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Effect of dopants on the optical Properties of Amino acid Crystal

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ABSTRACT

Recently an extensive research investigation has been carried out on semi organic because they share both the properties of organic and inorganic materials. In the case of organometallic complex materials the optical and properties are mainly dominated due to the presence of organic ligands. UV-Vis measurements were carried out to fetch the optical properties such as absorption, transmittance, reflectance, extinction coefficient and refractive index. The optical property confirms that the material is suitable for optical device fabrications.

Keywords: *L-Alanine, Reflectance, Refractive Index.*

1. Introduction

Crystal optics is the branch of optics that describes the behavior of light in anisotropic media, that is, crystal in which light behaves differently depending on which direction the light is propagating. Crystals are often naturally anisotropic, and in some media it is possible to in Optical Crystallography, branch of crystallography that deals with the optical properties of crystals [1]. It is of considerable interest theoretically and has the greatest practical importance. In the absence of external crystalline form, as with the minerals in a rock, a mineral often may be readily identified by the determination of some of its optical properties. Crystals, however, are often naturally anisotropic, and their atoms are closer together in some planes more than others. This means their optical properties are different depending on which way the light travels through them. In the case of organometallic complex materials the optical and structural properties are mainly dominated due to the presence of organic ligands [2]. Alanine is α-amino acid which contains amine, carboxyl and methyl group exist in a zwitterionic form [3]. In this emerging context organic non linear materials have been recognized as a forefront candidate for fundamental and applied investigations including, in a joint effort of chemists, material scientists and optical engineers [4-8].

2. Materials and methods

In order to study the optical properties of the crystals, three different crystals are chosen namely L-Alanine, cobalt and nickel doped L-Alanine. The transmittance data for all the three crystals were collected and theoretical calculations are performed to determine the optical parameters of the crystals. The optical constants were playing a prominent role it is used for the application of optoelectronics and photonics. When light passes through any crystal, it can be transmitted, reflected, or absorbed.

3. Result and Discussion

3.1. Transmittance

Transmittance is the quantity of light that passes through a crystal. It is the fraction of incident electromagnetic power that is transmitted through a crystal. The transmittance of a material is defined as the part of the light that moves through the other side of the surface. Transmittance is also defined as a ratio of the intensity of incident light (I_0) to the amount of intensity passes through the object (I). The transmittance is denoted as T.

$$T = \frac{I}{I_0}$$

I_0 is the intensity of incident light. I is the intensity of light that can pass through the material. Fig.1. shows the transmittance spectrum of the crystals.

