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Dielectric and Hardness Studies of L-Alanine Doped Cadmium Chlorides Crystals

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Abstract**:** Single crystals of L-alanine doped cadmium chloride (LACC), is an organometallic nonlinear optical material, have been grown by the slow evaporation technique. The grown crystals were subjected to various characterization techniques. In this work, give the information about Electrical and Mechanical properties of L-alanine doped Cadmium Chloride crystal. The mechanical properties of the crystals show that this material belongs to the category of hard materials. Second harmonic generation was confirmed by the Kurtz and Perry powder technique. Electrical parameters, such as dielectric constant, dielectric loss, AC conductivity and their corresponding activation energies have been studied. The low dielectric constant and dielectric loss suggest that this material is a good candidate for micro-electronic applications.

Keywords: *XRD; SHG; Dielectric; Microhardness*

I. INTRODUCTION

In the past decade, the crystals of the amino acids and their complexes have been subjected to many investigations by several researchers and a series of amino acids such as glycine, L-arginine, L-histidine, L-threonine etc.[1,2] L-alanine is one of the simplest amino acid often used as a model for the investigation of various types of intermolecular and intra molecular interactions, which are expected to be present in relatively complex and biologically relevant molecules.

L-alanine crystal is a nonlinear optical material which has second harmonic efficiency of 0.3 times that of KDP. In this work, L-alanine crystals are doped with cadmium chloride to improve the various properties of the host crystals. The crystals were grown by slow evaporation method and the harvested crystals were characterized by different studies.

II. SYNTHESIS

Commercially purchased L-alanine and cadmium chloride (Merck India) were used to prepare the cadmium chloride doped L-alanine salts. 1 mole%, 2 mole% and 3 mole% of cadmium chloride salts were added into L-alanine salts separately to get the doped L-alanine salts. Let the samples be abbreviated as LACC1, LACC2 and LACC3 respectively for 1 mole%, 2 mole% and 3 mole% doped L-alanine. Solution method with slow evaporation technique was adopted to grow the single crystals of the synthesized salts of L-alanine added with cadmium chloride. In accordance with the solubility data, the saturated solutions were prepared separately and the solutions were constantly stirred for about 2 hours using a magnetic stirrer. Then the solutions were filtered using the 4 micro Whatmann filter papers and the filtered solutions were kept in borosil beakers covered with porous papers. The grown crystals were harvested after a period of 35 days and they are displayed in the photograph.

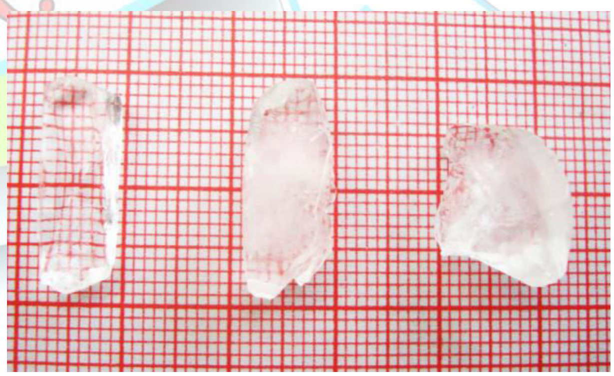

Fig 1: Fabricated Crystal

It is observed from the grown crystals that the transparency is getting decreased when the concentration of cadmium chloride in the L-alanine crystals is more.

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III. Dielectric and Hardness study of Cadmium Chloride Doped L-alanine crystal

A. Dielectric studies:

The dielectric properties like dielectric constant and loss factor of crystalline materials were measured using an LCR meter. The values of dielectric constant and the dielectric loss factor (tan δ) were obtained for various temperatures and frequencies. The frequency dependence of the dielectric constant for LACC1, LACC2 and LACC3 samples at different temperatures are shown in figures. 2-4. It is observed that the dielectric constant has higher values at lower frequencies and further it decreases with increase in frequency and become independent at higher frequencies. The dielectric constant of the materials is due to the contribution of electronic, ionic, dipolar or orientation and a space charge polarization which is high relay upon on the frequencies. The space charge polarization is generally active at lower frequencies and high temperatures [3-5].

