Investigation of structural, morphology, optical properties and electrical transport conduction of \( \text{Li}_{0.25}\text{Na}_{0.75}\text{CdVO}_4 \) compound

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Abstract: Polycrystalline \( \text{Li}_{0.25}\text{Na}_{0.75}\text{CdVO}_4 \) was synthesized via a solid-state technique under air atmosphere. It is found that X-ray diffraction peaks are listed as orthorhombic \( \text{Na}_2\text{CrO}_4 \) structure belonging to the space group Cmcm. Composition of elements was examined by energy dispersive X-ray analysis (EDX or EDS). Grains size and morphology of the present material were investigated by scanning electron microscopy (MEB) and atomic force microscopy (AFM). Electrical measurements were performed using complex impedance spectroscopy. Impedance curves confirm the presence of two contributions and an equivalent circuit was suggested. An electrical transport in the material as a thermally activated process has been achieved using DC conductivity. While; AC conductivity is analyzed by the non-overlapping small polar on tunneling (NSPT) conduction mechanism. Refractive index, extinction coefficient, and band gap energy were determined from ellipsometric measurements.

Keywords: \( \text{Li}_{0.25}\text{Na}_{0.75}\text{CdVO}_4 \), \( \text{Na}_2\text{CrO}_4 \) structure, EDS, MEB, AFM, impedance spectroscopy, AC conductivity, ellipsometric measurements.

1. Introduction

The search for new materials such as sodium-based NASICON battery and LISICON lithium battery type had a significance growing impact today in the scientific research. The latter are important devices for the storage of electrical energy and more particularly the lithium batteries have revolutionized the energy storage field due to their low high potential and weight. Indeed, Lithium batteries (LIB) have been successfully integrated in medical and military devices, hybrid electric vehicles and mobile phones thanks to their excellent electrochemical performances [1-6]. Nowadays, Hong et al. discussed the similarities and dissimilarities of lithium and sodium batteries based on positive and negative electrodes. They got it some of sodium batteries (NIBs) have even higher energy densities or comparable contrasted to Li batteries. Several vanadate-based materials and phosphate including \( \text{NaMPO}_4 \), \( \text{KMgPO}_4 \), \( \text{KPbPO}_4 \), \( \text{Na}_3\text{M}_2\text{O}_{44}\text{(P}_2\text{O}_7\text{)}_2 \), \( \text{Na}_2\text{FeP}_2\text{O}_7 \), \( \text{Na}_2\text{FePO}_4\text{F} \) and \( \text{Na}_3\text{V}_2\text{(PO}_4\text{)}_3\text{F}_3 \) have recently been introduced and have shown promising electrochemical performances [7-12].
Particularly, due to their diverse and excellent physical properties applications as cathodes for batteries and luminescent host materials, AMVO₄ compounds (A: an alkali metal and M: a divalent metal) have attracted attention of scientific researchers [13-17]. The origin of the intrinsic luminescence because of the charge transfer from the highest occupied molecular orbital level, which is consist of O (2p) non-bonding orbitals, to the lowest unoccupied molecular orbital level, consist of anti-bonding O (2p) orbitals and V (3d) orbitals in the [VO₄]⁻³ tetrahedral system.

In this work, vanadate based Li₀.₂₅Na₀.₇₅CdVO₄ was systematically prepared by solid-state technique. Then, we investigated structural, morphologic, electrical mechanism and optical parameters such as band gap energy, refractive index, and extinction coefficient.

