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A comparative analysis of chromium doped L-alanine cadmium chloride monohydrate single crystal using X-ray diffraction, thermal and optical techniques for nonlinear optical applications

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ABSTRACT

Single crystals of 1 and 3 mol% Cr^{3+} doped L-alanine cadmium chloride monohydrate were grown by slow evaporation solution technique using double distilled water as solvent. The amount of chromium incorporated into crystal lattice was found using atomic absorption spectroscopy and was found that actual concentration incorporated into lattice was few ppm only. Lattice dimensions of grown crystals were analysed using powder X-ray diffraction technique and found that the crystals crystallised in monoclinic system with space group C2. Crystalline perfection of grown crystals were assessed using High Resolution X-ray diffraction and X-ray topographic technique and was found that incorporation of chromium has significantly improved the crystalline perfection. Thermal stability of doped crystals were studied using thermogravimetric analysis and found that thermal stability was improved with the incorporation of chromium. Further there optical properties were analysed using UV–vis spectroscopy.

1. Introduction

There is a vast requirement of high speed transmission, optical data storage which lead to development in the field of photonics and nonlinear optics. The design and development of devices that requires photons instead of electrons for transmission has motivated the young scientists to search newer materials with enhanced optical properties. L-Alanine cadmium chloride monohydrate (LACCM) is potential material exhibiting the nonlinear optical properties. It has been observed that with the addition of suitable dopants in single crystal many properties like optical transparency, thermal stability, second harmonic generation (SHG) efficiency etc get enhanced. The dopants or additives also influence the crystalline perfection hence influencing the physical properties depending upon the extent of doping [1]. Effect of metal dopants like K^+ and Zn^{2+} on LACCM crystal have already been reported by Bright et al. [2,3]. Chromium being photorefractive element, has the tendency to alter optical properties of single crystal [4,5]. The present work focuses on analyzing the effect of metal dopant chromium on various properties of LACCM single crystal. In this regard, an attempt has been made by doping various concentration of chromium into LACCM material and then the growth of the crystals were carried out using slow evaporation solution technique (SEST). These crystals were then subjected to various characterization techniques in order to visualize the influence of dopants on various properties like crystalline perfection, optical transparency and thermal behaviour.

2. Experimental details

2.1. Synthesis and growth of single crystal

L-Alanine cadmium chloride monohydrate (LACCM) material was synthesised by mixing L-alanine & cadmium chloride monohydrate in proper stoichiometric ratio in double distilled water. The solution prepared was continuously stirred for homogenization for period of 1 hr at a temperature of 50 °C and was then filtered to remove the suspended impurities. The filtered solution was then divided into 2 parts and Cr(III) was doped in different concentrations (1 mol%, 3 mol%). The prepared solutions were filtered again and then the beakers were covered with perforated plastic sheet and housed in Eurotherm controlled (±0.01 °C accuracy) constant

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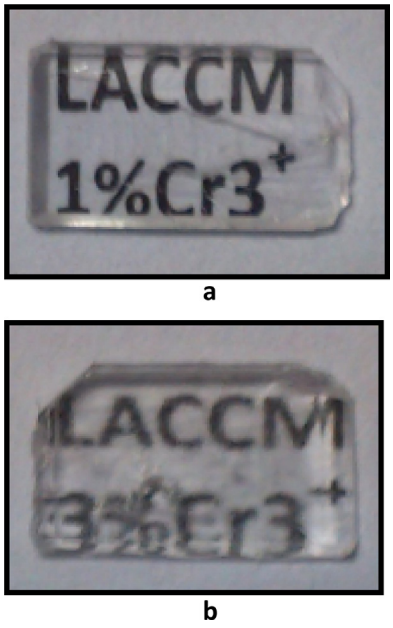

Fig. 1. (a) 1 mol% Cr^{3+} doped LACCM crystal. (b) 3 mol% Cr^{3+} doped LACCM crystal.

temperature bath (CTB) at 28 °C. Good quality single crystals were obtained after a period of 20 days. Fig. 1a and b depicts the photograph of 1 mol%, 3 mol% chromium doped LACCM single crystals.

2.2. Characterization techniques

The amount of chromium incorporated into the crystal lattice was confirmed by Atomic absorption spectroscopy AAS (Analytik Jena, Vario-6) having vapour-generation accessory. The lattice dimensions of the grown specimens were analysed using Bruker D-8 Advance X-ray powder diffractometer with Cu*K*α radiation of wavelength 1.54012 Å at a scan rate of 0.05 deg/s. The crystalline perfection of grown specimen were analysed using Rigaku double crystal X-ray diffractometer having 12 kW Rigaku rotating anode X-ray generator with topographic facility. Thermal analysis on the grown crystals was done using Mettler Toledo TGA/SDTA 851 with heating rate of 15 °C/min in nitrogen atmosphere. Absorption spectrum of the grown crystal was recorded using SHIMADZU UV–vis spectrophotometer (Model-1601) in the wavelength region ranging from 200 to 900 nm.

