, 7].

In this context, several theoretical and empirical models have been proposed to predict the $n{\sim}Eg$ relationship in advance. These models provide an initial framework for evaluating semiconductor materials and allow for preliminary analysis without relying on experimental data. The most frequently referenced models include: Moss [8], Ravindra [9], Herve–Vandamme [10], Reddy [11], and Kumar–Singh [12].

In the present study, the relationship between the refractive index (n) and the band gap energy (Eg) is systematically analyzed based on different theoretical models (Moss, Ravindra, Herve–Vandamme, Reddy, and Kumar–Singh). The selected interval of $2.0 \div 3.5\ eV$ is not arbitrary; it corresponds to the band gap energies of semiconductors widely used in modern optoelectronic devices, such as CdO, ZnO, CdS, ZnSe, GaN, TiO_2, SnO_2, and In_2O_3 [13–15]. These materials are widely integrated into practical applications across the photon energy spectrum, including solar cells, transparent conducting electrodes, UV sensors, gas and biosensors, as well as optoelectronic converters.

Therefore, the theoretical comparison of these models is significant not only from a fundamental scientific standpoint but also for the technological task of selecting the most suitable model for various optical systems and application scenarios. The primary objective of this research is to investigate how the $n{\sim}Eg$ dependence changes across each model, to identify its overall trend, and to define the applicability limits of each model. This approach aims to improve the accuracy of predicting the optical properties of materials and to provide theoretical support for the interpretation of experimental results.

The research is directed toward addressing the following key problems:

- How do the existing classical models (Moss, Ravindra, Herve–Vandamme, Reddy, Kumar–Singh) vary across different Eg intervals?
- Which of these models provide more realistic predictions for real materials within specific Eg ranges?
- Under what conditions does the practical predictive capability of each model weaken?

In addition, the study evaluates the reliability of these models in targeted optical calculations carried out for technological optimization. The aim is not only to compute the $n = f(Eg)$ functions, but also to scientifically highlight their comparative advantages and limitations.

2. Methodology

In this study, the relationship between the refractive index (n) and the band gap energy (Eg) for semiconductor and oxide-based materials was analyzed using various empirical and semi-theoretical models. The analysis was carried out in the following methodological stages:

2.1. Justification of the Selected Eg Interval

For this study, the interval $of\ 2.0 \div 3.6\ eV$ was chosen. This range is characteristic of wide-bandgap semiconductors and oxides, and it corresponds both to the stable applicability domain of theoretical models and to the practical applications of optoelectronic converters [5]. The materials that fall within the selected interval include:

- **III–V compounds:** AlAs (2.16 eV), GaP (2.26 eV), AlP (2.45 eV), GaN (3.40 eV)
- **II–VI compounds:** CdO (2.3–2.5 eV), CdS (2.42 eV), ZnTe (2.26 eV), ZnSe (2.70 eV)
- **Oxides and chalcogenides:** TiO_2 (3.00–3.20 eV), CuI (3.10 eV), In_2O_3 (3.20 eV), ZnO (3.37 eV), SnO_2 (3.60 eV)

The values of $Eg\ and\ n$ were determined under the same temperature conditions ($T \approx 300\ K$), identical crystal phases, and consistent measurement methods, and were obtained from reliable scientific sources [15, 16]. When multiple values under identical conditions were available, the median (central tendency) was used to ensure statistical stability.

Thus, the selection of this interval is justified both in terms of testing theoretical models and for their practical significance.

2.2. Calculation Procedure for Each Model

Model	Əsas düstur	Parametrlər
Moss (1950)	$n^4 E_g = K$	$K = 95$
Ravindra (1979)	$n = a + bEg$	$a = 4{,}084$ $b = -0.62$
Herve–Vandamme (1995)	$n = \sqrt{1 + (\frac{A}{E_g + B})^2}$	$A = 13{,}6$ $B = 3{,}47$
Reddy	$n = \sqrt{\frac{C}{E_g + D}}$	$C = 12{,}417$ $D = 0{,}365$
Kumar-Singh	$n = K \cdot E_g^m$	$K = 3{,}3668$ $m = -0.32234$

Here, the constants A, B, C, D, K, m, and others were taken as reported by the original authors of the respective models and applied to experimental data for validation. By using the functional expressions, the values of n were calculated within the interval of $2.0 \div 3.6\ eV$. [8, 10, 17–19].

2.3. Solution Algorithms and Tools Used

All calculations were performed using Microsoft Excel. In Excel, the functional formulas were arranged in columns, enabling the automatic calculation of n for any given Eg. Tables and graphs were dynamically constructed, which simplified the comparison between models. The obtained theoretical $n{\sim}Eg$ results were compared with the static refractive index values reported in the literature, and the consistency trends were visually analyzed through graphs. This approach allows users to replicate the computational framework and apply the models to different materials.

Alternatively, these models can also be easily coded in programming environments such as MATLAB or Python. However, in this study, the objective was to demonstrate the implementation of the methods in a simple and widely accessible environment.