2. Experimental Approach and Characterization Tools
The powder of the compound with general formula Li₀.₂₅Na₀.₇₅CdVO₄ was fabricated using a solid-state synthesis method. The starting materials with a high purity of sodium oxide (Na₂CO₃), lithium oxide (Li₂CO₃), cadmium oxide (CdO) and vanadium oxide (V₂O₅) were mixed in stoichiometric amounts following the synthesis reaction given as:

\[ x\text{Na}_2\text{CO}_3 + (1-x)\text{Li}_2\text{CO}_3 + \text{V}_2\text{O}_5 + 2\text{CdO} \rightarrow 2\text{Na}_x\text{Li}_{1-x}\text{CdVO}_4 + \text{CO}_2 \]

In a first step, the reagents were weighed in ground and a suitable proportion in an agate mortar before to be submitted to a preliminary heat treatment at 300 °C for 8 h under oxygen flow in the furnace. The goal is to remove CO₂. Then, acquired powder was regrounded, pelletized in a cylindrical form using heated at 720 °C during 12 h and a 3 T/cm² uniaxial pressure.

The crystal structure of Li₀.₂₅Na₀.₇₅CdVO₄ sample obtained using the solid state reaction was analyzed with a Panalytical Xpert X-ray diffractometer equipped with Cu-Kα1 (λ=1.5406 Å) X-ray source, operating at room temperature in 2θ/θ mode from 10° to 70° with a step Δ(2θ) = 0.017°.

Powder composition has been evaluated using analyzing the energy dispersive X-ray connected to Zeiss SEM instrument.

The average grains size was predicted by images possessed from Scanning Electron Microscopy type Zeiss (SEM) and the morphology was demonstrated by an atomic force microscopy (AFM) type a NanoScope IIIa, (Veeco Digital Instruments).

Impedance measurements were performed on pellet with a TEGAM 3550 ALF with AC voltage of 1 V (impedance analyzer) at different temperatures from 598 K to 720 K in frequency range of about (209 - 10⁶) Hz. The pellet was prepared by a uniaxial shaping followed by isostatic pressing at 3 T/cm² and sintering at 723 K during 2 h under air with a 5 K/min heating and cooling rates. The surface and the thickness of pellet were 0.503 cm² and 0.14 cm respectively with a geometric factor of e/S = 0.28 cm⁻¹. In order to ensure a good electric contacts; platinum electrodes were deposed on the two faces of the pellet with a platinum paste and the painted pellet was executed at stable condition temperatures. Impedance data were recorded while the pellet slowly cooled down from 720 K.

Ellipsometric measurements of studied compound was acquired by a phase modulated spectroscopic ellipsometry type (UV-VIS-NIR Horiba JobinYvon) with a 70° angle of incident in the spectral range of (200-800) nm with a 5 nm rate.

3. Results and Discussion
3.1. XRD Analysis
X-ray powder diffraction (XRD) patterns obtained at ambient temperature of Li₀.₂₅Na₀.₇₅CdVO₄ sample is shown in Figure 1. The crystal structure has been refined by the Rietveld’s profile-fitting method. The pseudo-Voigt function is utilized for peak shapes simulation. Atomic
position parameters and lattice parameters derived from the PCD software selected as initial atomic positions for the structural improvement. The profile improvement started with background parameters and a scale pressed by unit cell parameters. Then, preferred orientation corrections and the peak asymmetry are effected. Finally, the individual isotropic parameters and the position of the parameters are improved. The peaks of reflection corresponding to the values of $2\theta$ are listed in the orthorhombic system belongs to a $Cmcm$ space group. The physical parameters are summarized in Table 1.

![X-ray diffraction pattern](image)

**Figure 1.** X-ray diffraction pattern of Li$_{0.25}$Na$_{0.75}$CdVO$_4$ compound.

Table 1 Crystal parameters and conditions of data collection of Li$_{0.25}$Na$_{0.75}$CdVO$_4$ compound.

| **Formula** | Li$_{0.25}$Na$_{0.75}$CdVO$_4$ |
|-------------|-----------------------------|
| Formula weight | 247.82 |
| Color | Yellow |
| Cristallin System | Orthorhombic |
| Space Group | $Cmcm$ |
| Lattice Parameters | |
| $a$= 5.8393 (3) Å | |
| $b$= 9.1333 (4) Å | |
| $c$= 6.8694 (3) Å | |
| $V$=366.36 (3) Å$^3$ | |
| $Z$=4 | |
| Data Collection | |
| Temperature (K) | 298(2) |
| $2\theta$ range (°) | $5^\circ\leq\theta\leq70^\circ$ |
| Radiation, $\lambda$ (Å) | CuK$\alpha$, 1.54098 |
| GOOF | 3.99 |
| $R_B/R_F$ | 0.007/0.005 |