3. Results & discussions

3.1. Atomic absorption spectroscopy (AAS)

Concentration of chromium in doped crystal was found out with respect to elemental composition of pure LACCM. The amount of chromium which entered into the lattice of crystal was found to be much less than that present in solution during the growth process. For 1 and 3 mol% the actual amount of chromium entered into lattice was 0.43 ppm and 1.42 ppm only.

3.2. Powder X-ray diffraction (PXRD)

The X-ray diffraction pattern of 1 mol% and 3 mol% Cr^{3+} doped LACCM was recorded using Bruker D-8 Advance X-ray powder diffractometer. The pattern obtained are shown in Fig. 2a and b. From the pattern it may be concluded that no extra phases were present in doped crystals. The observed patterns were analysed using chekcell software and unit cell dimensions were calculated

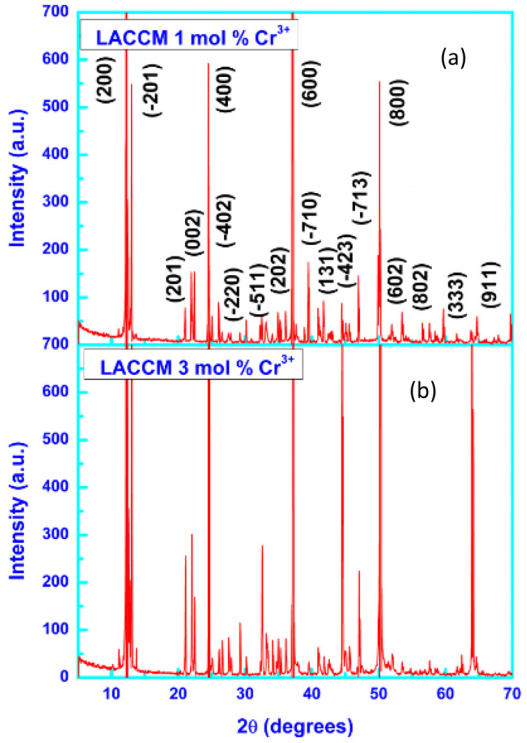

Fig. 2. (a) Powder XRD spectrum of 1 mol% Cr^{3+} doped LACCM crystal. (b) Powder XRD spectrum of 3 mol% Cr^{3+} doped LACCM crystal.

and found that for 1 mol% Cr^{3+} doped LACCM crystal $a = 16.2437$, Å, $b = 7.2755$ Å, $c = 7.9873$ Å, $\beta = 116.46$ & $V = 845.03$ Å^3 and for 3 mol% Cr^{3+} doped LACCM crystal $a = 16.2467$ Å, $b = 7.2736$ Å, $c = 7.9898$ Å, $\beta = 116.47$ & $V = 845.19$ Å^3. Slight change in dimensions of doped crystals compared to pure LACCM crystal (as reported in our earlier publication) [6] were observed which may be due to the incorporation of chromium into lattice but the results were in good agreement with reported literature [7]. Hence powder XRD analysis of doped LACCM crystal confirmed that there is no change in structure and morphology of crystals and they crystallised in monoclinic system with space group C2. Further the strain (η) in the lattice of doped crystals were calculated using Hall–Williamson relation as

$$\beta\cos\theta = \frac{K\lambda}{\tau} + \eta\sin\theta,$$

where β, θ, K, λ and τ are full width at half maxima (FWHM) of diffraction peak, Bragg diffraction angle of the peak, Scherrer constant, wavelength of X-rays and crystallite size, respectively. The corresponding values obtained are shown in Table 1. It was observed that with the increase in dopant concentration the strain increases which may be due to incorporation of chromium into the lattice of crystals.

3.3. High resolution X-ray diffraction (HRXRD) & X-ray topography (XRT)

Single crystals to be used for optical applications, the crystalline perfection must be reasonably good. In the present study, crystalline perfection of chromium doped crystals were assessed

Table 1
Strain in lattice of 1 and 3 mol% chromium doped LACCM crystal.

Sample name	Strain (η)
LACCM 1 mol% Cr^{3+}	-5.003×10^{-4}
LACCM 3 mol% Cr^{3+}	-2.15×10^{-4}