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Growth, Structural and Optical properties of organometallic nickel doped L-Alanine crystal

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ABSTRACT

The single crystal of nickel doped L-Alanine, an organometallic optical material is grown by slow evaporation technique. The structural parameters are identified by X-ray diffraction analysis. The crystalline nature was studied using the powder X-ray technique. To fetch the knowledge about the lattice parameters and crystallographic axis, single crystal diffraction studies was carried out. UV-Vis measurements were carried out to find the optical properties such as absorption, transmittance, reflectance, extinction coefficient and refractive index. Using the Tauc plot the energy gap of the organometallic compound was estimated. The structural and optical property confirm that the material is suitable for optical device fabrications.

Keywords: *L-Alanine, organometallic, energy gap.*

1. Introduction

Nowadays an extensive research investigation has been carried out on organometallic and coordination materials because they share both the properties of organic and inorganic materials. In the case of organometallic complex materials the optical and structural properties are mainly dominated due to the presence of organic ligands [1]. Among the VII B transition metals, the compound nickel has high transparency in the UV region. Therefore nickel compounds are used as a coatings, batteries, kitchen wares, mobile phones, power generation, ornaments etc. Nickel with electronic configuration [Ar] $3d^9 4s^1$ having more strength, greater toughness act as a better corrosion resistance material for electronic and magnetic materials. Alanine is α-amino acid which contains amine, carboxyl and methyl group exist in a zwitterionic form [2]. 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 [3-7]. In this paper, we have reported the growth, structural and optical properties of a nickel doped L-Alanine single crystals.

2. Experimental Procedures

Slow evaporation is a simple technique used to grow single crystals at ambient temperature and pressure. Deionised water was chosen as a solvent because the precursor materials are readily soluble in water. The selected precursor materials are L-Alanine and nickel chloride. The solution was prepared by dissolving 1:0.1 molar ratio of L-Alanine and nickel chloride. The L-Alanine nickel chloride was formed according to the following reaction.

$$C_3H_7No_2 + NiCl_2 \rightarrow C_3H_7No_2NiCl_2$$

Then the solution heated at 45^0 C using a temperature controlled stirrer to get the homogenized mixture. Afterwards the solution is filtered and then allowed for slow evaporation.

Nucleation occurs after 9 days and good quality crystals of 1.5×0.8×0.2cm size are harvested after 30 days.

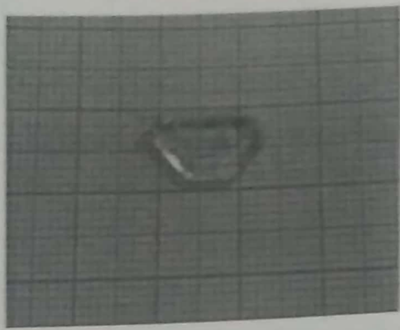

Figure: 1. Nickel chloride doped L-Alanine crystal

3. Result and Discussion

The grown organometallic crystals were characterized by powder X-ray diffraction technique to confirms the crystalline nature, Single crystal X-ray diffraction studies was carried out to identify the crystal structure and lattice parameters. The optical properties are determined using UV-Vis spectroscopy.

3.1. X-Ray Powder Diffraction Analysis

The structural characterization of nickel doped L-Alanine is carried out by powder X-ray diffraction method. Powder XRD patterns of the grown crystals were recorded using an X-ray diffractometer PAN Analytical XPERT-PRO. The intensity of the diffracted beam against 2θ is recorded in the range 10-80^0 with Cuk$_\alpha$ radiation (λ=1.54056Å). Using the observed Bragg angle and d spacing all the reflections of the powder XRD pattern for nickel doped L-Alanine has been indexed using the "INDEXING" software packages. The indexed X-ray powder diffraction pattern of the grown crystal is show in figure 2. The sharp peaks confirm the crystalline nature and purity of the crystal.

