www.sphinxsai.com

International Journal of ChemTech Research
CODEN (USA): IJCRGG ISSN : 0974-4290
Vol.6, No.3, pp 1563-1566, May-June 2014

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

Crystalline perfection and Mechanical properties of lithium sulphate monohydrate NLO single crystal

P. S. Latha Mageshwari[1], R. Priya[2], S. Krishnan[3]*, S. Mageshwari[4], G. Bhagavannarayana[5], V.Joseph[6], S. Jerome Das[6]

[1] Department of Physics, R. M. K. Engineering College, Kavaraipettai – 601206, India.
[2] Department of Physics, R. M. D. Engineering College, Kavaraipettai – 601206, India.
[3] Department of Physics, B. S. Abdul Rahman University, India.
[4] Bharathi Women's College, Broadway, Chennai, India.
[5] CGC section, National Physical Laboratory, NewDelhi -110012, India.
[6] Department of Physics, Loyola College, Chennai – 600034, India.

*Corres.author: skrishnanjp@gmail.com

Abstract: NLO active and optically transparent lithium sulphate monohydrate (LSM) single crystal was grown by slow evaporation technique and subjected to High resolution X-ray analysis (HRXRD) to determine the grown crystal is quite good for device fabrication. The microhardness study was carried out to verify the mechanical strength of the grown crystal and also to understand the mechanical behavior of LSM crystal. Vickers hardness, fracture toughness (K_c), brittle index (B_i), yield strength (σ_v) and the elastic stiffness constant (C_{11}) were calculated. Kurtz and Perry powder technique confirmed the NLO activity of the LSM crystal.
Keywords: HRXRD; Mayer's index; fracture toughness; brittle index; elastic stiffness constant, SHG.

1. Introduction and Experimental:

Recently, most of the researchers have shown phenomenal interest in synthesizing nonlinear optical materials (NLO), piezoelectric and ferroelectric materials which find extensive applications in all latest technologies. NLO materials play a pivotal role in emerging photonic and optoelectronic fields such as optical data storage systems, optical communications, optical information processing and optical interconnections [1-3]. Piezoelectric $Li_2SO_4.H_2O$ crystal possesses pyroelectric, non-linear and electro-optic properties were grown by slow evaporation technique at room temperature and the crystal crystallizes in the monoclinic polar space group $P2_1$ [4].

2. Result and Discussions:

2.1 High resolution X-ray diffraction analysis

High-resolution diffraction curves were recorded using the multicrystal X-ray diffractometer developed at NPL [5]. Fig. 1 shows the high resolution X-ray diffraction curve (DC) recorded for the grown LSM crystal using (1 1 0) diffraction planes using MoKα_1 radiation. On deconvolution of the diffraction curve, it is clear that the curve contains two additional peaks, which are 30 and 70 arcs away from the main peak (highest intensity peak). The FWHM (full width at half maximum) of the main peak and the two very low angle boundaries are respectively 21 and 34 and 30 arc s. The relatively low values of FWHM of the grains in comparison with that of the real life reasonably good crystal depicts that the crystalline perfection is quite good. It may be mentioned here that such a low angle boundaries could be detected in the diffraction curve only because of the high-resolution of the diffractometer used in the present investigations. The influence of such defects may not influence much on the NLO properties.

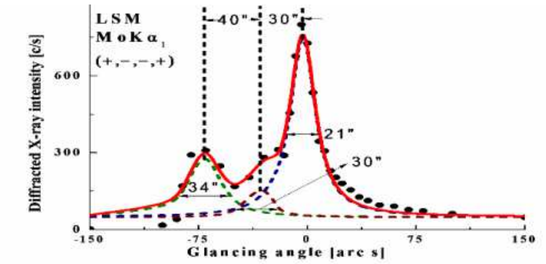

Fig. 1 Diffraction curve recorded for a typical LSM single crystal using (1 1 0) diffracting

2.2 Vickers hardness test

The Vickers hardness test for LSM crystal was carried out using the instrument MATSUZAWA MMTX- 7 SERIES. Hardness is a measure of resistance against lattice destruction or the resistance offered to permanent deformation or damage. The Vickers hardness (H_v) at different loads were calculated using $H_v = \frac{1.8544\,P}{d^2}$ kgmm^{-2}, where P is the applied load (in kg) and d^2 is the area of the indentation (measured in m^2). The value of hardness is found to increase with the increase of load for LSM crystal and the plot of log P versus log d yields a straight line and its slope gives the work hardening index n [4]. The grown crystal exhibits the reverse ISE in which the hardness values increases with increasing load. The work hardening coefficient (n) was found to be 2.44 and it is said to be soft material as mentioned by Onitsch [6].

The relation connecting the applied load and diagonal length 'd' of the indenter is given by Meyer's law, $P=K_1 d^n$, where K_1 is the standard hardness value which can be found out from the plot of P versus d^n (Fig 2). Since the material takes some time to revert to elastic mode, for every indentation a correction x is applied to the d value and the Kick's law is related as $P = K_2 (d+x)^2$, combining above two equations we get, $d^{n/2} = \left(\frac{K2}{K1}\right)^{1/2} d + \left(\frac{K2}{K1}\right)^{1/2} x$. For LSM crystal, the slope of $d^{n/2}$ versus d plot (Fig.3) yields $\left(\frac{K_2}{K_1}\right)^{1/2}$ and the intercept is a measure of x. The striking factor x is positive only when n<2 and negative for n>2 . The fracture toughness (K_1c) for LSM crystal is given by $K_c = \frac{P}{\beta C^{\frac{3}{2}}}$, where crack length measured from the centre of the indentation mark to the crack tip, P is the applied load and geometrical constant β =7 for Vickers indenter. The Mechanical behaviour is affected by another property called Brittle index (B_i).