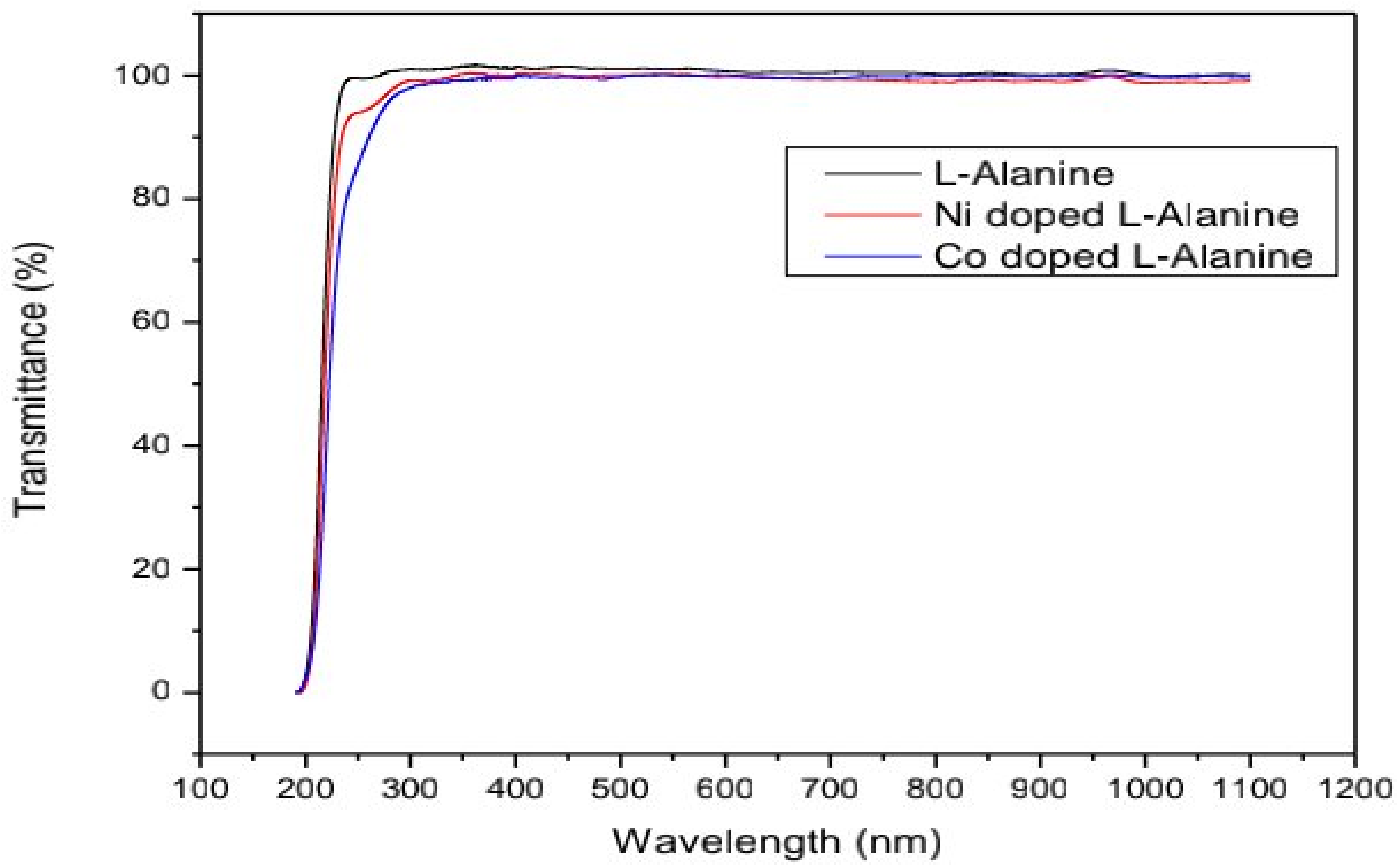

Fig.1. Transmittance spectrum of the crystals.

The transmittance spectrum confirms that, all the three crystals are highly transparent in nature. L-Alanine crystal shows maximum transmittance 100%. Due to doping with cobalt and nickel the transmittance percentage decreases. Nickel and cobalt doped L-Alanine crystal shows maximum transmittance of 99%. In the absence of strong conjugated bonds in L-Alanine amino acid crystal, the lower cut-off wavelength is 221 nm. Due to metal doping, strong conjugated bonds arises in which the lower cut-off wavelength shifted towards higher wavelength. The lower cut-off wavelength of Nickel and cobalt doped L-Alanine crystals are 232 nm and 246 respectively.

3.2. Absorbance

Absorbance (A), also known as optical density (OD), is the quantity of light absorbed by a crystal material.

$$A = \log_{10} (I_0/I)$$

where I_0 is the intensity of the incident light, and I is intensity of that light after it passed through the sample. The equation that allows one to calculate absorbance from % transmittance is

$$A = 2 - \log_{10} (\%T)$$

Fig.2. shows the absorbance spectrum of all the three crystals. From the absorbance spectrum it was known that all the three crystals experiences lower absorbance in percentage. Due to doping, there is small increase in the absorbance percentage.