A perspective view of the structure of Li$_{0.25}$Na$_{0.75}$CdVO$_4$ compound is presented in Figure 2. The structure can be depicted as a composite from [CaO$_6$] 5tetrahedral sharing parallel edges giving a little rolled chain along [001]. The chains are linked together by the [VO$_4$] 5tetrahedral and ordered in parallel planes normal to [010]. The different bond lengths and angles are summarized in Tables 2 and 3.
Figure 2 Perspective of the Li$_{0.25}$Na$_{0.75}$CdVO$_4$ structure

Table 2 The positions atomic for Li$_{0.25}$Na$_{0.75}$CdVO$_4$

| Atom | Wyckoff Position | x/a   | y/b   | z/c     |
|------|------------------|-------|-------|---------|
| Na   | 4c               | 0     | 0.67886 (7) | 1/4     |
| Li   | 4c               | 0     | 0.67886 (7) | 1/4     |
| Cd   | 4c               | 0     | 0     | 0       |
| V    | 4c               | 0     | 0.34999 (4) | 1/4     |
| O1   | 8g               | 0.22583 (10) | 0.46868 (8) | 1/4     |
| O2   | 8f               | 0     | 0.25665 (6) | 0.05379 (15) |

Table 3 Interatomic bond lengths (Å) and angles (°) for Li$_{0.25}$Na$_{0.75}$CdVO$_4$

| Distances (Å) | Angles (°) |
|---------------|------------|
| NaLi.O1       | 2.32 (2x)  | O2-NaLi-O1  | 102.94 (4x) |
| NaLi.O2       | 2.16 (2x)  | O1-NaLi-O1  | 68.97 (1x) |
| V-O1          | 1.59 (2x)  | O2-NaLi-O2  | 148.48 (1x) |
| V-O2          | 1.70 (2x)  | O1-V-O1     | 115.37 (2x) |
|               |            | O2-V-O2     | 109.84 (4x) |
|               |            | O1-V-O2     |             |
| Cd-O1         | 1.532 (2x) | O1-Cd-O1    | 85.20 (2x) |
| Cd-O2         | 1.579 (4x) | O1-Cd-O1    | 94.80 (2x) |
|               |            | O1-Cd-O1    | 180.00 (1x) |
|               |            | O1-Cd-O1    | 180.00 (1x) |
|               |            | O1-Cd-O1    | 90.37 (4x) |
|               |            | O1-Cd-O1    | 89.63 (4x) |

3.2. Chemical Analysis
The elemental composition of Li$_{0.25}$Na$_{0.75}$CdVO$_4$ annealed at 993 K is checked by the energy dispersive X-ray analysis (EDX). Figure 3 shows the EDX pattern of fabricated Li$_{0.25}$Na$_{0.75}$CdVO$_4$. This revealed component of the tested sample have been demonstrated of Na, Cd, V and O. Lithium is not observed in the EDS spectrum because it has a too low atomic
number to be detected with EDS. XRD and EDS results indicate our capacity of Li$_{0.25}$Na$_{0.75}$CdVO$_4$ synthesis.

![Figure 3](image_url) EDS profile of Li$_{0.25}$Na$_{0.75}$CdVO$_4$.

### 3.3. SEM and AFM Analysis

Figure 4 (a and b) shows typical SEM and AFM images of specimen. The AFM has been employed to determine the morphology and the surface roughness (RMS) of Li$_{0.25}$Na$_{0.75}$CdVO$_4$ sample. The root mean square (RMS) surface roughness is defined as the standard deviation of the surface height profile from the average height [18]. We notice in the Figure 4 (b) the shapes of micro particles with irregular sizes have been distributed at the surface with a surface roughness (RMS) of about 5.98 nm. This low roughness could be explained by the small grain size of the material.