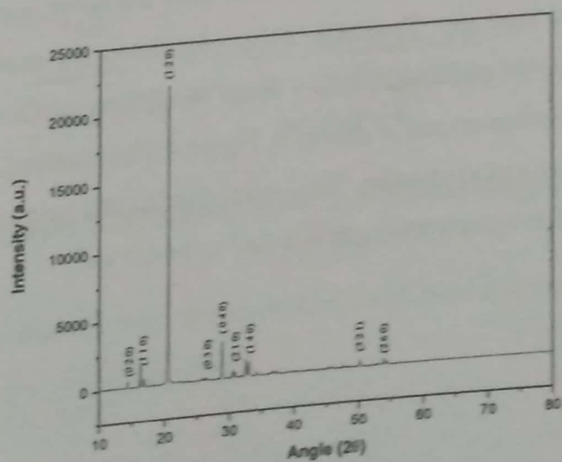

Figure:2. XRD pattern of nickel chloride doped L-Alanine

3.2. Single Crystal X-Ray Diffraction

Single crystal X-ray diffraction analysis of nickel doped L-Alanine crystal was carried outer using Bruker Kappa Apex II diffractometer. From the data, it was known that the crystal belongs to orthorhombic system with a=6.132Å, b=12.265 Å, c=0.478 Å, crystallographic axes $\alpha = \beta = \gamma = 90^0$ and space group $P2_12_12_1$.

3.3. UV-Vis Analysis

To study the optical properties of the grown crystals, UV-Visible spectrum of nickel doped L-Alanine crystal of 3 mm thickness was recorded by using UV/Vis/NIR spectrophotometer in the wavelength range of 200 - 900 nm. A graph of transmittance versus wavelength is shown in figure 3.

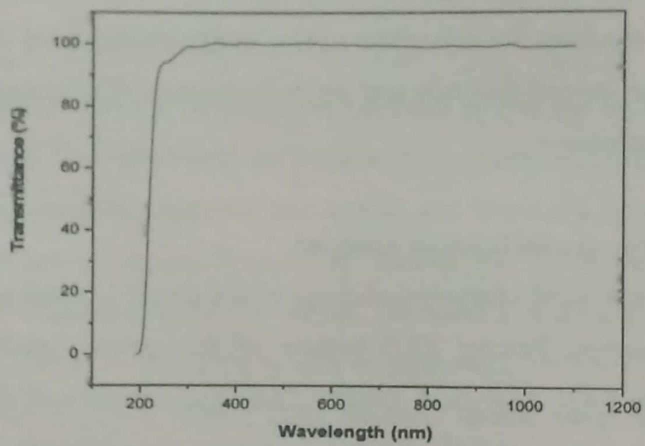

Figure: 3. Transmittance spectrum of nickel doped L-Alanine crystal

It was observed that the crystal has good transmittance and lower cut off wavelength is found to be 300 nm and its transparent power is 98%. The good transparency and lower cut off wavelength asserts the fact that the crystal can be used for lasser applications. A tauc plot is used to determine the optical band gap. Typically, a tauc plot shows the quantity energy on the abscissa and the quantity $(\alpha h\gamma)^2$ on the ordinate, where α is the absorption coefficient of the material. A tauc plot of nickel doped L-Alanine crystal is shown in Figure 4.The resultant plot has a distinct linear regime which denotes the onset of absorption. Thus extrapolating this linear region to the abscissa yields the energy of material. The optical band gap is found to be 6.3 eV.