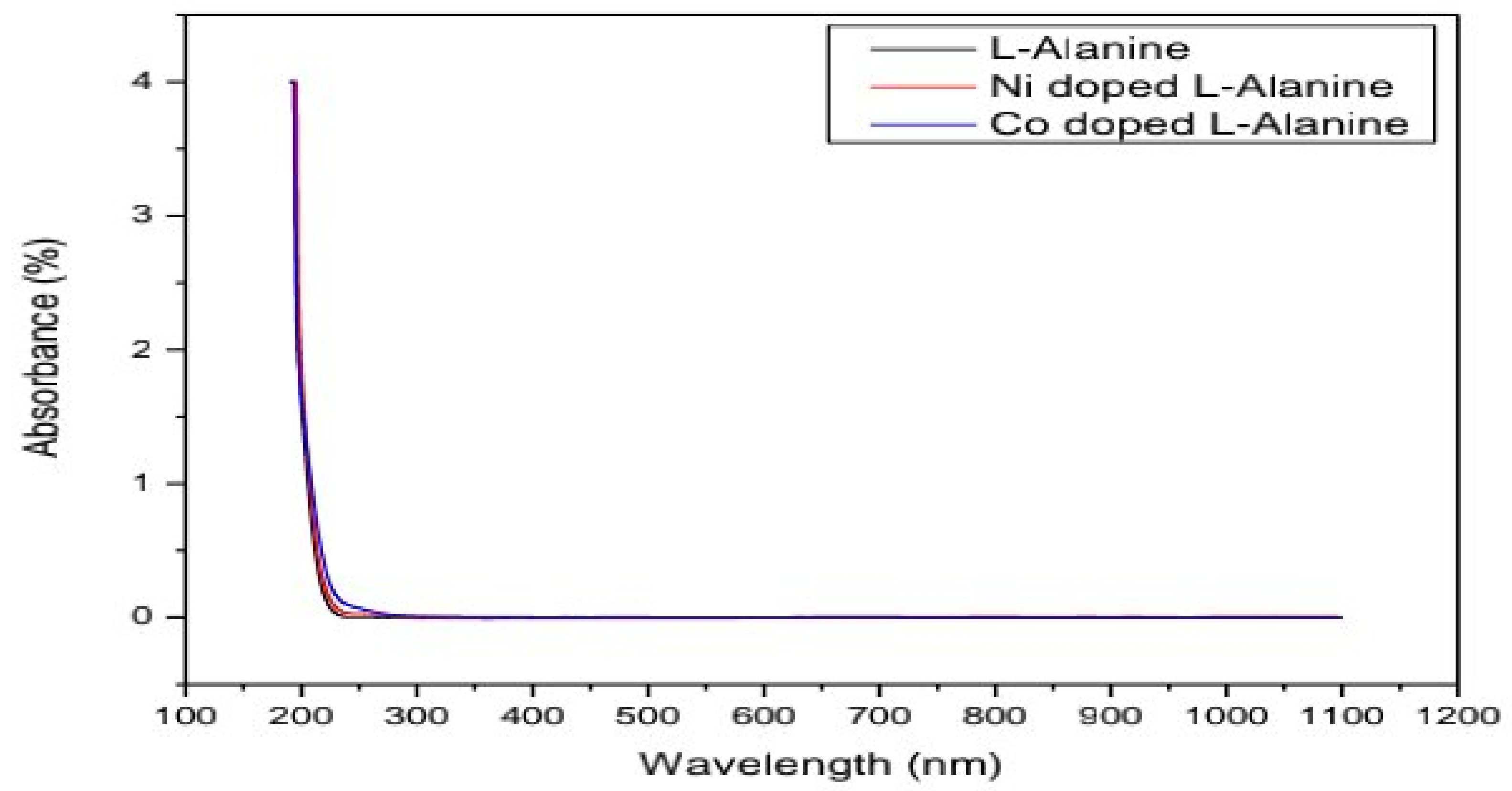

Fig.2. Absorbance spectra.

3.3. Absorption Coefficient (α)

The absorption coefficient determines how far into a material light of a particular wavelength can penetrate before it is absorbed. In a material with a low absorption coefficient, light is only poorly absorbed, and if the material is thin enough, it will appear transparent to that wavelength. Absorption coefficients of the crystals are determined using the following relation.