The variations of dielectric loss with the frequency at different temperatures are presented in the figures 5-7. It is observed that the dielectric loss decreases with the increasing frequency.

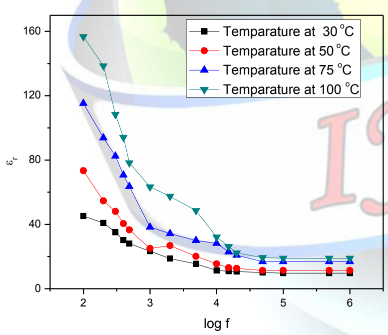

Fig 2: Frequency dependence of dielectric constant (εr) at different temperatures for LACC 1 crystal

The conductivity in a solid is due to the mobility of electrons or ions and imperfections which are charged. Although ionic solids are insulators, yet they conduct electricity to a very small extent. This arises due to the migration of ions, under an electric field to the vacancies or interstices in the ionic solids. Dielectrics actually exhibit a combined conduction, especially ionic and electronic conduction. As the temperature rises, more and more defects are produced which, in turn increases the conductivity.

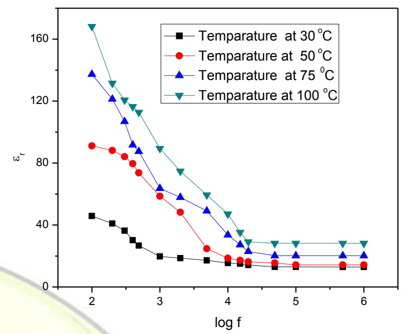

Fig 3: Frequency dependence of dielectric constant (εr) at different temperatures for LACC2 crystal

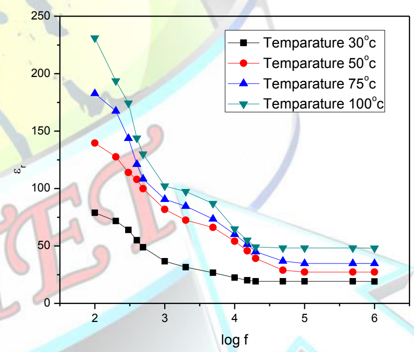

Fig 4: Frequency dependence of dielectric constant (εr) at different temperatures for LACC3 crystal

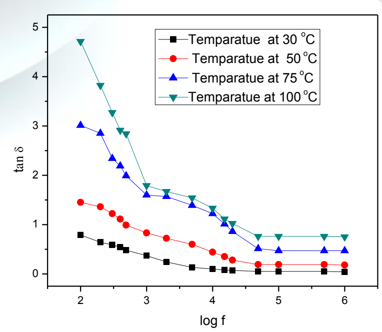

Fig 5: Frequency dependence of dielectric loss factor (tan δ) at different temperatures for LACC1 crystal

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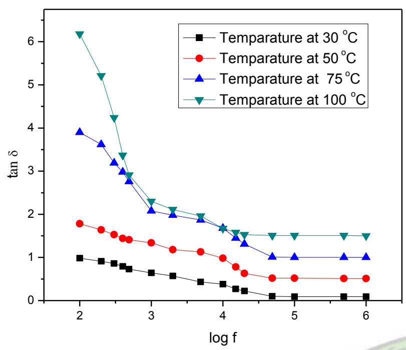

Fig 6: Frequency dependence of dielectric loss factor (tan δ) at different temperatures for LACC2 crystal

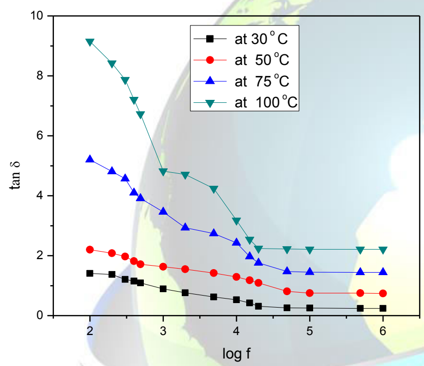

Fig 7: Frequency dependence of dielectric loss factor (tan δ) at different temperatures for LACC3 crystal

Using the data of dielectric constant and dielectric loss, AC electrical conductivity of a crystal was calculated using the formula σac = 2π f ε0εr tan δ where ε0 is the permittivity of free space, εr is the dielectric constant of the sample, tan δ is the dielectric loss of the sample and f is the frequency of AC signal. The variations of AC conductivity with frequency at different temperatures are shown in the figures 8- 10.

