IJISET - International Journal of Innovative Science, Engineering & Technology, Vol. 6 Issue 5, May 2019
ISSN (Online) 2348 – 7968
www.ijiset.com

Absorption Coefficient and Energy Gap of $Fe_3O_4$and Ni_2O_3 Nano-materials for Different Concentration

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Abstract

Thin film of (Fe_3O_4 and Ni_2O_3) Nano-material deposited on ITO glass substrate, have been prepared by spin coating method with different thicknesses (55.25, 78.7, 90.9 144.9 and 263.15) nm for each. The optical parameters like absorption coefficient and energy gap were found by using UV spectral technique. The absorption peaks is found to correspond to the energy gaps according to plank quantum. For all samples the absorption coefficient decreases upon increasing the concentration, while the energy gap increases with concentration.

Keyword: Absorption coefficient, energy gap, concentration.

Introduction

Nickel Oxide (NiO) is an important transition metal oxide with cubic lattice structure. Among the magnetic nanoparticles, fabrication of nickel nanoparticles is often more difficult than that of the other particles. This is because they are easily oxidized. To achieve pure nickel nano-crystals, numerous methods have been conducted in organic environments in order to prevent formation of hydroxide or oxidation [1]. Iron oxide nanoparticles (NPs) have attracted much consideration due to their unique properties, such as super paramagnetic, surface-to-volume ratio, greater surface area, and easy separation methodology. Various physical, chemical, and biological methods have been adopted to synthesize magnetic NPs with suitable surface chemistry [2].Optical property refers to a material's response to exposure to electromagnetic radiation and, in particular, to visible light. This section first discusses some of the basic principles and concepts relating to the nature of electromagnetic radiation and its possible interactions with solid materials. Next to be explored are the optical behaviours of metallic and non-metallic materials in terms of their absorption, reflection, and transmission characteristics. Electromagnetic radiation is considered to be wavelike, consisting of electric and magnetic field components that are perpendicular to each other and also to the direction of propagation; all electromagnetic radiation traverses a vacuum at the same velocity (3×10^8m/s).

Sometimes it is more convenient to view electromagnetic radiation from a quantum-mechanical perspective, in which the radiation, rather than consisting of waves, is composed of groups or packets of energy, which are called photons. The energy E of a photon is said to be quantized, or can only have specific values [3].Light Interactions with Solids: When light proceeds from one medium into another (e.g., from air into a solid substance), several things

happen. Some of the light radiation may be transmitted through the medium, some will be absorbed, and some will be reflected at the interface between the two media. For transparent materials, there is a relation between the index of refraction and the dielectric constant. The phenomenon of refraction is related to electronic polarization at the relatively high frequencies for visible light; thus, the electronic component of the dielectric constant may be determined from index of refraction measurements using Equation (9). Because the retardation of electromagnetic radiation in a medium results from electronic polarization, the size of the constituent atoms or ions has a considerable influence on the magnitude of this effect generally, the larger an atom or ion, the greater the electronic polarization, the slower the velocity, and the greater the index of refraction [4,5].Different attempts were made to account for optical properties of many metal oxides. In the work done by Khadija, it was shown that the increase of CuO concentration increase solar cell efficiency [6] where the efficiency is affected by the energy gap and absorption coefficient the work done by M.Dirar [7] shows that the solar cell efficiency increases when the ZnO concentration increases. Thowra and others [8] shows that the energy gab of CuO is lower than that of ZnO, where CuO acts as a p-type, where ZnO acts as an n-type semiconductor. The CuO and ZnO materials have low efficiencies. This requires searching for other materials which are abundant to study their absorption coefficient and energy gap.

Theoretical Background

The electric field E, displacement X, velocity V and acceleration a takes the

$$E = E_0 e^{-iwt} = E_m e^{i(kx-wt)}$$

$$x = x_0 e^{-iwt} \qquad v = \dot{x} = -iwx = v_0 e^{-iwt} \qquad a = \dot{v} = -iwv = -w^2 x \qquad (1)$$

The equation of motion of electrons or any charged particle is given by

$$m\ddot{x} = eE - \gamma_0 n_0 v \qquad (2)$$

Where n_0 is the medium number density hence

$$(\gamma_0 n_0 - iwm)v = eE$$

With γ_0 standing for the friction per particle. Therefore the velocity v is given

$$v = \frac{eE}{\gamma_0 n_0 - iwm} = \frac{e\,(\gamma_0 n_0 + iwm)E}{[\gamma_0^2 n_0^2 + w^2 m^2]} \qquad (3)$$

