African Journal of Advanced Pure and Applied Sciences (AJAPAS)
Online ISSN: 2957-644X
Volume 3, Issue 1, January-March 2024, Page No: 277-281
Website: *https://aaasjournals.com/index.php/ajapas/index*
معامل التأثير العربي 2023: (1.55) SJIFactor 2023: 5.689 ISI 2022-2023: 0.557

Study of Optical Properties and Calculation of the Energy Gap for $LINAWO_4$ Compound

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Received: January 14, 2024	Accepted: March 23, 2024	Published: March 26, 2024

Abstract:
In this study, the solid-state method was employed for the synthesis of the chemical compound $LiNaWO_4$. According to X-ray diffraction (XRD) analysis, it was found to crystallize in a triclinic crystal system with the parameters of the lattice (a = 12.82 Å, b = 17.49 Å, c = 7.25 Å, α = β = γ= 90°) and the P222 space group. Scanning electron microscopy (SEM) analysis revealed that the compound possesses a compact structure with some porosity. Furthermore, (UV-Vis) spectroscopy was utilized to investigate the optical properties of our compound. The study demonstrated the presence of an energy gap of 4.2 eV, confirming that this compound is a semiconductor material. The Urbach energy was discovered to be approximately 0.38 eV

Keywords: Optical properties, Energy gap, Urbach energy.

Cite this article as: M. Ben Yazid, M. Krimi, A. Ben Rhaiem, A. Elhams, A. Awhida, "Study of optical properties and calculation of the energy gap for the LiNaWO4 compound," *African Journal of Advanced Pure and Applied Sciences (AJAPAS)*, vol. 3, no. 1, pp. 277–281, January-March 2024.

دراسة الخواص البصرية وحساب فجوة الطاقة للمركب $LiNaWO_4$

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الملخص
تم استخدام طريقة الحالة الصلبة في هذه الدراسة لتحضير المركب الكيميائي $LiNaWO_4$. ووفقًا لتحليل الانحراف الزاوي للأشعة السينية (XRD)، تبين أن المركب يتبلور في نظام بلوري ثلاثي الأوجه بمعاملات الشبيكة التالية (a = 12.82 Å، b = 17.49 Å، c = 7.25 Å، α = β = γ = 90°) ومجموعة الفضاء P222. أظهر تحليل المجهر الإلكتروني الماسح (SEM) أن المركب يمتلك هيكلًا مدمجًا مع بعض المسامية. علاوة على ذلك، تم استخدام الطيفية (UV-Vis) لاستكشاف الخواص البصرية للمركب. أظهرت الدراسة وجود فجوة طاقة بمقدار 4.2 إلكترون فولت، مما يؤكد أن هذا المركب هو مادة نصف موصلة. تم اكتشاف طاقة Urbach بحوالي 0.38 إلكترون فولت.

الكلمات المفتاحية: الخواص البصرية، فجوة الطاقة، طاقة اورباخ.

Introduction

Due to the importance of advancements in applied industries across various fields of modern technology, research on new materials and the study of their operational properties is necessary. In recent years, tungsten has been an interesting topic for research due to its exciting characteristics that find applications in various practical uses [1-2]. Tungsten is considered a thermally stable material, with a melting point of approximately 3380

degrees Celsius and a boiling point of around 5900 degrees Celsius. It is also recyclable and is not considered harmful to health [3-5]. Additionally, tungsten trioxide (WO_3) is used as a non-crystalline inorganic material [5]. Moreover, it can be integrated into organic and inorganic compounds [6], which makes it useful in multiple applications, such as manufacturing NEM switches [7] and producing laser hosts and solid electrolytes [8,9]. Numerous tungsten-based materials can be produced, including those with the formula $ABWO_4$ (A, B = Li, Na, K, etc.), which vary in composition based on the ratios of the constituent compounds, resulting in differences in electrical, optical, and thermal properties. In this study, $LiNaWO_4$ compound was prepared using the solid-solid method [10], and analyzed using X-ray diffraction (XRD) to determine its structure and density, and scanning electron microscopy (SEM) was employed to examine its morphology. Furthermore, ultraviolet spectroscopy was utilized to investigate the optical properties, including energy band gap and Urbach energies, which make it an excellent candidate for a variety of uses

Material and methods

The compound $LiNaWO_4$ was prepared by the solid-state method, according to the following equation:

$$1/2Na_2CO_3 + 1/2\ Li_2CO_3 + WO_3 \Leftrightarrow LiNaWO_4 + CO_2$$

The high-purity oxides Na_2CO_3, Li_2CO_3, and WO_3 (99.99% purity) were used; they were ground in an agate mortar after being weighed in the proper ratios. To remove volatile compounds as CO_2, the resulting mix was raised to 723K for 16 hours in a furnace. The resulting powder was then formed into a cylindrical shape and heated once more for 16 hours at 773K to ensure its homogeneity. the sample was prepared for use in the study of its optical properties.