The results show that the conductivity of cadmium chloride doped L-alanine samples increases with increase in frequency and temperature and also it increases when L-alanine crystals are doped with cadmium chloride. For dielectrics, the dependence of AC conductivity on temperature usually obeys the well-known relation σac = σ exp (-Eac/kT) where k is the Boltzmann's constant, T is the absolute temperature, σ is the constant depending on the material and Eac is the AC activation energy and the equation can be written as ln σac = ln σ - Eac/kT .

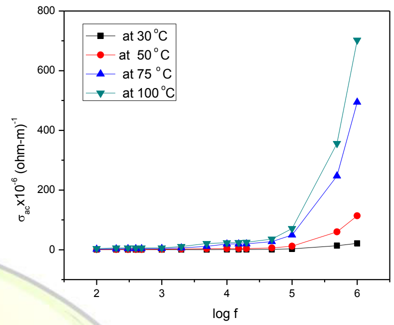

Fig 8: Frequency dependence of AC conductivity at different temperatures for LACC1 crystal

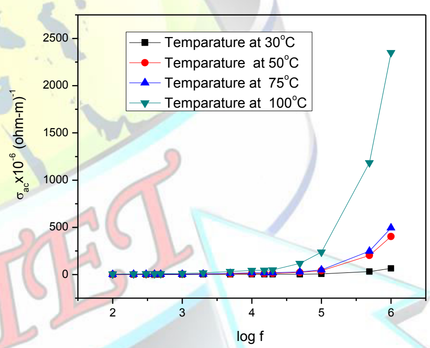

Fig 9: Frequency dependence of AC conductivity at different temperatures for LACC2 crystal

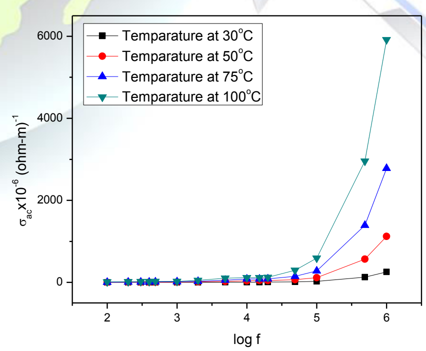

Fig 10: Frequency dependence of AC conductivity at different temperatures for LACC3 crystal

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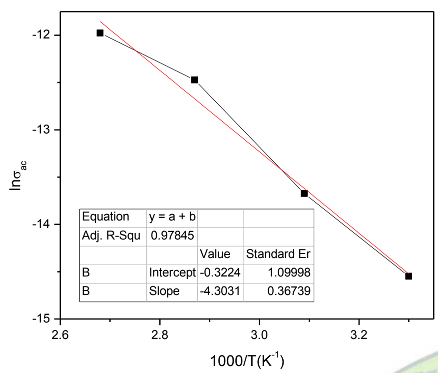

Figure 11: Plot of ln σ ac versus 1/T for LACC1 crystal at 1000 Hz

A plot of ln σac versus (1/T) gives Eac/kT as the slope and ln σ as the Y-intercept. The plots ln σac versus (1000/T) for LACC1, LACC2 and LACC3 crystals at the frequency of 103Hz are shown in the figures 10-12 and from the slope values, the values of the activation energy (Eac) were calculated. The obtained values of activation energy for LACC1, LACC2 and LACC3 samples are 1.02 eV, 1.08 eV and 1.14 eV respectively.

