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Optical and Mechanical Studies of γ-glycine Single Crystal in the Presence of Potassium Chloride

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Abstract

Single crystals of γ-glycine have been grown by slow evaporation method. The powder X-ray diffraction analysis determine the characteristic peak of γ-glycine and lattice parameters. Optical absorption spectrum reveals that the grown crystal has good optical transparency in the entire visible region with an energy band gap of 5.2 eV and lower cut off wavelength lies at 230 nm. The mechanical properties of the grown crystal was subjected to Vickers hardness test to find out the Brittleness index (B_i), Fracture toughness (K_c), Elastic stiffness constant (C_{11}).

Key words: γ-glycine, Optical properties, Mechanical properties

1. INDRODUCTION

Great efforts have been made to the research and design of highly efficient non-linear optical (NLO) materials due to widespread applications such as high speed information processing, optical communication and optical data storage [1]. Organic nonlinear optical materials formed from aminoacids have potential applications in second harmonic generation, optical storage, optical communication, optical modulators, optical switches etc [2]. Organic materials of glycine, a well-known amino acid, crystallizes in three different polymorphs: α, β and γ. While α and β forms crystallize in centrosymmetric space group and the γ-glycine crystallizes in non-centrosymmetric space group P32 making it a potential candidate for non-linear optical applications especially for effective optical second harmonic generation [3]. The growth of γ-glycine single crystal in the presence of potassium chloride was reported [4, 5]. But there is no investigation about the optical and mechanical properties. Hence the current communication deals with the single crystals of γ-glycine in the presence of potassium chloride and it has been grown by slow evaporation method. The grown crystal of γ-glycine were characterized by Optical and Mechanical properties.

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2. EXPERIMENTAL

The equimolar ratio of glycine and potassium chloride was dissolved in double distilled water. After the clear solution was filtered and the solution was poured in petri dish and kept in free atmosphere condition. The photograph of the harvested colorless γ-glycine crystal as shown in Figure.1.

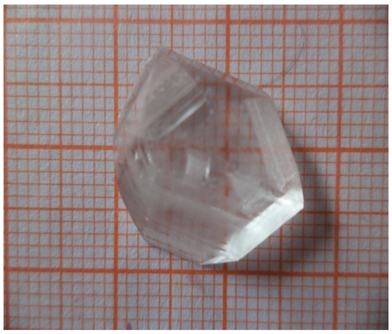

Fig.1: As grown crystal of γ-glycine

3. RESULTS AND DISCUSSION

3.1 Powder X-Ray Diffraction Analysis

The indexed powder X-ray diffraction pattern of the grown crystal as shown in Figure.2. The lattice parameters were calculated and the values are a = b = 7.02 Å, c = 5.50 Å and V = 235 A[3]. The determined values are in good agreement with the reported data available in JCPDS card No. 006 0230.

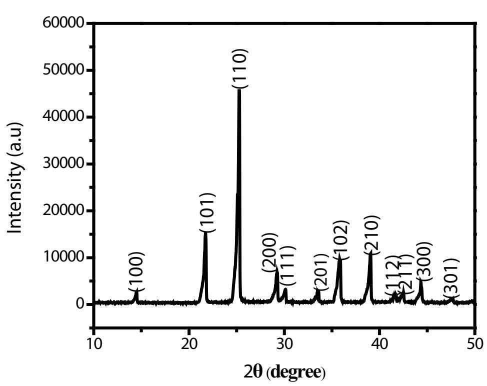

Fig.2: Powder XRD pattern of γ-glycine

3.2 Optical Properties

UV-visible-NIR spectral studies give information about the structure of the molecule and the absorption of UV and visible light involves the promotion of electrons from the ground state to higher energy state [6]. From the absorption spectrum it is observed that the lower cut off wavelength is 230 nm (Figure.3). The absence of absorption in the region between 241 nm to 800 nm is advantageous as it is the key requirement for materials having NLO properties and the SHG efficiency of the grown crystal is higher than that of KDP [5]. The E_g value could be estimated from the plot photon energy (eV) versus $(\alpha h\nu)^2$ (Figure.4) and energy band gap (E_g) value was obtained from the interception of the linear portion of the curve with X-axis. The direct band gap values around to be 5.2 eV. The energy band gap (E_g) has been evaluated from the absorption spectra and the optical absorption coefficient (α) [7]