Theoretical Background

The refractive index (n) is an important optical parameter that defines the propagation characteristics of electromagnetic waves as they pass through a material. In semiconductor materials, an inverse proportionality is typically observed between *n* and the band gap energy (Eg). This interdependence is analyzed using a number of empirical and semi-empirical models. The accuracy and reliability of these models vary depending on the type of material under consideration. The main features of these models and the corresponding computational results are presented below.

3.1. Moss Model (1950)

The Moss model is one of the earliest and most widely used empirical approaches expressing the inverse proportional relationship between the refractive index and the band gap energy. First proposed by T. S. Moss in 1950, this model attempted to establish a quantitative correlation between the optical and electronic properties of semiconductors [8]. It is formulated by the following simple expression:

$$n^4 E_g = const$$

Where:

n — refractive index of the material, Eg — band gap energy (eV), $const$ — an approximately constant value, independent of the material.

Moss suggested a constant value of about $95\ eV$; however, subsequent studies reported a wider range of $170 \div 300\ eV$. This inconsistency is a major limitation of the model and indicates that the constant may depend on the crystal structure, measurement method, and temperature [16, 17].

The main idea of the model is that materials with a wide band gap (e.g., ZnO, GaN, SnO_2) tend to be less polarizable and therefore possess a lower refractive index. Conversely, narrow-bandgap semiconductors (e.g., PbS, CdO) are optically denser and exhibit a higher n. This inverse relationship demonstrates the intrinsic link between electronic structure and optical response.

The application of the Moss model in the analyzed studies indicates that this model provides reasonable agreement only within a limited band gap range and for classical semiconductor systems. For example:

- Tripathy (2015) systematically analyzed the application of the model to different materials and obtained consistency with constants in the range of $170 \div 268\ eV$ [5].
- Reddy et al. (2006) demonstrated that the model lacks accuracy for low-band-gap materials and proposed a modified expression [18].
- Based on their results, Kumar and Singh (2012) reported that the Moss model shows less agreement with experimental data compared to power-law type theoretical approaches [19].

Nevertheless, the Moss model is still widely employed as a fundamental approach in the initial stage of $n{\sim}Eg$ analysis and serves as a baseline for the development of more complex models.

To demonstrate the application of this model, the refractive index (n) was calculated for five different Eg values:

$$n = \left(\frac{K}{E_g}\right)^{1/4}$$

If the Moss constant is taken as K = 95 eV:

(CdO): for $Eg = 2.5\ eV$

$$n = \left(\frac{95}{2{,}5}\right)^{1/4} \approx 2{,}48$$

(ZnO): for $E_g = 3{,}3\ eV$

$$n = \left(\frac{95}{3{,}3}\right)^{1/4} \approx 2{,}32$$

(ZnSe): for Eg ≈ 2.7 eV

$$n = \left(\frac{95}{2{,}7}\right)^{1/4} \approx 2{,}44$$

TiO_2: for Eg ≈ 3.2 eV

$$n = \left(\frac{95}{3{,}2}\right)^{1/4} \approx 2{,}33$$

In_2O_3: for Eg ≈ 2.9 eV

$$n = \left(\frac{95}{2{,}9}\right)^{1/4} \approx 2{,}39$$

These results show that, according to the Moss model, the refractive index (n) decreases as the band gap energy (Eg) increases. The structural simplicity of the model makes it practical and quick to apply compared to more complex approaches. At the same time, due to its ability to provide approximate agreement over a wide range, it is widely used in the optical analysis of similar semiconductor and oxide materials.

3.2. Ravindra Model (1979)

Following the Moss model, in order to provide a more realistic representation of the relationship between the refractive index and the band gap energy in semiconductors, Ravindra and Srivastava (1979) proposed a model based on a simple linear dependence [17]:

$$n = a - bEg$$

Where: n — refractive index, Eg — band gap energy (eV), a, b — empirical constants (for the Ravindra model: $a \approx 4.084, b \approx 0.62$).

This approach is based on the principle that the refractive index decreases linearly as Eg increases. The main advantage of the model lies in its computational simplicity and its better agreement with experimental data, especially for materials within the medium band gap range $(2 \div 3\ eV)$.

Compared to the Moss model, the Ravindra model can be applied to a broader class of materials and demonstrates higher accuracy particularly for II–VI and III–V semiconductors. Tripathy (2015) tested this model on a range of materials and reported high consistency for semiconductors such as CdS, ZnSe, and InP [5]. Similarly, Reddy et al. (2006) compared the Ravindra model with other nonlinear models and confirmed that within the $2 \div 3\ eV$ range, the linear trend aligns well with both theoretical predictions and experimental observations.

However, the drawback of the model is that for materials with very large band gaps (e.g., GaN, SnO_2, β-Ga_2O_3), the linear decrease may lead to negative values of n, which is physically unacceptable. Therefore, the applicability of the Ravindra model is considered reliable only within a limited band gap range.

Using this model, calculations can be performed to observe how *n* varies for different band gap energies Eg.