For very small mass m and high concentration n_0, such that

$$\gamma_0 n_0 > wm \qquad (4)$$

Equation (3) becomes

$$v = \left[\frac{e}{\gamma_0 n_0} + \frac{iwme}{\gamma_0^2 n_0^2}\right] E \qquad (5)$$

But the current density is given by

$$J = n\,e\,v = n\,e\,\frac{dx}{dt} = \frac{dnex}{dt} = \frac{dp}{dt} = x\,\frac{dE}{dt} = -iwxE = -iw\,(x_1 + ix_2)E$$

Where x represents electric susceptibility

Using (5) gives

$$ne^2 = \left[\frac{1}{\gamma_0 n_0} + \frac{iwm}{\gamma_0^2 n_0^2}\right] E = [wx_2 - iwx_1]E \qquad (6)$$

Equating real and imaginary parts gives

$$x_1 = \frac{-m}{\gamma_0^2 n_0^2} x_2 = \frac{ne^2}{w\gamma_0 n_0} \qquad (7)$$

The absorption coefficient is related to the complex wave number

$$k = k_1 + ik_2 \qquad (8)$$

Where the intensity takes the form

$$I = |E|^2 = E\, m^2 e^{-k_2 x} = I_0 e^{-2k_2 x} = I_0 e^{-\alpha x} \qquad (9)$$

Thus the absorption coefficient is given by

$$\alpha = 2k_2 \qquad (10)$$

Using the relation between wave number with electric permittivity and magnetic permeability, one gets

$$k^2 = (k_1 + ik_2)^2 = k_1^2 - k_2^2 + 2k_1 k_2 i = \frac{w^2}{v^2} = w^2 \mu \varepsilon = w^2 \mu[\varepsilon_1 + i\varepsilon_2]$$
$$= w^2 \mu \varepsilon_1 + w^2 \mu \varepsilon_2 \qquad (11)$$

Thus equation real and imaginary parts, yields

$$k_2 = \frac{w^2 \mu \varepsilon_2}{2k_1} = \frac{w^2 \mu \varepsilon_0 (1 + x_2)}{2k_1} \qquad (12)$$

In view of equations (7) and (12), one gets

$$k_2 = \frac{w^2 \mu \varepsilon_0 \left(1 + \frac{ne^2}{w\, r_0 n_0}\right)}{k_1} \qquad (13)$$

Thus according to equation (10) the absorption coefficient takes the form

$$\alpha = 2k_2 = \frac{2w^2 \mu \varepsilon_0}{k_1}\left(1 + \frac{ne^2}{w\, r_0 n_0}\right) \qquad (14)$$

Material and Method

Samples Preparation

Nickel oxide thin films were prepared by spraying a 0.1 M solution of nickel nitrate of doubly distilled water onto the pre-heated amorphous glass substrates kept at (390˚C ± 10˚)C. Iron oxide thin films were prepared by spraying a 0.1 M solution of ferric nitrate of doubly distilled water onto the pre-heated amorphous glass substrates kept at (390˚C±10˚C). Film concentration or thickness was measured by using the weight difference method considering the substrate surface area and the density of the bulk nickel oxide. As the density of thin films was certainly lower than the bulk density, the actual film thickness would be larger than the estimated values the thickness of the thin film thus reflects the concentration. The structural, optical characterization of the films deposited at optimized preoperative parameters was carried out.

