International Journal of ChemTech Research
CODEN (USA): IJCRGG ISSN : 0974-4290
Vol.6, No.6, pp 3262-3264, Aug-Sep 2014

ICMCT-2014 [10th – 12th March 2014]
International Conference on Materials and Characterization Techniques

Influence of Mg^{2+} and Cu^{2+} metallic ions on the Structural, Mechanical and Optical Properties of L-Arginium Maleate Single Crystals

P. Shanmugam[1], V. Kathiravan[2], J. Madhavan[3] and S. Pari[1]*

[1]Department of Physics, National College, Tiruchirapalli – 620 001, India
[2]Department of Physics, Government Arts College, Karur – 639 005, India
[3]Department of Physics, Loyola College, Chennai – 600 034, India

*Corres.author: sparimyur@gmail.com

Abstract: Good quality pure and metal doped nonlinear optical L-Arginium Maleate (LArM) single crystals are grown by low temperature solution growth using slow evaporation technique. The grown crystals are subjected to powder X-ray diffraction studies to identify the structure. The presence of the dopants did not alter the triclinic structure of LArM. The dopant concentrations in the doped crystals are estimated by Atomic Absorption Spectroscopic analysis. The UV cut of range of the pure and the doped crystals are determined by optical absorption study. The NLO behaviors of the grown crystals are studied by Kurtz-Perry technique. The mechanical studies showed that the doped crystals are harder than the pure crystal.
Keywords: LArM, UV, NLO, XRD.

Introduction

Some organic compounds exhibit large NLO response than widely known inorganic materials. They also offer the flexibility of molecular design and the promise of virtually an unlimited number of crystalline structures. Among organic crystals for non linear optics (NLO) applications, amino acids display specific features of interest such as (i) molecular chirality, which secures acentric crystallographic structures; (ii) absence of strongly conjugated bonds, leading to wide transparency ranges in the visible and UV spectral regions; (iii) zwitterionic nature of the molecule, which favours crystal hardness [1-2].

The second harmonic generation (SHG) efficiency of LArM is about thrice that of potassium dihydrogen phosphate (KDP), the knowledge of studying the properties is very important since L- Arginine can be considered as the fundamental building block of more complex amino acids [3-5]. Hence, it may be useful to synthesize the amino acid complexes with other carboxylic acids and study their properties. This paper discusses the growth of single crystals of pure and doped LArM by slow evaporation technique. Structural and second harmonic efficiency were carried out and the results were presented and discussed.

Synthesis

L-Arginine Maleate ($C_6H_{15}N_4O_2^+ C_4H_3O_4^-.2H_2O$) LArM was synthesized by the reaction between a weak organic maleic acid ($C_4H_4O_4$) and the strong basic amino acid, L-arginine (Merck) taken in equimolar proportions. Purification of the synthesized salt was done by repeated crystallization until optically clear crystals (Fig .1) were obtained.

Fig 1. Photograph of LArM Pure and doped single crystals

Results and Discussion

Powder XRD studies

The structural properties of single crystals of pure and doped LArM have been studied by X-ray powder diffraction technique. Powder X-ray diffraction studies of pure, $Mg^{2+}$and Cu^{2+} doped LArM crystals were carried out, using Siemens D500 X-ray diffractometer with Cu K_{α} (λ = 1.5406 Å) radiation. The samples were scanned for 2θ values from 10˚ to 50˚ at a rate of 2˚ /min. Figure 2 shows the Powder XRD pattern of the pure and doped LArM crystals. There are slight variations in the lattice parameters and cell volume of the pure and doped crystals. These variations are due to the incorporation of $Mg^{2+}$and Cu^{2+} in the LArM crystal lattice.