CdO for $Eg = 2{,}5eV$: $n = 4{,}084 - 0{,}62 \cdot 2{,}5 = 4{,}084 - 1{,}55 \approx 2{,}53$

ZnO for $Eg = 3{,}3eV$: $n = 4{,}084 - 0{,}62 \cdot 3{,}3 = 4{,}084 - 2{,}046 = 2{,}03$

ZnSe for $Eg = 2{,}7eV$: $n = 4{,}084 - 0{,}62 \cdot 2{,}7 = 4{,}084 - 1{,}674 = 2{,}41$

TiO_2 for Eg ≈ 3.2 eV: $n = 4{,}084 - 0{,}62 \cdot 3{,}2 = 4{,}084 - 1{,}984 = 2{,}10$

In_2O_3 for Eg ≈ 2,9 eV: $n = 4{,}084 - 0.62 \cdot 2{,}9 = 4{,}084 - 1{,}798 = 2{,}29$

As a result, although the Ravindra model is useful in providing a simple and remarkably practical relationship between the refractive index and the band gap energy, it exhibits theoretical inconsistencies at extreme Eg values and must be complemented by more sophisticated models.

3.3. Herve–Vandamme Model (1995)

Proposed by Herve and Vandamme in 1994–1995 [10, 16], this model explains the relationship between the refractive index and the band gap energy based on the theory of electromagnetic wave propagation in solids. It is primarily theoretically justified for wide-band-gap semiconductors and is expressed by the following empirical relation:

$$n(E_g) = \sqrt{1 + \frac{A}{E_g + B}}$$

Where: n — refractive index; Eg — band gap energy (eV); $A \approx 13.6\ eV$ — a constant close to the ionization energy of the hydrogen atom; $B \approx 3.47\ eV$ — an empirical correction constant.

The main idea of the model is that optical conductivity and the real part of the dielectric function are related to the band gap energy and atomic-level transitions of high-frequency photons. The fact that A is $13.6\ eV$ indicates that the model is linked to the ground-state energy of the hydrogen atom in quantum mechanics, while B serves as a correction factor depending on the crystal structure and binding energies.

The primary advantage of the Herve–Vandamme model is its high accuracy for wide-band-gap semiconductors (e.g., ZnO, GaN, TiO_2). It shows broad agreement with experimental data, particularly within the $2.5 \div 4.0\ eV$ range.

However, the model also has certain limitations. For narrow-band-gap semiconductors (e.g., PbS, InSb), their accuracy is low. In systems with high carrier concentrations and a strong Burstein–Moss effect, the constants need to be re-optimized [15].

Tripathy (2015) tested this model across a wide range of semiconductors and demonstrated that the Herve–Vandamme relation provides higher accuracy compared to the Moss and Ravindra models, especially for oxides and III–V semiconductors. Reddy et al. (2006) also emphasized that the model works well for wide-band-gap II–VI compounds [18].

The strength of this model lies in the fact that the relationship between the refractive index (n) and the band gap (Eg) is explained not only empirically but also because of physical principles of electron–photon interactions.

CdO $for\ Eg \approx\ 2{,}5eV$:

$$n = \sqrt{1 + \frac{13{,}6}{2{,}5 + 3{,}47}} \approx \sqrt{1 + 2{,}13} \approx 1{,}76$$

ZnO for $Eg \approx\ 3{,}3eV$:

$$n = \sqrt{1 + \frac{13{,}6}{3{,}3 + 3{,}47}} \approx \sqrt{1 + 1{,}88} \approx 1{,}70$$

TiO_2 for $Eg \approx\ 3{,}2eV$:

$$n = \sqrt{1 + \frac{13{,}6}{3{,}2 + 3{,}47}} \approx \sqrt{1 + 2{,}039} = \sqrt{3{,}039} \approx 1{,}74$$

$İn_2O_3$ for $Eg \approx\ 2{,}9eV$:

$$n = \sqrt{1 + \frac{13{,}6}{2{,}9 + 3{,}47}} \approx \sqrt{1 + 2{,}135} = \sqrt{3{,}135} \approx 1{,}77$$

(ZnSe) for Eg ≈ 2.7 eV

$$n = \sqrt{1 + \frac{13{,}6}{2{,}7 + 3{,}47}} \approx \sqrt{1 + 2{,}204} = \sqrt{3{,}204} \approx 1{,}79$$

These results indicate that the model can be applied to wide-band-gap oxide semiconductors such as CdO, ZnO, TiO_2, and In_2O_3. By providing a more realistic and physically grounded variation of the refractive index, the Herve–Vandamme model can play an important role in modeling the optical properties of materials with large band gaps.

3.4. Reddy Model (1992, 1995)

The models proposed by Reddy and co-workers emerged as modifications of the Moss model and aimed to more accurately represent the relationship between the refractive index (n) and the band gap energy (Eg).