Results and Discussion

1. X-ray diffraction and structural analysis

The diffraction examination using X-rays of the $LiNaWO_4$ ceramic was conducted at room temperature. Subsequently, the structure completion was performed using the CELLREF software. Through structural completion, it was confirmed that $LiNaWO_4$ possesses an orthorhombic structure with the P222 space group and lattice parameters (a = 12.82 Å, b = 17.49 Å, c = 7.25 Å, $\alpha = \beta = \gamma = 90°$). with a unit cell volume of 1628.03 Å3, as shown in Figure (1). the scanning electron microscopy (SEM) technique and energy dispersive X-ray spectroscopy (EDX) were utilized with an accuracy of 40 µm (A) and 9 µm (B), respectively. These techniques were employed to study the structure and composition of our compound, enabling the identification of elements or phases present in it and the detection of backscattered electrons. Figure (2) demonstrates the cohesive distribution of particles on the surface with some pores present. The sample consists of homogeneous particles with dimensions of approximately 3.5 µm, with some particle agglomeration observed due to moisture, attributed to the presence of lithium. Through (EDX) analysis, it is evident that all the elements are present in the compounds shown in the Figure (2).

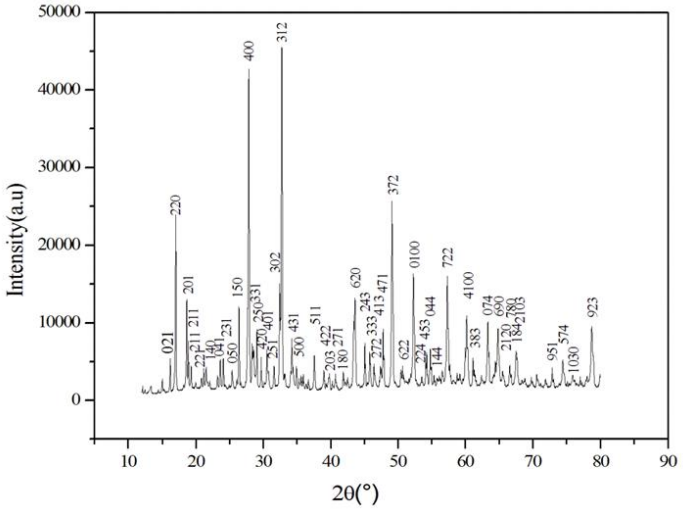

Figure 1 X-ray powder diffraction pattern of $LiNaWO_4$.

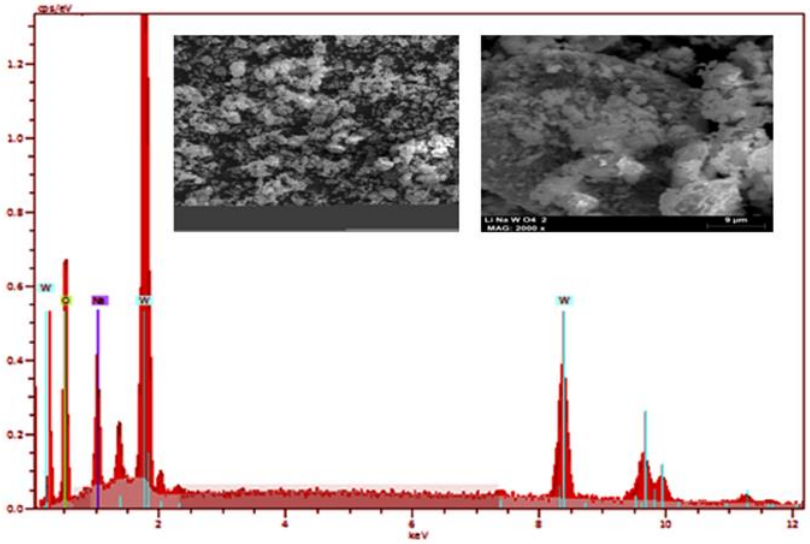

Figure 2 SEM coupled to the EDX result of $LiNaWO_4$ compound.

2. Optical Characterization

We used visible ultraviolet spectroscopy (UV-Vis) to investigate gap and Urbagh energies and the absorption coefficient α Al these parameters allow us to study the optically induced transition and to have more information about the band structure of our compound. The gap energy is a significant parameter for describing materials in the solid state (for disordered materials, it is linked either to a direct or indirect transition through an optical forbidden band) [11].

As shown in Figure (3), an absorption spectrum was conducted at room temperature in the wavelength range of (200-900 nm) to determine the absorption range of the compound. It was observed that $LiNaWO_4$ absorbs visible light with a wavelength of approximately 245 nm. This absorption can be explained by the internal electronic transition (WO)-2 [12-13].