![Figure 4](image_url) SEM and AFM images of Li$_{0.25}$Na$_{0.75}$CdVO$_4$ sample.

The image of scanning electron microscope (SEM) for Li$_{0.25}$Na$_{0.75}$CdVO$_4$ compound fabricated using solid-state technique see Figure 4 (a). It can be seen that the Li$_{0.25}$Na$_{0.75}$CdVO$_4$ particles present irregular polygons with a wide size distribution, resulting from the grain aggregation
during the solid-state reaction process. According to this image, the grain sizes estimated with image J software are mainly (0.02-0.08) μm (20-80) nm as shown in the Figure 5.

![Figure 5 Size distribution histogram for Li$_{0.25}$Na$_{0.75}$CdVO$_4$ compound](image)

3.4. Electrical Properties

3.4.1. Nyquist Plots and Equivalent Circuit

Complex impedance plots of Li$_{0.25}$Na$_{0.75}$CdVO$_4$ at several temperature are given in the Figure 6. Nyquist plots are characterized by the presence of double semicircular arcs in the pattern because of grain boundary conduction and the bulk. These semicircles exhibit some depression below the x-axis that shows a non-Debye type of relaxation. Electric response material is modeled by an equivalent circuit formed by two cells: (R//C//CPE)+(R//CPE).

The extracted data (EXP.) for the imaginary (-Z") and real (Z') compound for whole impedance was measured using theoretical terms confirmed with the proposed equivalent circuit:

$$Z' = \frac{R_1^{-1} + Q_1 \omega^\alpha \cos(\alpha_1 \pi/2)}{(R_1^{-1} + Q_1 \omega^\alpha \cos(\alpha_1 \pi/2))^2 + (C \omega^\alpha \sin(\alpha_1 \pi/2))^2} + \frac{R_2(1 + R_2 Q_2 \omega^\alpha \cos(\alpha_2 \pi/2))}{(1 + R_2 Q_2 \omega^\alpha \cos(\alpha_2 \pi/2))^2 + (R_2 Q_2 \omega^\alpha \sin(\alpha_2 \pi/2))^2}$$

$$-Z'' = \frac{C \omega + Q_1 \omega^\alpha \sin(\alpha_1 \pi/2)}{(R_1^{-1} + Q_1 \omega^\alpha \cos(\alpha_1 \pi/2))^2 + (C \omega^\alpha \sin(\alpha_1 \pi/2))^2} + \frac{R_2^2 Q_2 \omega^\alpha \sin(\alpha_2 \pi/2)}{(1 + R_2 Q_2 \omega^\alpha \cos(\alpha_2 \pi/2))^2 + (R_2 Q_2 \omega^\alpha \sin(\alpha_2 \pi/2))^2}$$

In order to check for the equivalent circuit chosen, we have shown in the Figure 7 the variations of Z' and Z" (experimental values) compared to patterned (simulated) ones. It was noticed that plots have a linear conducted for the slope nearly equal to unity which shows that the proposed circuit is correctly described the electrical model of the synthesized material.
Figure 6 Impedance curves for Li$_{0.25}$Na$_{0.75}$CdVO$_4$ compound at different temperatures.

Figure 7 Impedance variation of simulated versus calculated values ones of un imaginary and real parts.
3.4.2. D.C Conductivity
Based on the crystal structure, the activation energy appears the ease of ion hopping practically to the openness of the conduction passage.

D.C conductivity $\sigma_{dc}$ of the compound is calculated based on impedance data by the expressions [19]

$$\sigma_g = \frac{e}{S \times R_g}$$

$$\sigma_{gb} = \frac{e}{S \times R_{gb}} \times \frac{C_g}{C_{gb}}$$

Figure 8 presents dependence of the DC conductivity as a function of temperature. It is shown that the dc conductivity increases with an increasing of the temperature and it exhibits a typical Arrhenius behaviour following the relation [20]

$$\sigma_{dc} T = A_0 \exp\left(\frac{E_a}{k_B T}\right)$$

$A_0$: a pre-exponential factor corresponding to 1/T=0, $E_a$: activation energy for the charge transfer and $k_B$: Boltzmann constant.