The first model, proposed by Reddy and Anjaneyulu in 1992, is expressed in a form like the Moss relation and is constructed on a simple empirical basis. Later, in 1995, Reddy and Nazeer Ahammed modified this expression by introducing a second constant, which improved the agreement for materials with lower band gap energies.

$$\mathrm{n} = \sqrt{\frac{\mathrm{C}}{\mathrm{E_g} - \mathrm{D}}}$$

where: $n -$ refractive index,

Eg- band gap energy (eV),

C and D — empirical constants; for Reddy et al. [1] üçün C≈12,417, D≈0,365.

This expression resembles the square-root form of the Moss model; however, the inclusion of the constant D prevents the occurrence of near-zero or negative arguments at low band gap energies and ensures better agreement with experimental values.

One of the main advantages of the Reddy model is its high accuracy for a wide range of II–VI and III–V semiconductors with band gaps in the range of $1.5 \div 3.5\ eV$ [18]. Owing to its simple structure, it is computationally as convenient as the Moss and Ravindra models. For low-band-gap materials (CdO, PbS, CdSe), it provides more accurate results compared to the Moss model.

Along with these advantages, the Reddy model also has certain drawbacks. As $Eg \rightarrow C$ (very narrow-band-gap materials), the model may yield unrealistically high n values, which are physically unacceptable. For wide-band-gap oxides (e.g., ZnO, Ga_2O_3), its accuracy may deteriorate unless the parameters are re-optimized.

Tripathy (2015) applied this model to various semiconductors and found a higher correlation coefficient in the range of $2.0 \div 3.3\ eV$ compared to the Moss model. Reddy et al. (2006) [18] also emphasized that, in most cases, the difference between experimental and theoretical n values is less than ± 0.05, as shown in tabulated results.

CdO $for\ Eg \approx 2{,}5eV$:

$$n = \sqrt{\frac{12{,}417}{\mathrm{E_g} - 0{,}365}}$$

ZnO $for\ Eg \approx 3{,}3eV$:

$$n = \sqrt{\frac{12{,}417}{\mathrm{E_g} - 0{,}365}}$$

$ZnSe\ for\ Eg \approx 2{,}7eV$:

$$n = \sqrt{\frac{12{,}417}{\mathrm{E_g} - 0{,}365}}$$

$TiO_2\ for\ Eg \approx 3{,}2\ eV$:

$$n = \sqrt{\frac{12{,}417}{\mathrm{E_g} - 0{,}365}}$$

$In_2O_3\ for\ Eg \approx 2{,}9\ eV$:

$$n = \sqrt{\frac{12{,}417}{\mathrm{E_g} - 0{,}365}}$$

The refractive index (n) values obtained through this model provide useful analytical opportunities both for comparison with other theoretical models and for evaluating experimental agreement.

3.5. Kumar–Singh Model (2012)

Proposed by Kumar and Singh in 2012 [19], this model establishes an empirical power-law type dependence between the refractive index and the band gap energy. Unlike the rigid forms of the earlier Moss and Ravindra models, this approach allows for flexible adjustment to experimental data by optimizing two parameters.

The model is expressed by the following general relation:

$$n = K \cdot E_g^m$$

where: n — static refractive index, Eg — band gap energy (eV), K — scaling factor, m - exponent (power index), which varies depending on the class and structure of the material.

The power-law approach describes a monotonic decrease of the refractive index with increasing Eg. The coefficients $K\ and\ m$ are optimized through regression analysis of experimental data. This provides greater flexibility in the modeling process and allows for the selection of specific parameters for different groups of semiconductors.

The advantages of the Kumar–Singh model include the possibility of determining suitable parameters for different band gap ranges. It can be applied to a broader spectrum of materials compared to other models. Due to parameter optimization, it provides high correlation with experimental data.

As for its limitations, the parameters are not universal - $K\ and\ m$ must be re-determined for each new material group. Its physical meaning is not as explicit as that of fixed models (e.g., Moss, Herve–Vandamme); rather, it has a more empirical fitting character.

Tripathy (2015) [5] applied this model to oxides and II–VI semiconductors and obtained high R^2 (correlation) values in the range of $2.0 \div 3.5\ eV$ compared to other models. Kumar and Singh (2012) [19] used the least-squares method to calculate the optimal values of $K\ and\ m$ presenting results for a wide class of materials.

The accuracy of each model depends on the type of material, the band gap range, and the experimental conditions. In this study, the chosen $2.0 \div 3.5\ eV$ range covers semiconductors such as ZnO, TiO_2, In_2O_3, ZnSe, CdS, and GaN, which enables a direct comparison of the models' outcomes within the same window.

RESULTS AND DISCUSSION

In this study, the dependence of the refractive index (n) on the band gap energy (Eg) for semiconductor materials was comparatively analyzed based on five different theoretical models— Moss, Ravindra, Herve–Vandamme, Reddy, and Kumar–Singh. The variations observed in the results across different models arise from the diversity of the theoretical principles and methodological approaches underlying each model.

Table 1 presents the calculated static refractive index (n) values corresponding to different band gap energies (Eg) using the Moss, Ravindra, Herve–Vandamme, Reddy, and Kumar–Singh models. These values were systematically arranged to facilitate a comparative analysis of the $n{\sim}Eg$ dependence among the models.