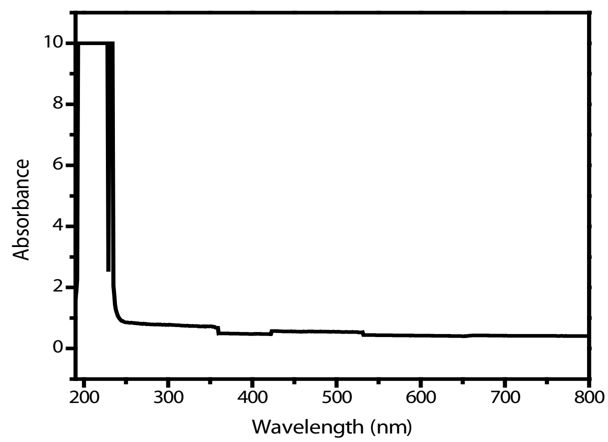

Fig.3: Absorption Spectrum of γ-glycine

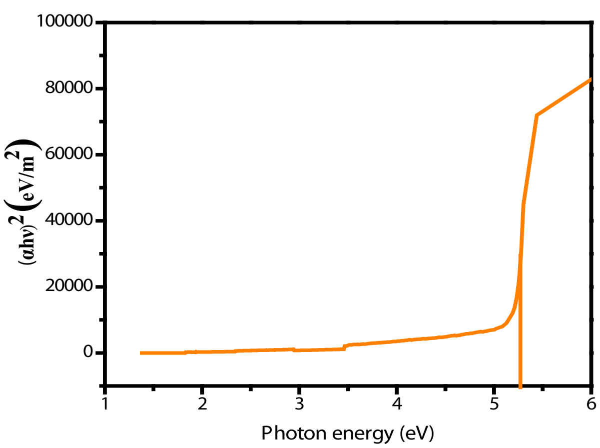

Fig.4 Tauc's plot for γ-glycine

3.3 Mechanical Properties

Mechanical property of the samples was studied by measuring microhardness number with various loads from 10, 25, 50 and 100 g. The hardness of a material is a measure of its resistance to plastic deformation. The hardness value increases with increasing load is normally termed as reversed indentation size effect (RISE). The plot of P versus H_v as shown in Figure.5.

The work hardening coefficient (n) is measure the strength of the materials. According to Onitsch and Hanneman, n should lie between below 1.6 for hard materials and above 1.6 for soft materials. For the normal ISE behavior, the exponent $n < 2$. When $n > 2$, there is reverse ISE behavior [8]. The value of n is found to be plot of log p versus log d (Figure.6) from the slope of the graph value of 5.1 because γ-glycine crystals which belongs to soft materials.Hence the title crystal exhibits reverse ISE behavior. The Meyer's law, gives an expression regarding load and size of indentation [9].