Nature of pattern suggests the electrical conduction in the material is a thermally activated procedure; values of activation energies of different contributions such as bulk and grain boundary are given in the Figure 8.

![Figure 8](image)

**Figure 8** Curves of $\ln(\sigma_{dc, gb, tot} \times T)$ against $(1000/T)$ for the conductivity data of Li$_{0.25}$Na$_{0.75}$CdVO$_4$ compound

Figure 9 shows the experimental results of the electrical conductivity for NaCdVO$_4$, LiCdVO$_4$ and Li$_{0.25}$Na$_{0.75}$CdVO$_4$ samples. These results display an increase of the conductivity with rising of the sodium content over the complete studied temperature range, which confirms the results founded by Hong et al the battery-based sodium can be a good candidates for battery applications.
3.4.3. AC Conductivity

The ac conductivity $\sigma_{ac}$ is calculated from the impedance data using the following relation [21]

$$\sigma_{ac} (\omega) = \frac{e}{S} \times \frac{Z'}{Z'^2 + Z''^2}$$

where: $Z'$ and $Z''$: real and imaginary parts of the impedance, respectively.

The ac conductivity increases with an increasing of both the angular frequency and the temperature. AC conductivity of variation presents high frequency dispersion and a low frequency plateau. When the dispersion happened, the hopping frequency has been recognized. Then, when the temperature increases, the hopping frequency is tend to a shift toward higher frequencies. This disposal proposes the electrical conduction in compound happened by means of the mechanism of hopping dominated using Almond-West expression defined [22]

$$\sigma_{ac} (\omega) = \sigma_{dc} [1 + \left( \frac{\omega}{\omega_h} \right)^{\frac{1}{s}}]$$

where: the hopping frequency $\omega_h$ is expressed by

$$\omega_h = \left( \frac{\sigma_{dc}}{A} \right)^{\frac{1}{s}}$$

The values of $\sigma_{dc}$, $\omega_h$ and $s$ are obtained by fitting the frequency dependent conductivity data $\sigma_{ac}$. The temperature dependence of the exponent $s$ is given in Figure 10.

The hopping frequency is a temperature dependent and it obeys the Arrhenius equation

$$\omega_h = \omega_0 \exp \left( - \frac{E_h}{k_B T} \right)$$
Figure 10 Temperature dependence of hopping frequency $\omega_h$.

where: $\omega_o$ and $E_h$ are the hopping frequency and the activation energy, respectively. The variation of $\ln(\omega_h)$ versus $1000/T$ is shown in the Figure 11. The activation energy obtained from a linear fit of data is the order of 1.04 eV. This activation energy is different from the one determined from DC conductivity study indicating the transportation is not explained using a simple hopping mechanism.

Figure 11 Curve for $(\sigma_{ac}/\sigma_{dc})$ against $(\omega/\omega_h)$ at various temperatures.

The frequency and conductivity axes are scaled using hopping frequency and DC conductivity, respectively following scaling form

$$\frac{\sigma_{ac}}{\sigma_{dc}} = \frac{\omega}{\omega_h}$$

where: $\sigma_{ac}$: DC conductivity and $\omega_h$: a crossover frequency separating dc regime (plateau region) from the dispersive conduction [23].
A completely superposed master plot for the spectra of conductivity is acquired of titled compound see Figure 12. Therefore, the relaxation mechanism is temperature independent with the conductivity formalism.

![Figure 12](image-url)

**Figure 12** Theoretical and experimental AC conductivity analysis based on the NSPT model for NaCdVO₄, LiCdVO₄ at different frequencies.