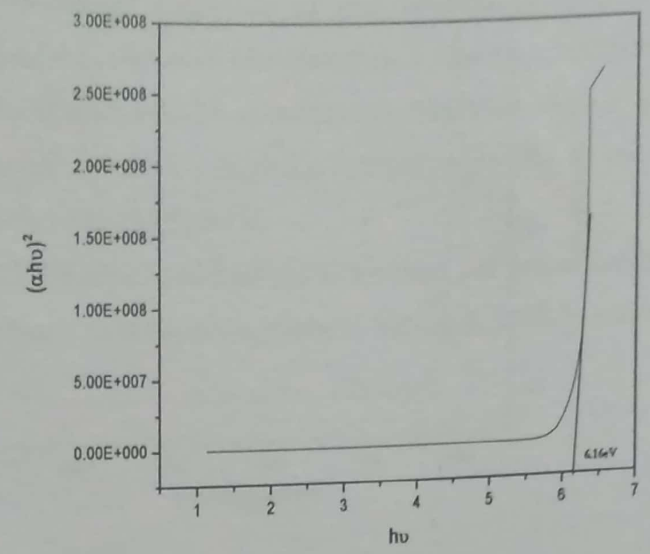

Figure: 4. Tauc plot

The optical properties of the crystals are governed by the interaction between the crystal and the electric and magnetic fields of the electromagnetic waves. Extinction coefficient is the fraction of light lost during scattering and absorption per unit distance in a participating medium. The variation of extinction coefficient and wavelength is shown in Figure 5. The extinction coefficient (K) can be obtained from the relation, $K=\frac{\lambda\alpha}{4\pi}$

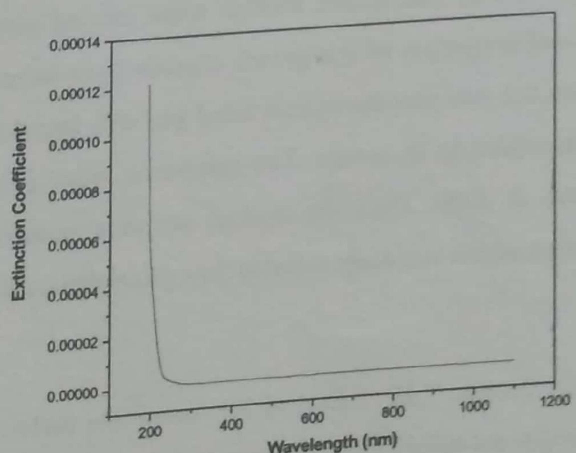

Figure.5. Extinction coefficient Vs wavelength

The reflectance is obtained from the absorption coefficient and is calculated by the equation

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

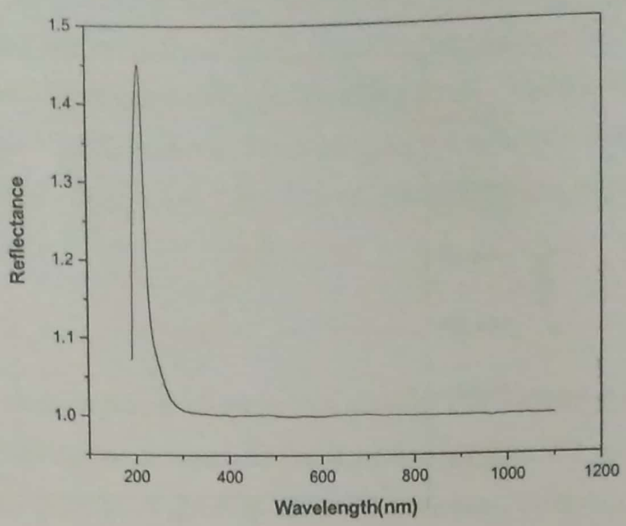

Figure: 6. Reflectance Vs wavelength

The refractive index is evaluated from reflectance using the given equation,

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

The value of the refractive index (n) is found to be 2.09 at 300nm.

4. Conclusion

An organometallic optical crystal, nickel doped L-Alanine was successfully grown by slow evaporation method. X-Ray diffraction studies were carried out and the lattice parameters are evaluated. The optical properties of the grown crystals have been analyzed from UV-Vis spectral measurements. From the tauc plot the optical band gap was found to be 6.3 eV which confirms that the crystal is semiconducting in nature. The refractive index (n) calculated at the lower cut off wavelength 300 nm is 2.09. Thus the optical property confirms that the crystal belongs to semiconducting nature which is mainly suitable for optical device fabrications.

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