$$\alpha = \frac{2.303 \times \log \frac{1}{T}}{t}$$

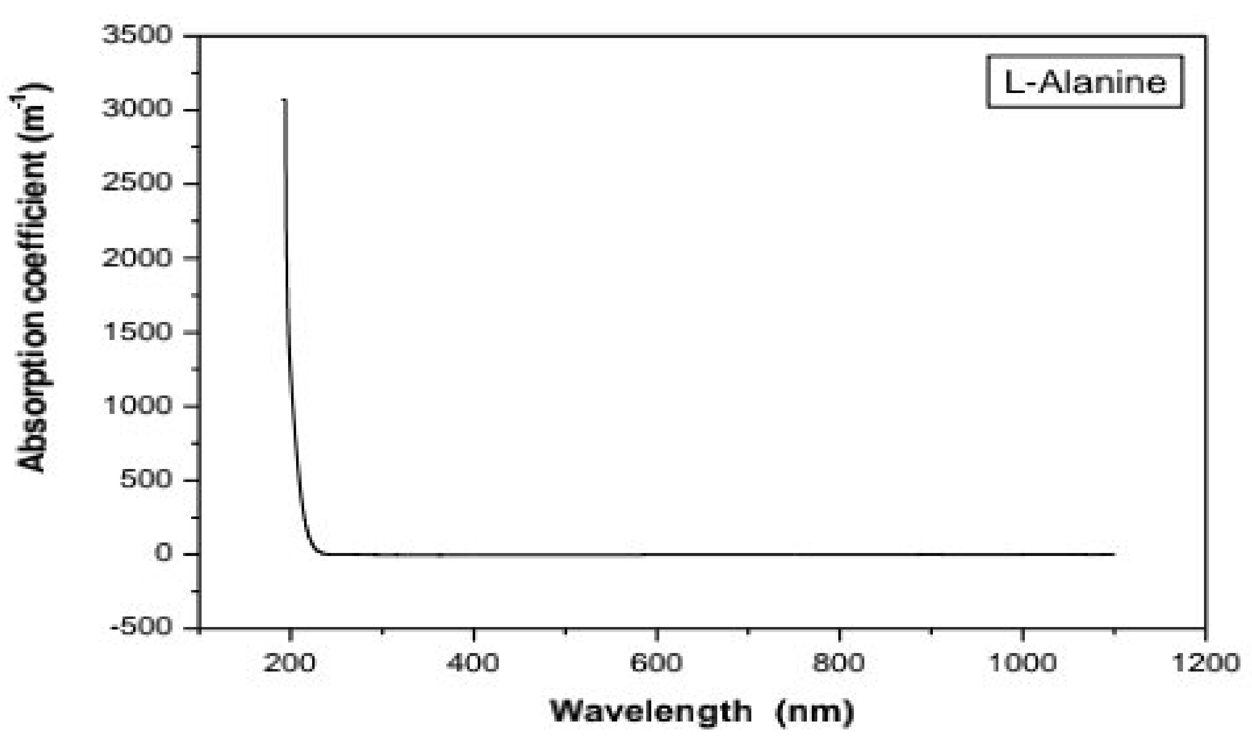

Fig.3. Absorption coefficient of L-Alanine crystal

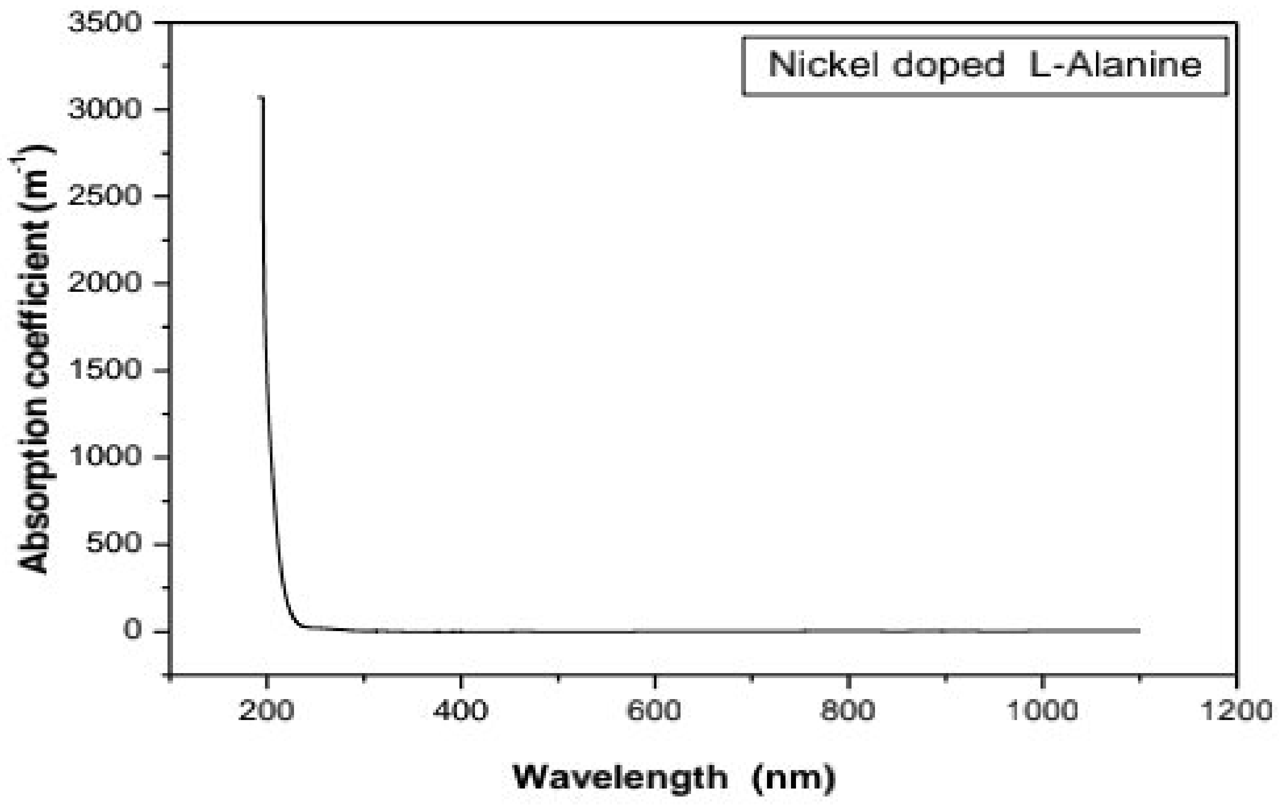

Fig. 4. Absorption coefficient of Nickel doped L-Alanine crystal

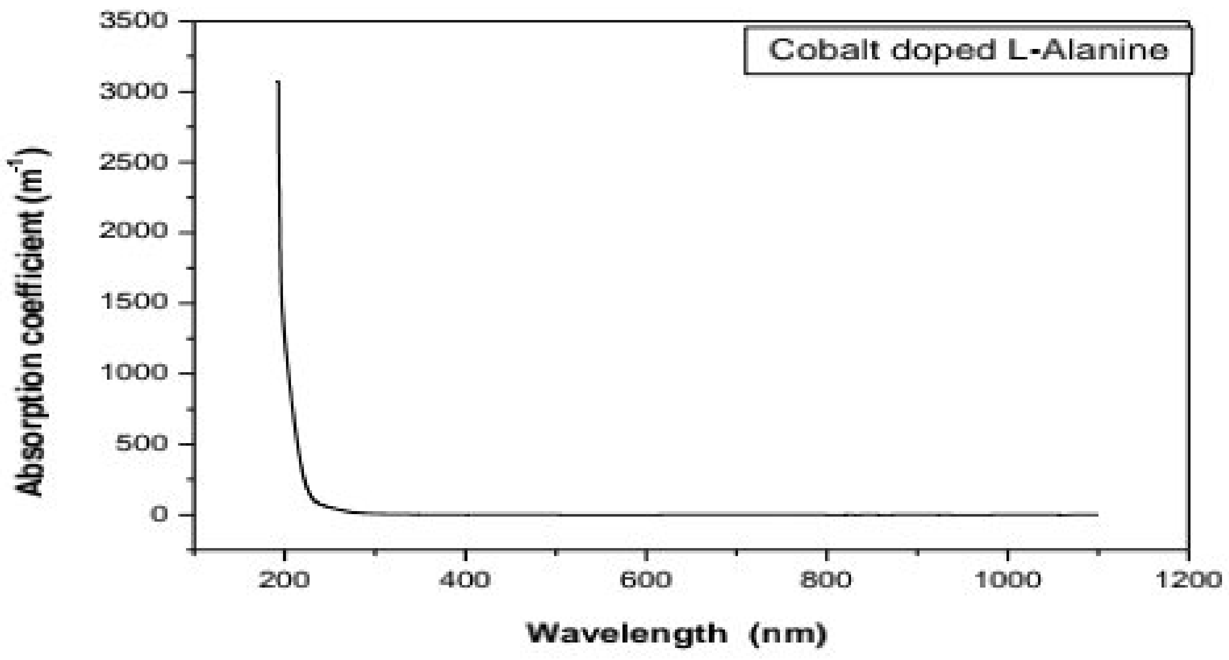

Fig.5. Absorption coefficient of Cobalt doped L-Alanine crystal

The absorption coefficient depends on the material and also on the wavelength of light which is being absorbed. At lower wavelength region (200-300 nm) all the three crystals having higher absorption coefficients, which means crystals readily absorb more photons, which excite electrons into the conduction band. The wavelength above 300 nm the crystal experience low absorption coefficients which means crystal did absorb more photons. Knowing the absorption coefficients of materials aids engineers in determining which material to use in their solar cell designs. For photons which have energy very close to that of the band gap, the absorption is relatively low since only those electrons directly at the valence band edge can interact with the photon to cause absorption. As the photon energy increases larger number of electrons interact with the photon and result in the photon being absorbed.

3.4. Photon Energy