### 3.4.4. Theoretical Fitting of AC Conductivity Data With NSPT Model

It is well known that dependence of the exponent $s$ with the temperature can highlight the conduction mechanism. If $s$ increases with the temperature, small polar on tunneling is the predominant mechanism. A minimum value of $s$ followed by an increase suggests that the predominant conduction is obtained by overlapping a large polar on tunneling mechanism. Under such circumstances $s$ is independent of the temperature and quantum mechanical tunneling is possible. The correlated barrier hopping is usually associated with a decrease of $s$ with temperatures [24-26].

In our composition, the value of $s$ is found to be increasing with the rising of the temperature. This behavior is a characteristic of a small polar on tunneling and ac conduction in this case can be explained based on small polar on tunneling model. Considering this model the frequency exponent $s$ and the ac conductivity are expressed as [25]

$$s = 1 - \frac{4}{\left[ \ln \left( \frac{1}{\omega \tau_0} \right) - \frac{W_H}{k_B T} \right]}$$

$$\sigma_{ac} = (\pi e)^2 k_B T \omega \alpha^{-1} [N(E_F)]^2 \frac{R^4_{\omega}}{12}$$

where: $N(E_F)$: the density of states near the Fermi level, $e$: the electronic charge and $\alpha$: the spatial extension of the polar on ($\alpha = 1(\text{Å})^{-1}$) [27]

$$R_{\omega} = \frac{1}{2 \alpha} \left[ \ln \left( \frac{1}{\omega \tau_0} \right) - \frac{W_H}{k_B T} \right]$$

The variation of ac conductivity as a function of temperatures at selective frequencies see Figure 13, one can see, experimental data (points) are in a good agreement with theoretical curves (lines) ones. The results of refinement parameters are listed in Table 4.
The dependence of $R_\omega$ with temperature at various frequencies, see Figure 14. One can see, for a given temperature, $R_\omega$ decreases as a function of the frequency. However, at high frequencies the parameter $R_\omega$ reaches low values. This behavior can be explained by the fact that beyond a certain frequency for the external field the charge carriers cannot follow the applied electric field. It is therefore likely that hopping of charge carriers go from a long distance to a short distance.

Figure 14 Dependance of $R_\omega$ with temperature at different frequencies.
As $R_\omega$ is in the order of the angstrom and the structural arrangement of demonstrated compounds presents Na$^+$/Li$^+$ ions are located in tunnels along [100] direction. Moreover, Na/Li-Na/Li distance in the range of 5.83 Å, thus one can conclude that the motion of small polar on s is because of the displacement of Na$^+$/Li$^+$ ions in tunnels along [100] direction for a high frequency.

According to the standard polar on model of H. Frohlich the polar on radius is connected to it’s effective mass as [28]

$$R = \frac{\hbar}{\sqrt{2m^*\omega}}$$

where: $\omega_{LO}$ is the phonon energy.

The polaron radius can be evaluated using the relation [29]

$$r_p = \frac{1}{2} \frac{\pi}{6N}^{1/3}$$

The calculated values of $m^*$ and $r_p$ for the considered compound are found to be 2.25 Å and $1.03 \times 10^{-28}$ Kg. Since the polar on radius is lower than the hopping distance (inter ionic distance along the tunnels). It confirms that small polar on hopping is a possibility in this material.

3.5. Ellipsometric Study

The refractive index $n$ and extinction coefficient $k$ of the corresponding Li$_{0.25}$Li$_{0.75}$CdVO$_4$ samples determined by a phase modulated spectroscopic ellipsometer. The ellipsometer measures the change of the light’s polarization transmitted or reflected from materials. Polarization change is performed as aphase difference ($\Delta$) and an amplitude ratio ($\Psi$). On the other hand, it can be applied to investigate crystallinity, doping concentration, roughness composition, and other properties of materials deals with optical response changing [30-35]. Fresnel reflection and transmission coefficients are the proportions component amplitudes of an electric field. Fresnel reflection coefficients $r_s$ and $r_p$ indicate s- (perpendicular) and p- (parallel) direction of polarized light, which are utilized to confirm states of polarization of an electromagnetic wave, which can be separated by means of transmitted of reflected electric field components from samples.