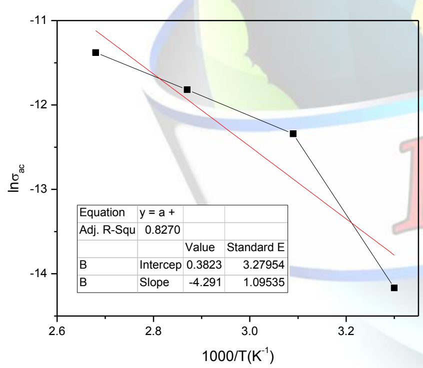

Figure 12: Plot of ln σ ac versus 1/T for LACC2 crystal at 1000 Hz

B. Microhardness Studies:

Hardness is an important solid-state property and plays a vital role in device fabrication. The hardness studies were carried out for cadmium chloride doped L-alanine crystal by applying loads ranging from 25 to 100 g. The microhardness number (Hv) was calculated for the samples as given the procedure in the previous chapters. Figure 13 shows the variation of microhardness number with the loads. It is observed that the hardness increases with increase of load. The increase in hardness with the load can be considered due to reverse indentation size effect which involves a release of the indentation stress along away from the indentation site because of crack formation, dislocation activity or elastic deformation of tip of the indenter [6, 7]. The hardness is found to be greater for cadmium chloride doped L-alanine single crystals. The work hardening coefficient (n) of the crystals is determined by plotting the graphs between log P and log d. Here P is the applied load in kg, d is the mean diagonal length of the indentation in mm.

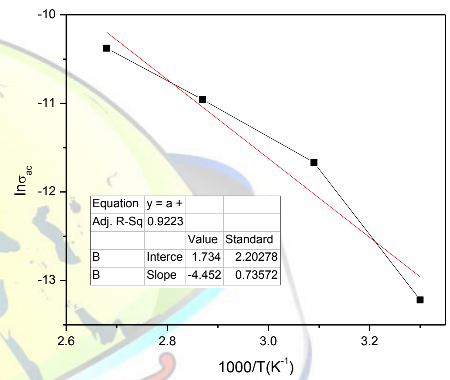

Figure 13: Plot of ln σ ac versus 1/T for LACC3 crystal at 1000 Hz

The increase in hardness with the load can be considered due to reverse indentation size effect which involves a release of the indentation stress along away from the indentation site because of crack formation, dislocation activity or elastic deformation of tip of the indenter [6, 7]. The hardness is found to be greater for cadmium chloride doped L-alanine single crystals. The work hardening coefficient (n) of the crystals is determined by plotting the graphs between log P and log d. Here P is the applied load in kg, d is the mean diagonal length of the indentation in mm. The plots of log P versus log d are given in the figures 14-16. The work hardening coefficient values are found to be 3.433, 3.278 and 3.227 respectively for LACC1, LACC2 and LACC3 samples respectively. As given in the chapter-4, the yield strength of the material and stiffness constant has been determined. A graph is drawn between yield strength and load as shown in the figure 18. It is observed that yield strength increases with increase of load and increase of dopant concentration. The plots of stiffness constant with the load are given in figure 19.

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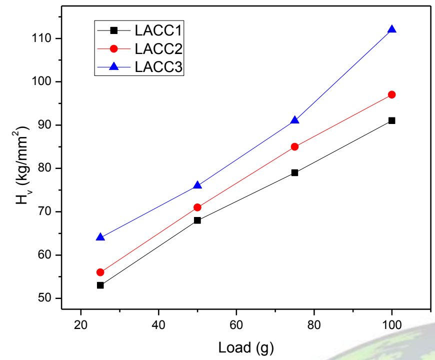

Fig 14: Variation of Vickers microhardness number (Hv) with the applied load for cadmium chloride doped L-alanine crystals