Table 1. Theoretical dependence between the band gap energy (*Eg*) and the static refractive index (*n*) according to different models. Calculations were carried out using the Moss, Ravindra, Herve–Vandamme, Reddy, and Kumar–Singh models.

Eg (eV)	Moss modeli	Ravindra modeli	Herve-Vandamme modeli	Reddy modeli	Kumar - Singh
2,00	2,63	2,84	3,52	2,76	2,69
2,10	2,59	2,78	3,47	2,68	2,65
2,20	2,56	2,72	3,43	2,60	2,61
2,30	2,54	2,66	3,39	2,53	2,57
2,40	2,51	2,60	3,34	2,47	2,54
2,50	2,48	2,53	3,31	2,41	2,51
2,60	2,46	2,47	3,27	2,36	2,48
2,70	2,44	2,41	3,23	2,31	2,45
2,80	2,41	2,35	3,19	2,26	2,42
2,90	2,39	2,29	3,16	2,21	2,39
3,00	2,37	2,22	3,13	2,17	2,36
3,10	2,35	2,16	3,09	2,13	2,34
3,20	2,33	2,10	3,06	2,09	2,32
3,30	2,32	2,04	3,03	2,06	2,29
3,40	2,30	1,98	3,00	2,02	2,27
3,50	2,28	1,91	2,97	1,99	2,25
3,60	2,27	1,85	2,94	1,96	2,23

Based on the $Eg\ and\ n$ values presented in Table 1, Figure 1 illustrates the variation of the refractive index with the band gap energy for each theoretical model. The graphs provide a comparative representation of how the different models evaluate this dependence and clearly highlight the trends, agreements, and divergences among the models.

It is evident from the figure that there is a negative correlation between the refractive index and the band gap energy. In other words, as Eg increases, the refractive index decreases across all models, which is consistent with the general optical behavior reported in the literature [8, 20, 21].