Results

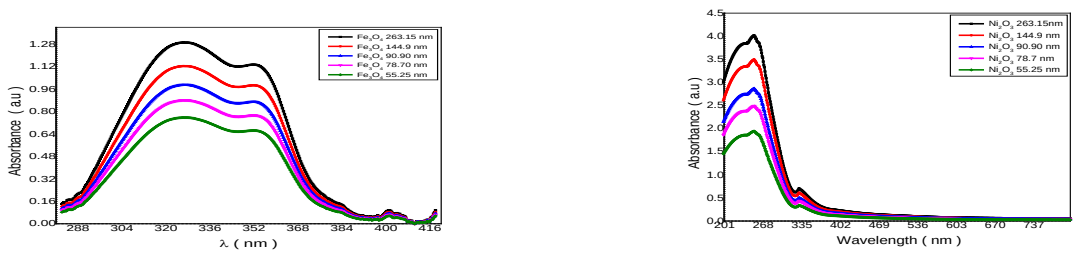
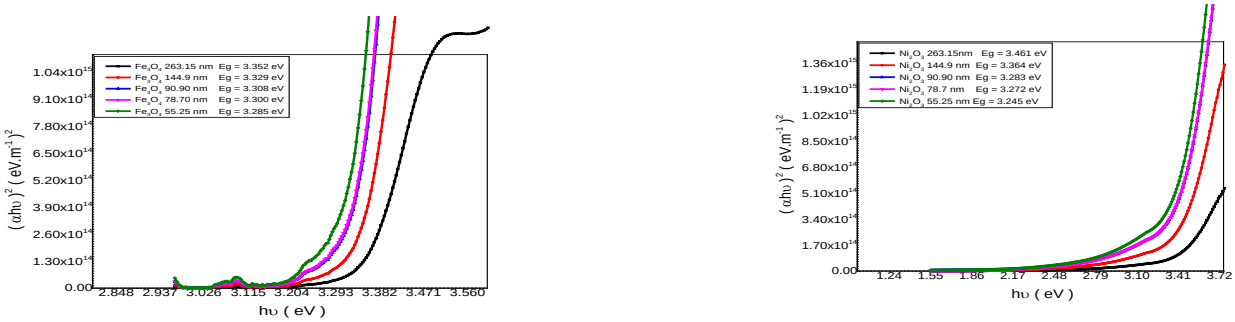
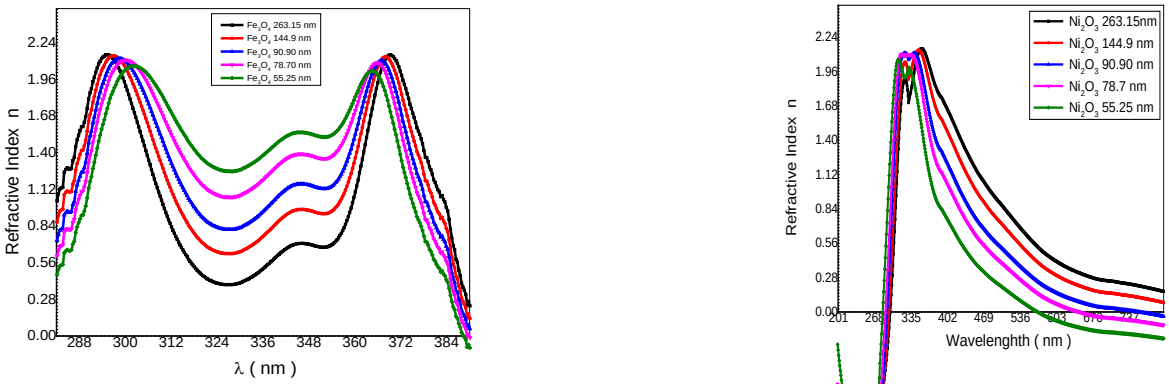


Fig:(1):relation between absorbance and wavelengths of five sample that is made by Ni_2O_3 in and five sample made by (Fe_3O_4) different thickness

Fig(2): relation between absorption coefficient and wavelengths of five sample that made by Ni_2O_3 and five sample made by (Fe_3O_4) in different thickness



Fig(3):The optical energy band gab of five sample that made by Ni_2O_3 and five sample made by (Fe_3O_4) in different thickness



Fig(4) :relation refractive index and wavelengths of five sample that made by Ni_2O_3 and five sample made by (Fe_3O_4) in different thickness

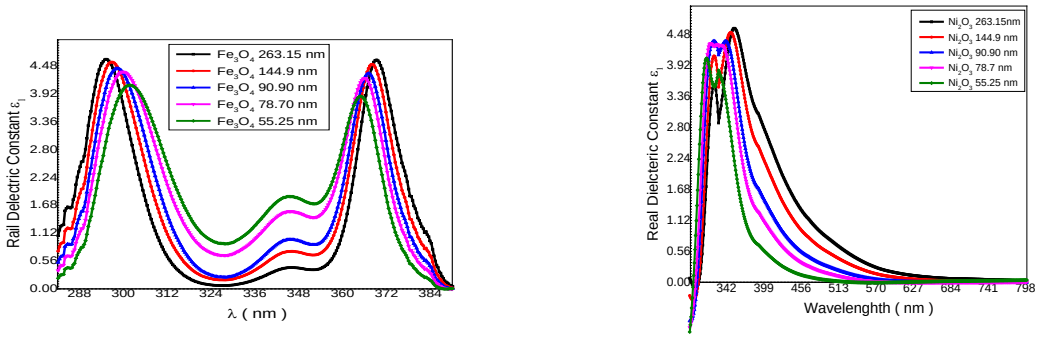


Fig (5): relation between reail dielectric constant and wavelengths of five sample that made by Ni_2O_3 and five sample made by (Fe_3O_4) in different thickness