The photon energy or optical band gap is the threshold for photons to be absorbed, while the transport gap is the threshold for creating an electron–hole pair that is not bound together. The optical band gap (Eg) at the wavelength (λ) for the crystal is evaluated using the relation, $Eg = \frac{hc}{\lambda}$

Table 1

Photon energy

Wavelength (nm)	Photon energy (eV)
200	6.21
250	4.968
300	4.14
350	3.548571
400	3.105
450	2.76
500	2.484
550	2.258182
600	2.07
650	1.910769
700	1.774286
750	1.656
800	1.5525
850	1.461176
900	1.38
950	1.307364
1000	1.242
1050	1.182857
1100	1.129091

3.5. Extinction Coefficient

As extinction coefficient (k) is a measure of light lost due to scattering and absorption per unit volume, hence, high values of k in lower wavelength range show that these films are opaque in this range. The extinction coefficient k is related to the absorption coefficient α, by the following formula:

$$k=4\pi / \lambda\alpha$$

where λ is the wavelength. The unit of absorption coefficient is m^{-1}. Fig. 6. shows the Variation of Extinction coefficient and photon energy, a small value of extinction coefficient in the lower energy region reveals that the all the crystal permitting the free passage of electromagnetic radiation, while the high energy region indicates greater degrees of opacity. The coefficient of attenuation depends on the type of material and radiation intensity. A low extinction coefficient is apt for use as an optical material in processing devices.