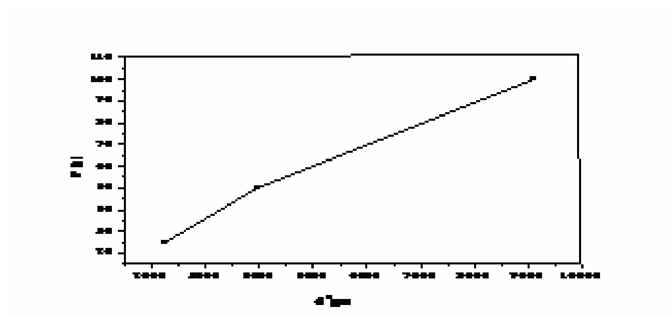

Fig.2 Plot of load (P) versus d^n

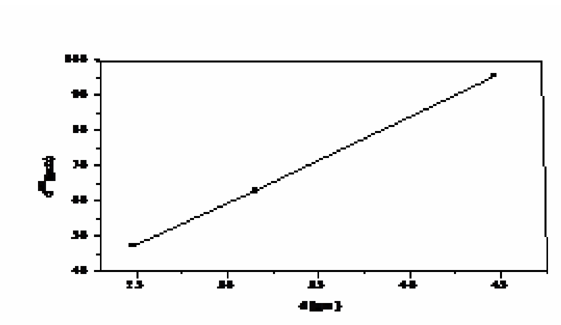

Fig.3 Plot of $d^{n/2}$ versus d

The Brittle index (B_i) for LSM crystal is given by $B_i = \frac{\mathbf{H_v}}{K_c}$. From the hardness value, the yield strength (σ_v) of the material was found using the relation, $\sigma_v = \frac{\mathbf{H_v}}{2}.9\left\{1-(n-2)\right\}\left[\frac{12.5(n-2)}{1-(n-2)}\right]^{n-2}$ and the first order elastic stiffness coefficient C_{11} for LSM crystal gives the idea about the tightness of bonding between neighboring atoms were calculated using Wooster's empirical relation $C_{11} = (\mathbf{H_v})^{\frac{7}{4}}$ and the high value of C_{11} indicates that the binding forces between the ions are quite strong [7] and hence, the mechanical strength is estimated as sufficiently large enough to withstand the stresses developed locally in the materials.

Table 1 Mechanical parameters of LSM crystal

Parameters	n	$\mathbf{K_1}$ (kg m^{-1})	$\mathbf{K_2}$ (kg m^{-1})	$\mathbf{H_v}$ (kg mm^{-2})	**x** (ìm)	K_c (kg $m^{-3/2}$)	B_i ($m^{-1/2}$)	σ_v (M Pa)	C_{11} (10^{12} Pa)
Values	2.44	10.61	53.65	95	-0.08	11.03 x 10^4	8 x 10^2	447.86	2.478

2.3 NLO test

Second harmonic generation of the grown crystal was estimated using Kurtz and Perry powder technique. The sample was illuminated with high intense beam of laser wavelength 1024 nm and pulse width of 8 n s. The emission of green radiation from the sample confirms the NLO activity of LSM crystal.

2.4 Conclusions

NLO active and good quality single crystal was grown successfully from aqueous solution by slow evaporation technique. HRXRD confirmed the perfection of grown crystal. The Vickers hardness studies revealed that the hardness number increased with load and grown crystal was found to be soft material and also several hardness parameters had been calculated for the grown crystal. The calculation of stiffness constant reveals that the binding forces between the ions are strong and thus NLO active LSM crystal is quite suitable for device fabrications.

3. References

1. Long N. J., Organometallic compounds for nonlinear optics-the search for enlightenment, Angew. Chem. Int. Ed. Engl., 1995, 34, 21-38.
2. Zhang X., Li M. and Cui Z., Prepare organic/inorganic hybrid non linear material containing two-dimensional spindle-type chromophers, Materials Letters., 2011, 65, 1404-1406.
3. Xieu Ren, Dongli Xu and Dongfeng Xue., Crystal Growth of KDP, ADP and KADP, J. Cryst. Growth., 2008, 310, 2005-2009.

4. Priya R., Krishnan S., Justin Raj C., and Jerome Das S., Growth and Characterization of NLO Active Lithium Sulphate Monohydrate Single Crystals, Cryst. Res. Technol., 2009, 44, 1272-1276.
5. Lal K., and Bhagavannarayana G., J. Appl. Cryst., 1989, 22, 209-215.
6. Onitsch M., Mikroskopie, 1947, 2, 131.
7. Ravishankar M.N., Chandramani R., and Gnanaprakash A.P., Evaluation of Stiffness constant C_{11} and yield strength (σ_v) of Solution Growth Semi organic NLO crystals, J. Optoelectronics and Biomedical Materials., 2011,3, 101-106.

****