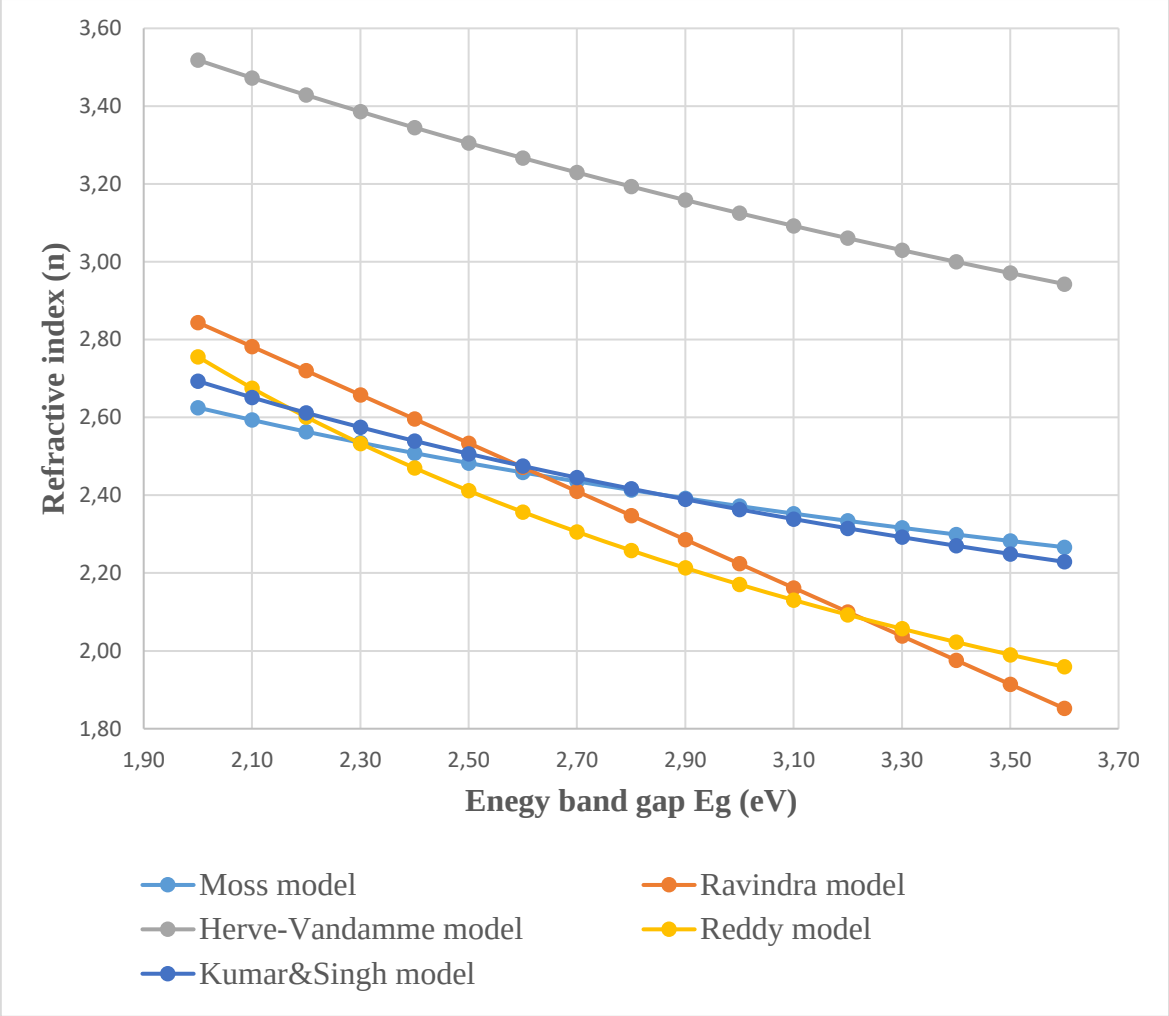

Figure 1. Graphical representation of the dependence of the refractive index (n) on the band gap energy (Eg) according to different theoretical models (Moss, Ravindra, Herve–Vandamme, Reddy, and Kumar–Singh). The graph demonstrates the inter-model differences and the nonlinear nature of the $n(Eg)$ relationship.

The Herve–Vandamme model differs fundamentally from the others. The n values obtained from this model are not only the highest but also show no intersection points with the other models. The main reason why different models predict the relationship between refractive index and band gap energy differently lies in their varying physical foundations. For example, some models (Moss, Ravindra) are based on empirical observations and provide simple mathematical relations, whereas others (Herve–Vandamme, Kumar–Singh) employ more complex physical concepts, such as electron–photon interactions, optical response functions, and high-frequency dielectric constants.

Therefore, the outcomes predicted by different models may significantly diverge. In particular, the parabolic dependence observed in the Herve–Vandamme model exhibits a distinct trend without intersecting the other models. This stems from the model's consideration of both polarizability and the quantum-mechanical approach to light–matter interaction. While such models have stronger theoretical justification over a wider energy range, they may not always fully align with experimental results.

Thus, inter-model differences are a direct consequence of their theoretical foundations—namely, which physical effects are included or excluded—and this factor must always be taken into account when analyzing the results. Because the Herve–Vandamme model incorporates polarization effects and frequency dependence more extensively, its outcomes stand apart from those of the other models [10].

The Moss model, based on classical quantum mechanics, explains the $Eg{\sim}n$ relationship in a straightforward way and provides intermediate values of the refractive index compared to other models. While it shows good accuracy at low Eg, it becomes less reliable at higher Eg values.

In the Ravindra model, a sharp decrease in the refractive index is observed as Eg increases. However, at high Eg values, this may lead to unrealistic n predictions. For example, in the range of $3.5 \div 3.6\ eV$, the predicted n falls to $\sim 1.85 \div 1.90$, which does not agree with experimental data [20].

The Reddy model presents an empirical relation between Eg *and* n, and in some cases yields results closer to experimental observations. Its accuracy is particularly higher in the range of $2.2 \div 3.2\ eV$ [21].

The Kumar–Singh model shows a relatively stable variation of n compared to the other models, with weaker changes in refractive index. This indicates that

the model has been optimized for certain classes of materials [22].

Table 2 presents the band gap energies (*Eg*) and refractive index (*n*) values of various semiconductor materials as predicted by the five different theoretical models (Moss, Ravindra, Herve–Vandamme, Reddy, and Kumar–Singh). For materials with identical *Eg* values, the predicted *n* values are compared, and the behaviors and inconsistencies of the models are analyzed. Based on this data, graphs were constructed to visually evaluate the trends of the models.

	Eg (eV)	Moss modeli	Ravindra modeli	Herve-Vandamme modeli	Reddy modeli	Kumar - Singh
AlAs	2,16	2,58	2,74	3,45	2,63	2,63
ZnTe	2,20	2,56	2,72	3,43	2,60	2,61
CdS	2,42	2,50	2,58	3,34	2,46	2,53
AİP	2,45	2,50	2,57	3,32	2,44	2,52
CdO	2,50	2,48	2,53	3,31	2,41	2,51
ZnSe	2,70	2,44	2,41	3,23	2,31	2,45
GaP	2,80	2,41	2,35	3,19	2,26	2,42
TiO2	3,00	2,37	2,22	3,13	2,17	2,36
CuI	3,10	2,35	2,16	3,09	2,13	2,34
In_2O_3	3,20	2,33	2,10	3,06	2,09	2,32
ZnO	3,37	2,30	1,99	3,01	2,03	2,28
GaN	3,40	2,30	1,98	3,00	2,02	2,27
SnO2	3,60	2,27	1,85	2,94	1,96	2,23

Based on the theoretical calculations presented in Table 2, the $Eg{\sim}n$ dependence according to the different models is illustrated in Figure 2. Through this graph, the effect of variations in the band gap energy on the refractive index of semiconductor materials can be visually compared for each model. The differences among the models as well as the overall trends can be observed more clearly in this representation.