Ellipsometric angles $\Psi$ and $\Delta$ are related to the Fresnel coefficients through the following equation [36-39]

$$\rho = \frac{|r_p|}{|r_s|} = \tan \Psi e^{i\Delta}$$

where: $\Psi = \frac{|r_p|}{|r_s|}$ and $\Delta = \delta_p - \delta_s$.

The Figure 15 shows the spectral dependencies of $\Psi$ and $\Delta$ for Li$_{0.25}$Li$_{0.75}$CdVO$_4$. 
Figure 15 Ellipsometric parameters spectra, and Δ and Ψ against wavelength λ for Li$_{0.25}$Li$_{0.75}$CdVO$_4$.

The complex refractive index is connected directly to the ellipsometric angles Ψ and Δ, for bulk isotropic samples and the angle of incidence θ can be expressed by the equation [40]

\[
n^2 - k^2 = n_0^2\sin^2 \theta \left( 1 + \tan^2 \theta \frac{\cos^2 2\Psi - \sin^2 2\Psi \sin^2 \Delta}{(1 + \sin 2\Psi \cos \Delta)^2} \right)
\]

\[
2nk = n_0^2\sin^2 \theta \tan^2 \theta \frac{\sin 4\Psi \sin \Delta}{(1 + \sin 2\Psi \cos \Delta)^2}
\]

The calculation of Δ and Ψ for a fixed λ and incidence angle of incident is adequate to extract two unknown parameters (refractive index n and extinction coefficient k).

Optical absorption coefficient is calculated from the acquired k data using the following expression [41]

\[k = \frac{\alpha \lambda}{4\pi}\]

Figure 16 presents the variation of extinction coefficient and refractive index as a function of incident wavelength. It is obvious that the refractive index n of sample decreases with wavelength increasing. Indeed, in the ultraviolet region, the opacity value decreases until it reaches a rather low value in the visible range of the spectrum. One can deduced from these results and as this compound presents a fort absorption in the UV region, demonstrated compound can be utilized like UV sensor application in this research.
Figure 16 Plots extinction coefficient and refractive index against λ for Li$_{0.25}$Li$_{0.75}$CdVO$_4$ specimen.

The exact band gap value of the compound is determined by the Tauc relation [42]

$$(\alpha h \nu) = B (h \nu - E_g)^m$$

where: $h \nu$: incident photon energy, $A$: a constant characteristic of the material, $(E_g)$: optical energy gap , $m$=2 or 1/2: direct and indirect transitions respectively, and $\alpha$: absorption coefficient.

The incident photon energy is determined by means of the following expression [42]

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

Figure 17 presents the curves of $(\alpha h \nu)^2$ and $(\alpha h \nu)^{1/2}$ as a function of the photon energy $(h \nu)$ of Li$_{0.25}$Li$_{0.75}$CdVO$_4$ sample. The behaviours of these plots favour the direct transition. The optical energy gap $E_g$ is calculated by the extrapolation of the best fit line of $(\alpha h \nu)^2$ versus $(h \nu)$. It is found to be 4.5 eV. This compound labelled as a semi-conductor has a large gap compared to other ones.
4. Conclusion

Li_{0.25}Li_{0.75}CdVO_{4} powder was prepared by the solid-state reaction method. X-ray diffraction analysis confirmed that the prepared compound is crystallized with the Na_{2}CrO_{4} structure. The analysis of frequency dependence of Nyquist curves allowed calculating an equivalent electrical circuit for the electrochemical cell with the considered compound. The ac conductivity showed a variation with frequencies following a Jonscher power law. The NSPT model has theoretically supported the electrical conductivity of the present compound.

The phase modulated spectroscopic ellipsometry was used in the goal to extract some important optical parameters such as refractive index, extinction coefficient and the band gap energy. The extinction coefficient and refractive index development as a function of λ for samples follows to the absorbing Cauchy law. The optical band gap of the material was evaluated to be 4.5 eV.

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