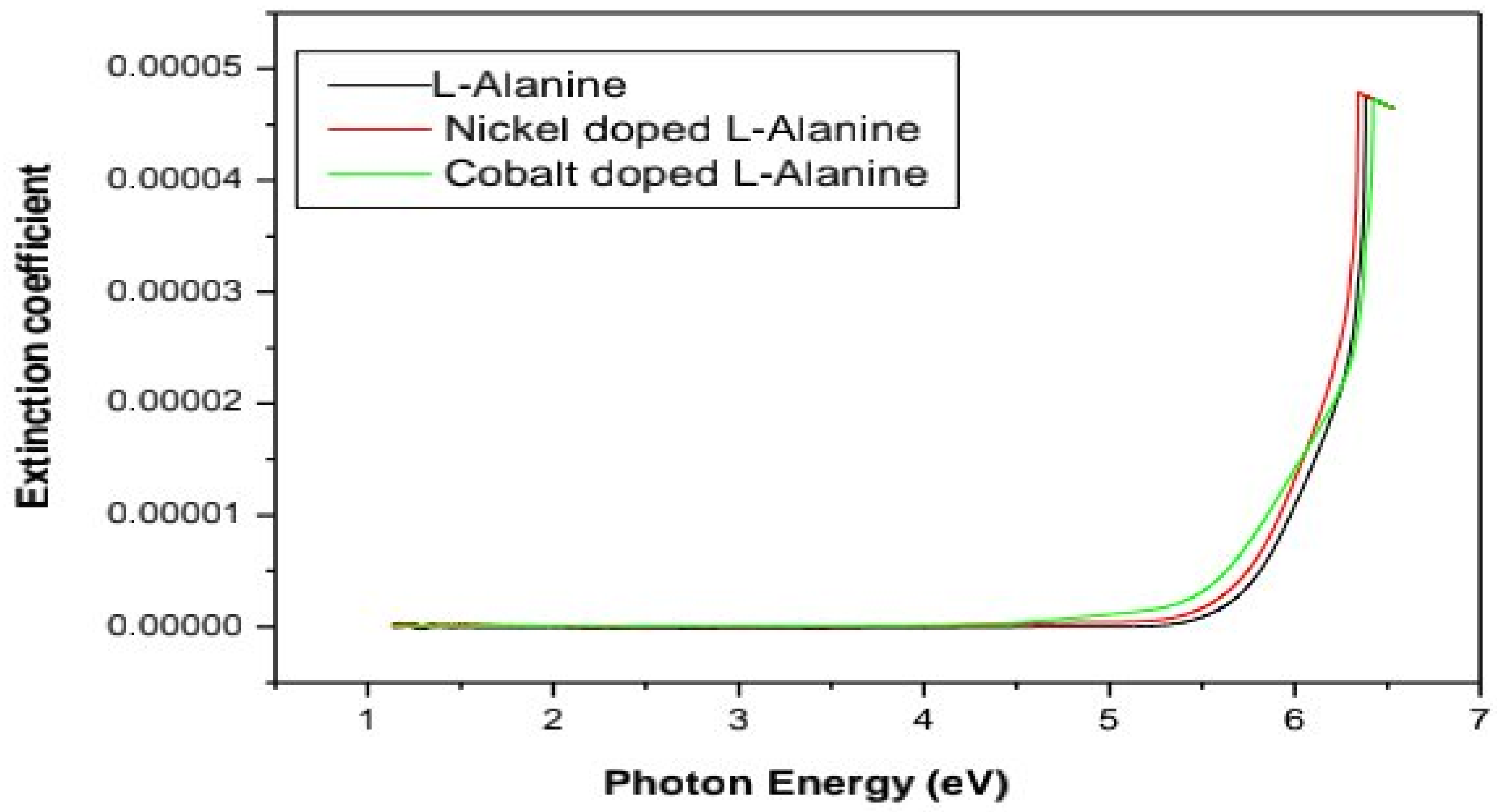

Fig .6. Variation of Extinction coefficient and photon energy

3.6. Reflectance

The reflectance of the surface of a crystal is its effectiveness in reflecting radiant energy. It is the fraction of incident electromagnetic power that is reflected at the boundary. Reflectance is a component of the response of the electronic structure of the material to the electromagnetic field of light, and is in general a function of the frequency, or wavelength, of the light, its polarization, and the angle of incidence. The dependence of reflectance on the wavelength is called a reflectance spectrum or spectral reflectance curve. The reflectance of the crystals are calculated using the following relation,

$$R=\frac{\exp(-\alpha t)+\sqrt{\exp(-\alpha t)T-\exp(-3\alpha t)T+\exp}(-2\alpha t)T^2}{\exp(-\alpha t)+\exp(-2\alpha t)T}$$

From the reflectance spectra it was known that the reflectance value increases due to doping and the maximum value obtained for a nickel doped L-Alanine crystal at higher photon energy.