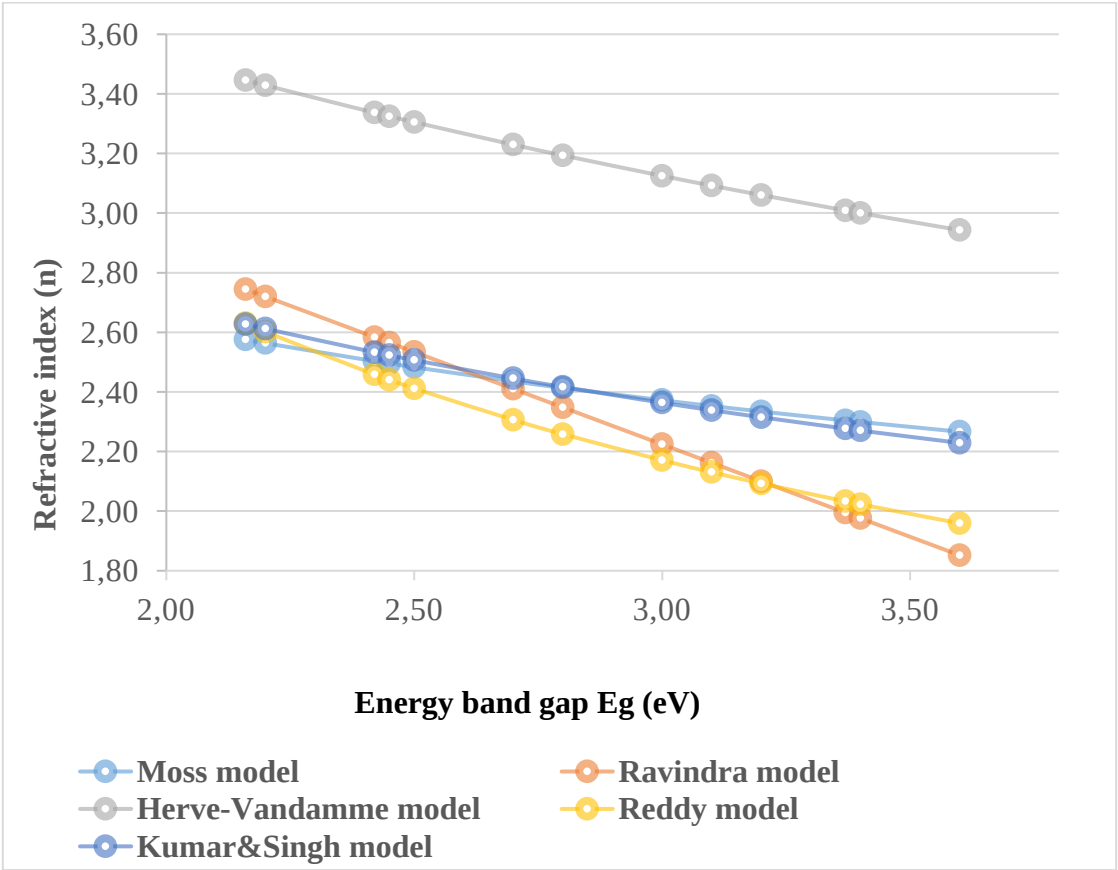

Figure 2. Dependence of the refractive index (n) on the band gap energy (Eg) constructed according to different theoretical models (Moss, Ravindra, Herve–Vandamme, Reddy, and Kumar–Singh). As seen from the graph, n exhibits a decreasing trend with increasing Eg for all models. The Herve–Vandamme model, in contrast to the others, is characterized by higher n values and distinct behavior, which is attributed to its different approach based on the optical dielectric constant.

For materials such as CdO, ZnO, ZnTe, SnO_2, and GaN, the n values obtained from the Herve–Vandamme model were higher than the actual experimental indicators. The Reddy and Kumar–Singh models, on the other hand, often show closer agreement with experimental data. For example, the experimental refractive index of ZnO is approximately $2.0 \div 2.1$, which is in close agreement with the Reddy (2.03) and Kumar–Singh (2.28) models. The Moss model provides acceptable results particularly for relatively narrow-band-gap materials such as GaP and CdS.

These results demonstrate that since the applicability and accuracy of each model differ, no single model can be universally applied to all semiconductors. The choice of model should be made according to the band gap energy and structural properties of the material under investigation.

Conclusion

In this study, the relationship between the refractive index (n) and the band gap energy (Eg) was comparatively analyzed based on five different theoretical models— Moss, Ravindra, Herve–Vandamme, Reddy, and Kumar–Singh. For Eg values in the range of $2.3 \div 3.3\ eV$, the refractive index values were calculated for each model and compared.

The results show that the refractive index decreases inversely with the band gap energy across all models, a trend explained by optical dispersion. Comparative analysis revealed that the Herve–Vandamme model, due to its theoretical and physical foundation, systematically diverges from the others and does not intersect with them in the graphical representation. The Reddy and Kumar–Singh models demonstrated closer agreement with experimental data, especially in the medium and wide band gap ranges, making them more suitable for practical applications.