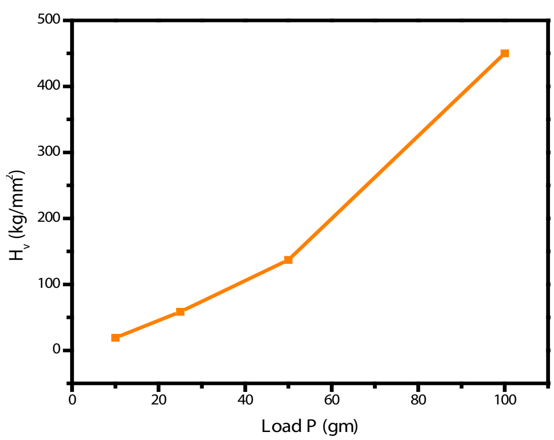

Fig. 5 : Plot of P versus H_v

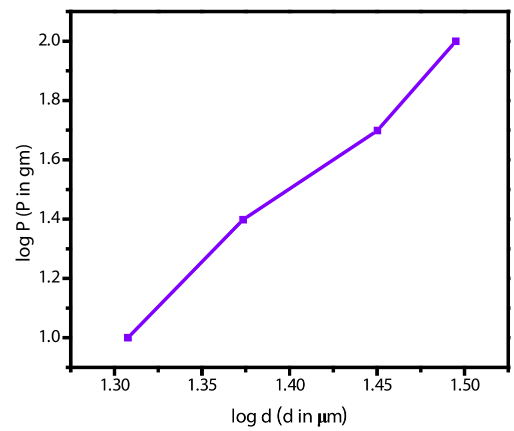

Fig.6 : Plot of log d versus log p

Using Meyer's relation, the material constant k_1 is computed as 2.332 kg/mm from the Figure.7. The elastic stiffness constant (C_{11}) was calculated for various loads by using Wooster's relation and the values are tabulated (Table.1). It gives an idea about the bond strength and it is clear from the result that the bond strength increases with increase in load.

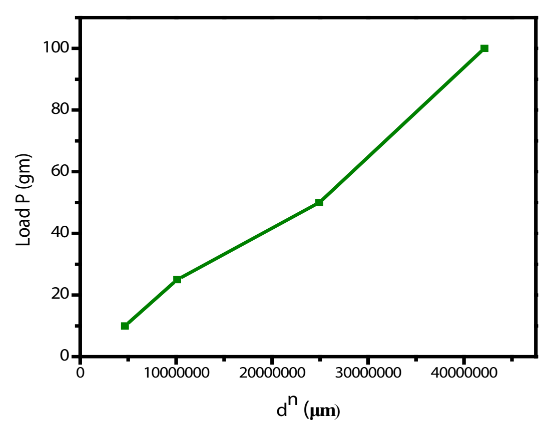

Fig.7 : To determine material constant

The fracture mechanics in the field of mechanics concerned with the study of the propagation of cracks in materials. The crack was measured from the center of indentation mark up the tip of crack in μm. The resistance to fracture indicates the toughness of a material and the fracture toughness K_c [10].

Brittleness is an important property that affects the mechanical behavior of a material and gives an idea about the fracture induced in a material without any appreciable deformation [11].

The elastic stiffness constant is calculated using Wooster's empirical formula [12]. Which gives an idea about the tightness of bonding between the neighboring atoms. The calculated values of Fracture mechanics (K_c), Brittleness index (B_i) and Elastic Stiffness Constant (C_{11}) are given in Table 1.

Table -1: Mechanical related constant for γ-glycine

Load (g)	$C_{11}X10^{14}$ (Pa)	c/a	Nature of crack	Fracture mechanics ($MNm^{-3/2}$)	Brittleness index ($m^{-1/2}$)
10	2.4208	-	-	-	-
25	7.0738	-	-	-	-
50	12.8146	-	-	-	-
100	30.0588	2.1	Palmqvist	4.9842	38.0666

3.4 SHG Confirmation

The second harmonic generation efficiency of the powdered sample was analyzed by Q-switched Nd:YAG laser wavelength of 1064nm and green light was emitted. The SHG efficiency of γ-glycine crystal is higher than that of KDP (The SHG efficiency of KDP is12.9 and that of γ-glycine is 13.08).

4. CONCLUSIONS

Optical transparent of γ-glycine single crystals were grown by slow evaporation method. The lattice parameters were calculated by powder X-ray diffraction analysis, they agree well with reported values. The optical absorption spectrum shows that the lower cut off wavelength 230 nm and energy band gap value was found to be 5.2 eV. The mechanical properties were carried out to understand the hardness parameters such as Work hardening coefficient, Fracture mechanics, Brittleness index and Elastic stiffness constant were calculated. Second harmonic generation (SHG) test were analyzed.

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