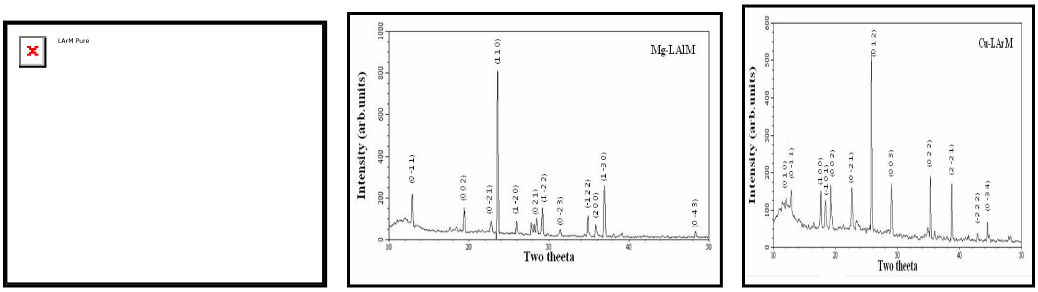

Fig 2. XRD pattern of of LArM Pure and doped single crystals

UV-Vis-NIR spectra

Using a Varian carry 5E model dual beam spectrophotometer, optical absorption data were taken between 200–1200 nm on the pure and doped LArM polished crystal samples of about 4 to 6 mm thickness. The spectra (Figure 3) indicate that the pure and doped LArM crystals have minimum absorption in the region between 250–1000 nm. It is seen that the doped LArM crystals have better lower cut-off wavelengths than the pure one. Both the Mg^{2+} and Cu^{2+} doped crystals have decreased absorption. In the doped crystals, minimum absorption and low cut-off wavelength, which are the required key properties are enhanced in both the doped crystals.

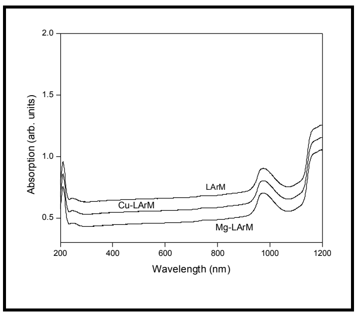

Fig 3. Optical absorption spectra of pure and doped LArM crystals

Atomic Absorption studies

The exact weight percentage of the $Cu^{2+}$and Mg^{2+} present in doped crystals is determined. 10mg of fine powder of the doped LArM crystals were dissolved in 100ml of triple distilled water respectively and the prepared solutions were subjected to Atomic Absorption Spectroscopy (AAS) Analysis. The results shows that only 0.96 % of $Cu^{2+}$and 1.33 % of Mg^{2+} are present in the respective samples, out of 2 % of the dopant. It is seen that the amount of dopant incorporated in to the doped crystal is less than the concentration of the dopant in the corresponding solution. It is also seen that more Mg ions have gone into the LArM lattice compared to Cu ions. This may be due to the radius of Mg (0.65 Å) compared to Cu ions (0.72 Å).

NLO studies

Kurtz SHG tests were carried out on the pure and doped LArM samples using the Nd:YAG Q-switched laser beam as a source [6]. For a laser input of 6.2 mJ, the second harmonic signal (532 nm) of 91.66 mW, 292.12 mW, 382.48 mW and 494.39 mW were obtained for KDP, pure LArM, Mg^{2+} and Cu^{2+} doped LArM respectively. Thus, the SHG efficiencies of pure, Mg^{2+} and Cu^{2+} doped crystals are 3.2, 4.2 and 5.4 times respectively higher that of KDP. Thus, the $Mg^{2+}$and Cu^{2+} metals have increased the efficiency of pure LArM.

Conclusion

Single crystals of pure, $Mg^{2+}$and Cu^{2+} doped L-Arginine Maleate (LArM) were grown successfully by slow evaporation technique. Powder X-ray diffraction studies were carried out and the lattice parameters are calculated. NLO studies showed that the metal doped crystals have efficiency greater than that of the pure LArM. Thus, it is concluded that the metal doped crystals can be effectively used as promising NLO material for device fabrication for the desired applications.

References

1. Sankar D, Vinay Raj Menon, P.Sagayaraj, J. Madhavan, Physica B, Jan, 405 (2010)192.
2. Sujatha T, A. Cyrac Peter, M. Vimalan , J. Merline Shyla , J. Madhavan, Physica B , 405 (2010) 3365.
3. Sujatha T, A. Cyrac Peter, M. Vimalan , J. Merline Shyla , J. Madhavan, Physica B, 405 (2010) 3365.
4. Victor Antony Raj M, J. Madhavan, M. Gulam Mohamed, J. Comput. Method. Mol.Design, 1(4) (2011)57.
5. Atkins P W, Physical Chemistry, Oxford University Press, Oxford, 2001.
6. Kurtz S.K and Perry T.T., J. Appl. Phys., 1968, 39, 3798.

*****