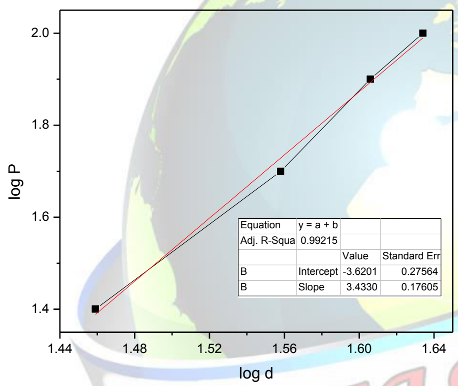

Fig 15: Graph of ln P versus ln d for LACC1 crystal

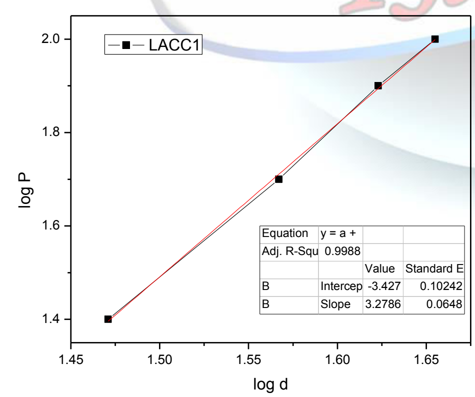

Fig 16: Graph of ln P versus ln d for LACC2 crystal

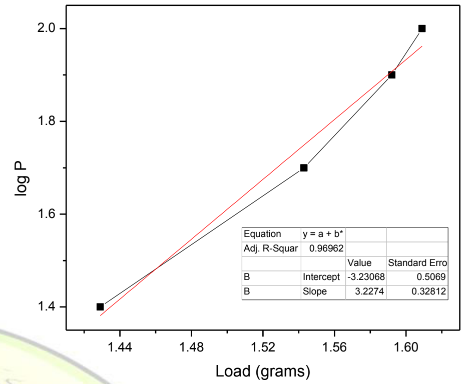

Fig 17: Graph of ln P versus ln d for LACC3 crystal

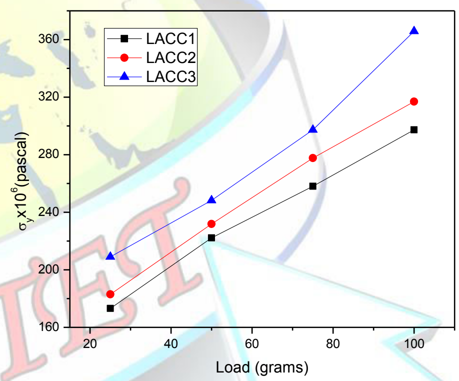

Fig 18: Plots of yield strength versus the applied load for cadmium chloride doped L-alanine crystals

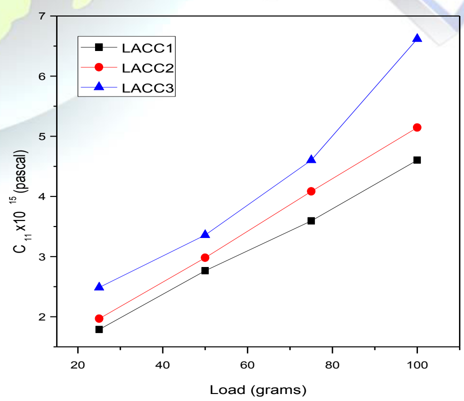

Fig 19: Plots of stiffness constant versus the applied load for cadmium chloride doped L-alanine crystalsparagraphs

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IV. CONCLUSION

Dielectric studies for the cadmium chloride doped L-alanine crystals have been measured at various frequencies in the range 102 – 106 Hz and at different temperatures ranging from 30oC to 85oC.The values of dielectric constant and loss are found to decrease with increase in frequency. The values of dielectric constant and loss are low at higher frequencies because domains of larger relaxation times may not be able to respond to these frequencies. The low value of dielectric loss with high frequency for cadmium chloride doped L-alanine crystals suggests that the grown crystals are of good quality with lesser defects. Lower values of dielectric constant will increase the efficiency of SHG and this is called as the Miller's rule and hence the lower value of dielectric constant at higher frequencies for the samples is an important parameter for the improvement of SHG coefficient.

AC conductivity and activation energy values were determined from the dielectric data and the behavior of the conduction was analyzed. Microhardness measurements were carried out using a Vickers microhardness indenter and this study gives an idea about the mechanical strength of the grown crystals. Microhardness studies reveal that the doped L-alanine crystals are harder than the undoped crystal. Values of work hardening coefficient, stiffness constant and yield strength for the samples have been determined and from the obtained data it is found that the grown crystals of this work are the category of soft materials.

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BIOGRAPHY

Photograph

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