Tauc's relation provides the relationship between gap energy (Eg) and coefficient absorbance (α) near the band edge [14-15]:

$$\alpha h\nu = A(h\nu - E_g)^n$$

Where A is a constant dependent on the material properties, (n) equals 2 for an indirect transition and a direct transfer, equals 1/2 [16]. Additionally, α is the absorption coefficient and ($h\nu$) represents the incident photon energy, which can be calculated using the following expression [17]:

$$h\nu = \frac{1240}{\lambda(nm)}$$

In Figure (3), a graph of $(\alpha h\upsilon)^{1/2}$ and $(\alpha h\upsilon)^2$ as a function of photon energy ($h\upsilon$) is depicted. This graph allows for the determination of the optical band gap (Eg) for both direct and indirect allowed transitions by extrapolating the linear portion of the curves to intersect ($h\upsilon$). The direct band gap is estimated to be approximately 3.57 eV, while the indirect band gap is estimated to be around 4.28 Ev.

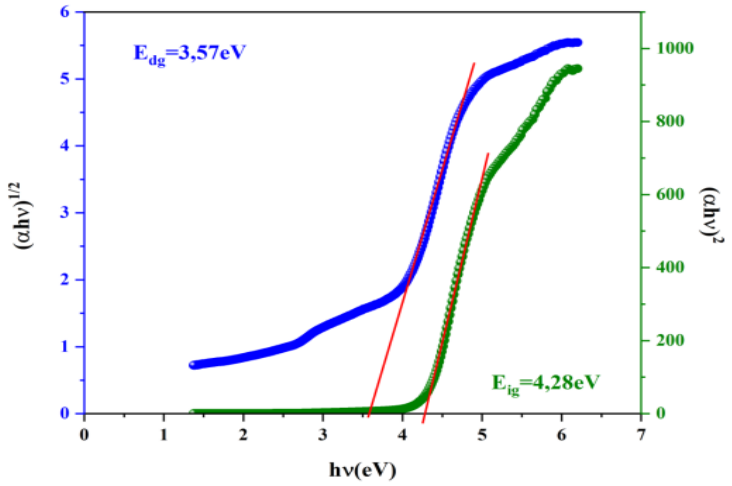

Figure 3 Direct and indirect band gap of $LiNaWO_4$ compound.

The Urbach energy represents the transition between the extended state in the valence band and the localized states in the conduction band, and it also indicates the degree of disorder in the material. In some studies, the width of a state localized in the band gap is used to determine the Urbach energy. Generally, the Urbach energy follows the empirical relation [18-19]:

$$\alpha = \alpha_0 \exp(\frac{h\nu}{E_U})$$

Where α_0 is a constant and (E_U) is the Urbach energy, The Urbach energy can be obtained from the slope of the straight line when plotting Ln (α) against the photon energy (hν), as shown in Figure (4), and it was approximately 0.38 eV

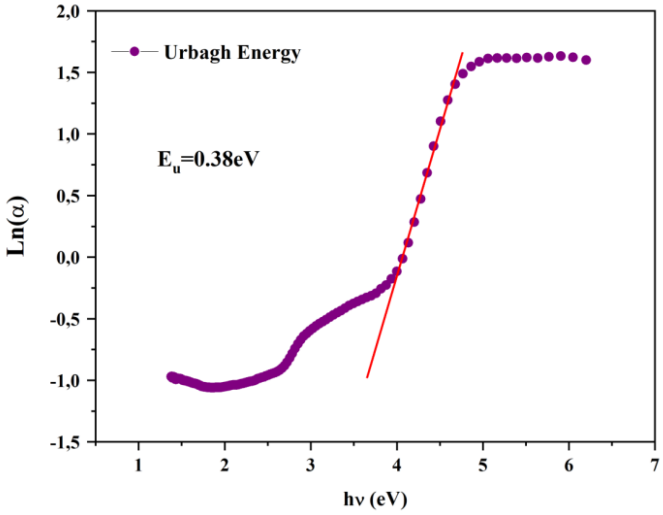

Figure 4 Ln (α) as a function of (hν) for $LiNaWO_4$ compound.

Conclusion

The solid-state method was successfully utilized in the synthesis of the $LiNaWO_4$ compound. Its crystalline nature was confirmed through X-ray diffraction analysis, revealing a triclinic crystal structure. The presence of lithium was observed in the compact structure, exhibiting some clustering and porosity as evident from SEM imaging. Furthermore, the optical properties of the compound were investigated at room temperature using (UV-Vis) spectroscopy. It was found that the molecule absorbs visible light with a wavelength of approximately 245 nm. Additionally, the Urbach energies and optical energy gap of the compound were calculated.

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