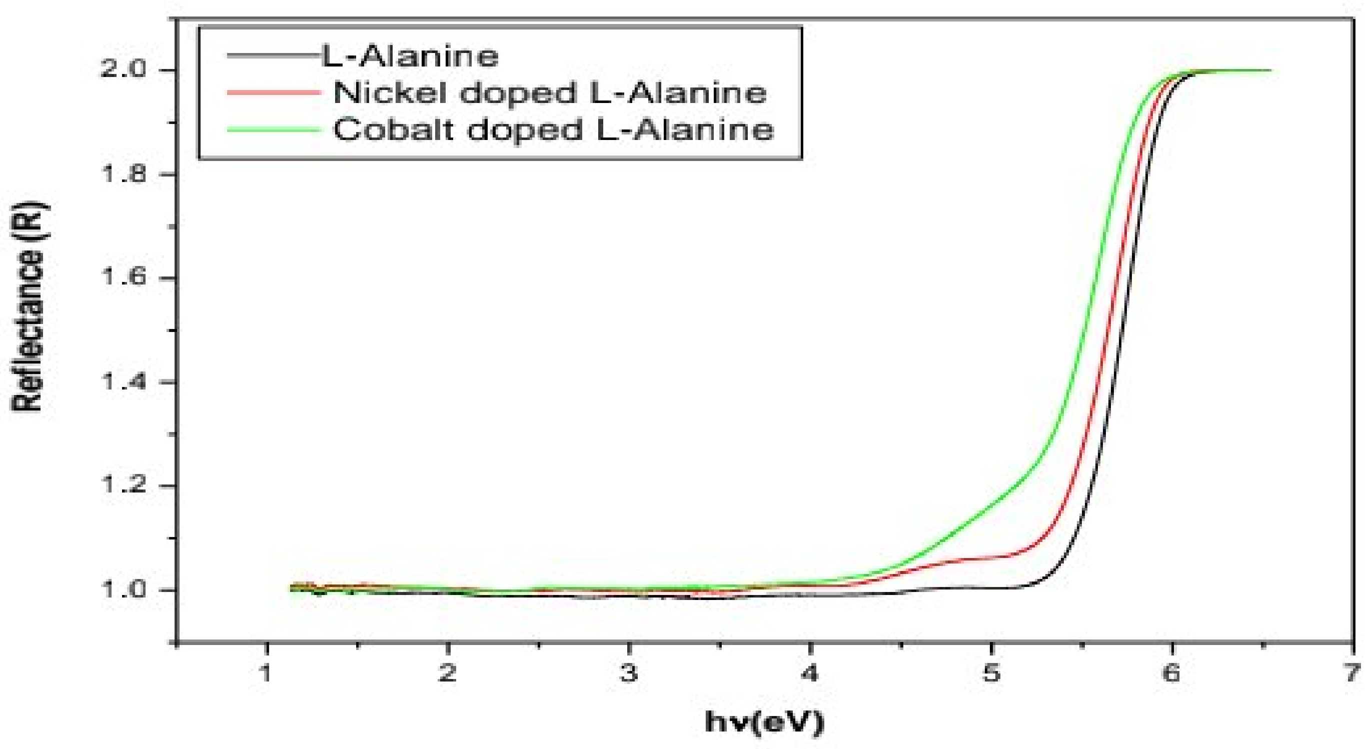

Fig. 7. Reflectance spectrum

3.7. Refractive Index

In optics, the refractive of a material is a dimensionless number that describes how fast light travels through the material. The refractive index determines how much the path of light is bent, or refracted, when entering a material. Light propagation in absorbing materials can be described using a complex-valued refractive index. The imaginary part then handles the attenuation, while the real part accounts for refraction. For most materials the refractive index changes with wavelength by several percent across the visible spectrum. The refractive index can be calculated using the relation

$$n = -\frac{(R+1)+\sqrt{3R^2+10R-3}}{2(R-1)}$$

For smaller photon energy, the refractive index of all the three crystals experience lower value which corresponds to increasing speed of light in the crystal. At higher photon energy, increasing refractive index corresponds to decreasing speed of light in the material. Moreover due to the addition of dopants the refractive index increases.