The analysis confirms that each model provides more accurate results within specific *Eg* intervals; therefore, the optimal choice of model for a given material should be made based on its optical parameters and band gap characteristics. Since the accuracy of results in optical structure design and simulation depends on the selected model, the differences among models emphasize the importance of choosing the most appropriate one.

These theoretical evaluations are consistent with results reported in other studies indexed in Scopus and Web of Science and can be effectively used in analyzing the optical properties of materials such as $CdO, ZnO, SnO_2, ZnSe, TiO_2, and\ In_2O_3$. Future research combining these models with DFT and experimental data could provide more precise assessments and broaden the scope of conclusions in optoelectronic applications.

Abstrakt

This study analyzes the relationship between the refractive index (n) and the energy band gap (Eg) using Moss, Ravindra, Herve–Vandamme, Reddy, and Kumar–Singh models. Results were compared through tables and graphs. All models show an inverse relation between Eg and n, attributed to optical dispersion. Herve–Vandamme deviates due to its theoretical basis, while Reddy and Kumar–Singh agree better with experimental data, especially for medium and wide Eg ranges.

References:

1. Sze, S. M., & Ng, K. K. (2006). *Physics of Semiconductor Devices* (3rd ed.). Wiley-Interscience.

2. Ginley, D. S., Hosono, H., & Paine, D. C. (Eds.). (2010). *Handbook of Transparent Conductors*. Springer.

3. Green, M. A. (2008). Self-consistent optical parameters of intrinsic silicon at 300 K. *Solar Energy Materials and Solar Cells*, 92(11), 1305–1310. https://doi.org/10.1016/j.solmat.2008.06.009

4. Ravindra, N. M., Ganapathy, P., & Choi, J. (2007). Energy gap–refractive index relations in semiconductors – an overview. *Infrared Physics & Technology*, 50(1), 21–29. https://doi.org/10.1016/j.infrared.2006.02.005

5. Tripathy, S. K. (2015). Refractive indices of semiconductors from energy gaps. *Optical Materials*, 46, 240–246. https://doi.org/10.1016/j.optmat.2015.04.038

6. Fox, M. (2010). *Optical properties of solids* (2nd ed.). Oxford University Press.

7. Palik, E. D. (Ed.). (1998). *Handbook of optical constants of solids*. Academic Press.

8. Moss, T. S. (1950). The interpretation of the properties of indium antimonide. *Proceedings of the Physical Society. Section B, 63*(3), 167. https://doi.org/10.1088/0370-1301/63/3/302

9. Ravindra, N. M., Ganapathy, P., & Choi, J. (2007). Energy gap–refractive index relations: A review. *Infrared Physics & Technology, 50*(1), 21–29. https://doi.org/10.1016/j.infrared.2006.02.006

10. Herve, P. J. L., & Vandamme, L. K. J. (1995). General relation between refractive index and energy gap in semiconductors. *Infrared Physics & Technology, 35*(4), 609–615. https://doi.org/10.1016/1350-4495(94)00085-X

11. Reddy, P. J., et al. (1991). Refractive index of semiconductors: Relation to energy gap. *Journal of the Optical Society of America B, 8*(4), 776–778. https://doi.org/10.1364/JOSAB.8.000776

12. Kumar, A., & Singh, K. (2012). Estimation of refractive index from energy gap. *Optik - International Journal for Light and Electron Optics, 123*(6), 535–536. https://doi.org/10.1016/j.ijleo.2011.01.020

13. Morkoç, H., & Mohammad, S. N. (2009). Fundamentals of Zinc Oxide as a Semiconductor. In Zinc Oxide: Fundamentals, Materials and Device Technology.

14. Ohta, H. (2008). Transparent oxide semiconductors. Materials Today, 11(6), 44–50.

15. Özgür, Ü., et al. (2005). A comprehensive review of ZnO materials and devices. Journal of Applied Physics, 98(4), 041301.

16. Herve, P. J. L., & Vandamme, L. K. J. (1995). General relation between refractive index and energy gap in semiconductors. *Journal of Applied Physics*, 77(10), 5476–5477.

17. Ravindra, N. M., et al. (1979). Energy gap–refractive index relations in semiconductors. *Infrared Physics*, 19, 603–604.

18. Reddy, R. R., et al. (2006). Empirical relationship between refractive index and energy gap of semiconductors. *Optoelectronics and Advanced Materials – Rapid Communications*, 10, 1359–1361.

19. Kumar, S., & Singh, N. (2012). Empirical modeling of refractive index for semiconductors. *Optik*, 123, 1654–1656.

20. Ravindra, N.M., et al. (1980). "Energy gap–refractive index relations in semiconductors." *Infrared Physics*, 19(1), 51–52.

21. Reddy, R.R., et al. (2007). "Empirical relation between refractive index and energy gap of semiconductors." *Optics Materials*, 29(10), 1220–1223.

22. Kumar, V., & Singh, A. (2014). "New empirical relation between refractive index and energy gap of materials." *Optik*, 125(17), 4980–4983.