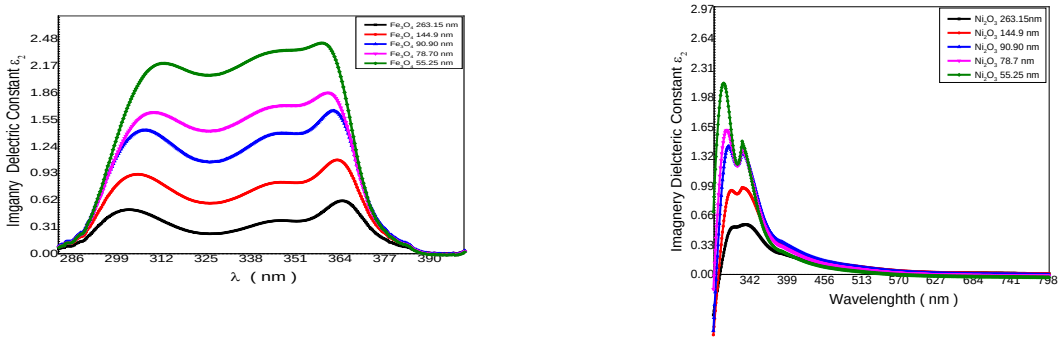


Fig (6): relation between imaganry dielectric constant and wavelengths of five sample that made by Ni_2O_3 and five sample made by (Fe_3O_4) in different thickness

Discussion

The absorption spectral pattern, the absorption coefficient and energy gap for Fe_3O_4 and Ni_2O_3 show very interesting properties. For Fe_3O_4, fig (1) shows that the absorption peak for all thicknesses is around the wavelength 320 nm. However slight wavelength decrease upon increasing concentration is observed. This means that the absorption peak and pattern are slight dependent on material density and thickness. This means that increasing Fe_3O_4 concentration decrease the absorbed photon wavelength thus increases the minimum photon threshold energy which cause electrons to transfer from valence to conduction band. This means that the increase of Fe_3O_4 concentration increase the energy gab. This agrees with energy gab curve in fig (3). According to fig (1) the increase of concentrations to take the values (55.25, 78.7, 90.9 144.9 and 263.15) mg/cm^2 causes the wavelength to take values 323, 321, 320, 318 and 317 nm which decreases upon increasing the Fe_3O_4 concentration. The energy gab increases also when the concentration increases and wavelength decrease where it takes the values (3.285, 3.300, 3.308, 3.329 and 3.352) ev respectively. The absorption peaks in the range of 320 nm corresponds to energy gab having order of 3.3 ev. The same hold for Ni_2O_3 where the increase of Ni_2O_3 concentration to take the values (55.25, 78.7, 90.9 144.9 and 263.15) mg/cm^2 causes the wavelengths to decrease to take the values (268, 267, 266, 265 and 264) nm respectively with increase of energy gab to assume the values (3.245, 3.272, 3.283, 3.364 and 3.461) ev respectively. It is very interesting to note

that the absorption peaks in the range of 360 nm correspond to energy gabs having order of magnitude in the range of 3.2 ev. Fig (2) shows that the absorption coefficient increases when the Fe_3O_4 and Ni_2O_3 concentration decrease. This feature can be easily described by using equation (14) which shows inverse relation between the concentrations and absorption coefficient. The fact that the Fe_3O_4 and Ni_2O_3 have large energy gaps in the range $(\sim 3ev)$, means that increasing their concentrations n_0 does not increase the concentrations of free carriers n, Thus upon increasing n_0, n remains constant, thus α decrease according to the relation (14)

$$\alpha \sim \frac{n}{n_0} \quad (15)$$

This may be also explained by suggesting that Fe_3O_4 and Ni_2O_3 are more transparent than the substrate, since they contain a lot of oxygen thus they reemit the absorbed radiation. It is also very interesting to note that the increasing $Fe_3O_4$and Ni_2O_3 concentration increases the energy gap. This may be explained by bearing in mind that increasing concentrations decrease the absorption α. But

$$\alpha = (hf)^{-1} C^{\frac{1}{2}} (hf - E_g)^{\frac{1}{2}} \quad (15)$$

According to this relation α decrease as the energy gap increases. The increase of energy gap when the Fe_3O_4 and Ni_2O_3 concentrations increase can also be explained by using generalized statistical mechanical laws, by assuming that Nano crystal potential of each Nano particle is an attractive force. Thus the number of particles which is proportional to the concentration is given by:

$$n_0 = A\, e^{\frac{-\beta E_g}{\overline{E}}} = A\, e^{\frac{\beta E_g}{v}} \quad (16)$$

Where: $\overline{E} = -v$

Hence $E_g = \frac{v}{\beta} \ln \frac{n_0}{A}$

Conclusion

The change of Fe_3O_4 and Ni_2O_3 concentrations affects both absorption coefficient and energy gap. The increase of concentration increases the energy gap and decreases the absorption coefficient.

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