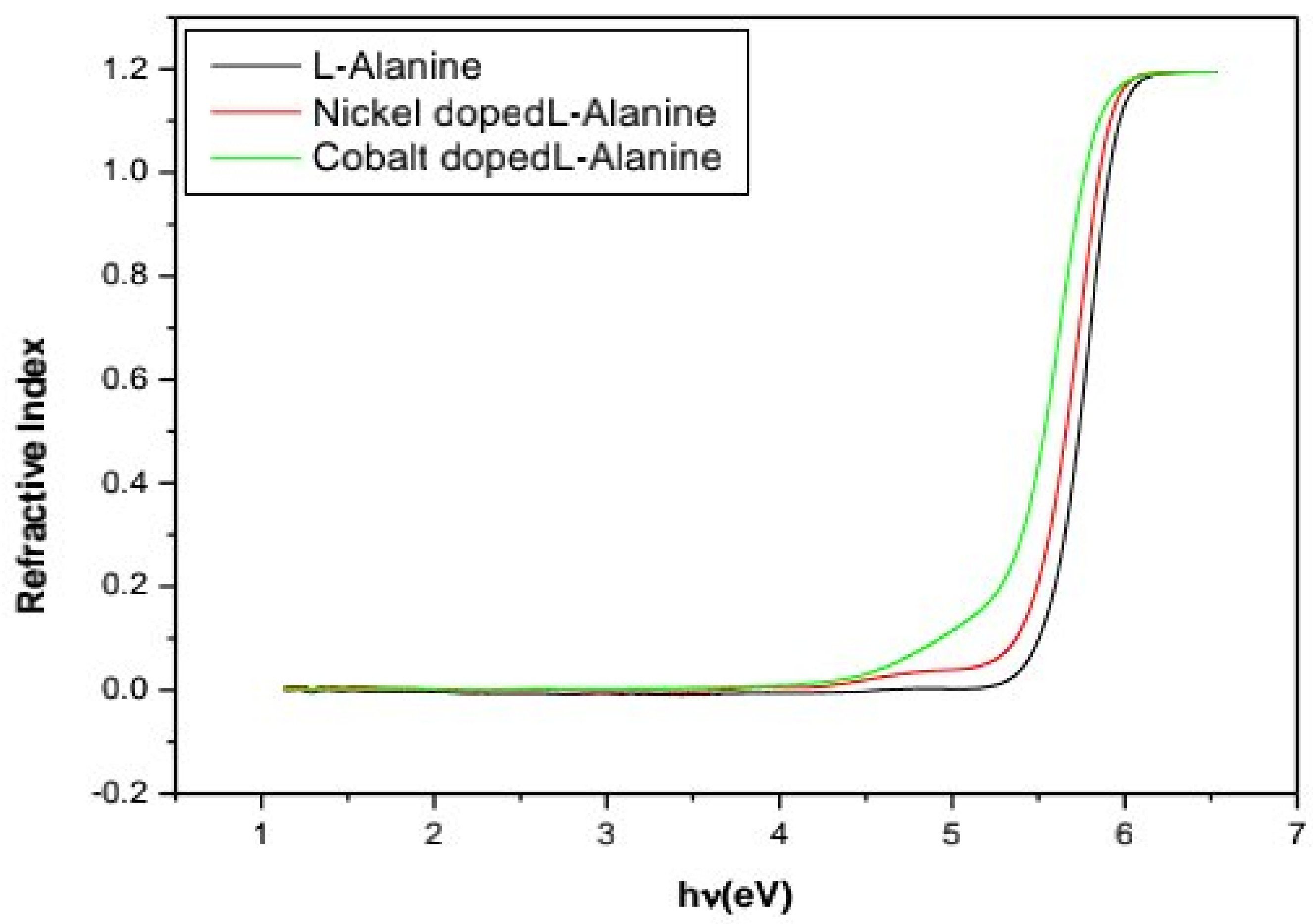

Fig. 8. Refractive index

4. Conclusion

The optical properties of the semi organic crystals are analyzed by calculating the optical parameters of three different crystals namely L-Alanine, cobalt and nickel doped L-Alanine. The transmittance data for all the three crystals were collected and theoretical calculations were performed to determine the optical parameters of the crystals. The optical constants were playing a prominent role it is used for the application of optoelectronics and photonics. The transmittance spectrum confirms that, all the three crystals are highly transparent in nature. Due to doping with cobalt and nickel the transmittance percentage decreases and the lower cut-off wavelength shifted towards higher wavelength. The absorption coefficient depends on the material and also on the wavelength of light. At lower wavelength region (200-300 nm) all the three crystals having higher absorption coefficients. The wavelength above 300 nm the crystal experience low absorption coefficients. The reflectance value increases due to doping and the maximum value obtained for a nickel doped L-Alanine crystal. Refractive index plays an important role in crystal optics, the refractive index of all the three crystals experience lower value near lower photon energy region and higher photon energy increasing refractive index. Moreover due to the addition of dopants the refractive index increases. Thus due to doping the optical properties enhances which is highly recommended for optical device fabrications.

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