www.sphinxsai.com

ChemTech

International Journal of ChemTech Research
CODEN (USA): IJCRGG ISSN : 0974-4290
Vol.6, No.14, pp 5604-5607, Nov-Dec 2014

Mechanical behaviour of Nonlinear Optical (NLO) single crystal

Suresh Sagadevan[1]*, Priya Murugasen[2]

[1]Department of Physics, Sree Sastha Institute of Engineering and Technology, Chembarambakkam, Chennai-600 123, India
[2] Department of Physics, Saveetha Engineering College, Chennai, India

*Corres.author : Email-sureshsagadevan@gmail.com

Abstract: L-Leucinium Oxalate (LLO) single crystals were synthesised and grown by slow evaporation solution growth method. Good optical transparency crystal were harvested and subjected to microhardness studies. The microhardness test was carried out to verify the mechanical strength of the grown crystal and also to understand the mechanical behavior of LLO crystal. Vickers microhardness study was carried out on the surface of the single crystal with various loads at room temperature with the indentation time as 5 s. Vickers hardness numbers (H_v) were calculated and it is found to increase with the applied load. Mayer's index number 'n' was also calculated. Vickers hardness, fracture toughness (Kc), brittle index (Bi), yield strength (σv) and the elastic stiffness constant (C_{11}) were calculated and presented in this paper.
Keywords: Vickers hardness, fracture toughness (Kc), brittle index (Bi), yield strength (σv) and Elastic stiffness constant (C_{11}).

1. Introduction

The structure and composition of the crystalline solids are inviolably related to the mechanical hardness. Microhardness testing is one of the best methods of understanding the mechanical properties of materials such as fracture behaviour, yield strength, brittleness index, and temperature of cracking [1, 2]. Superhard materials have attracted great attention because of their important industrial applications. In order to explore new super hard materials, the nature of hardness was extensively investigated with numerous models, proposed to predict the hardness of materials. Organic crystals were intensively investigated due to their high nonlinearities, high mechanical properties, rapid response in electro-optic effect and tailor made flexibility [3]. In the present work the mechanical behaviour of LLO crystal was studied using Vickers microhardness tester. Vickers hardness number H_v, Mayer's index number 'n', crack length, elastic stiffness constant, yield strength, fracture toughness and Brittle index were calculated. Hardness measurement is very important for device fabrications. The results are discussed in detail.

2. Materials and Methods

The LLO crystal was synthesized by taking Leucine and oxalic acid in the appropriate ratio. The calculated amounts of Leucine and oxalic acid were thoroughly dissolved in double distilled water using a temperature controlled magnetic stirrer. The solution was stirred well and slightly warmed using magnetic stirrer and filtered using filter paper and transferred to Petri dish. The prepared solution was allowed to evaporate at room temperature, which yield the salt of LLO. The purity of the synthesized salt was further improved by re-crystallization process. The temperature was maintained at 35°C and solutions were allowed to evaporate. Transparent crystals were grown in a period of 45 days. The mechanical characterization of LLO crystal was made by Vickers microhardness test. The grown crystal with flat and smooth faces and free from any defects was chosen for the static indentation tests. The surface was polished gently with methanol and mounted properly on the base of the microscope. Now the selected face was indented gently by varying the loads for a dwell period of 10s using Vickers indenter attached to an incident ray research microscope.

3. Vicker's Microhardness Measurement

Hardness is an important factor in the choice of ceramics for abrasives, bearings, tool bits, wear resistance coatings etc. Hardness is a measure of resistance against lattice destruction or the resistance offered to permanent deformation or damage. Measurement of hardness is a destructive testing method to determine the mechanical behaviour of the materials. As pointed out by Shaw (1973) [4], the term hardness is having different meanings to different people depending upon their areas of interest. For example, it is the resistance to penetration to a metallurgist, the resistance to cutting to a machinist, the resistance to wear and tear to a lubrication engineer and a measure of flow of stress to a design engineer. All these actions are related to the plastic stress of the material. For hard and brittle materials, the hardness test has proved to be a valuable technique in the general study of plastic deformation [5]. The mechanical strength of a material plays a key role in device fabrication. It is a measure of the resistance the lattice offers to local deformation [6]. Hardness is one of the important mechanical properties of the materials [7-9]. It can be used as a suitable measure of the plastic properties and strength of a material [10]. Stillwel (1938) [11] defined hardness as resistance against lattice destruction, whereas Ashby (1951) [12] defined it as the ability of a crystal to resist a structural breakdown under applied stress. This resistance is an intrinsic property of the crystal. The hardness properties are related to the crystal structure of the material and microhardness tests have been carried out to understand the plasticity of the crystals. Also, the hardness of the crystal is dependent on the type of chemical bonding, which may differ along the crystallographic directions. Hardness is generally taken as a ratio of the applied load to the area of indentation. The measurement of hardness is very important, as far as the fabrication of devices is concerned. The mechanical strength of the grown crystal was found out using Reichert MD 4000E ultra microhardness tester fitted with a Vickers diamond pyramidal indenter. The indentations were made at room temperature with a constant indentation time of 5s. The diagonal length of the indentation impression was measured using a microscope. In order to get accurate results for each applied load, several indentations were made on the sample and the average diagonal length (d) of the indenter impressions were measured. The Vicker'smicrohardness number H_v of the crystal was calculated using the equation

$$H_V = 1.8544\, P / d^2 (Kg / mm^2) \qquad (1)$$

where P is the applied load and d is the mean diagonal length of the indenter impression. Hardness measurements were taken for applied loads 10 to 50 g keeping the time of indentation constant at 5 sec for all the cases. The relation between hardness number and applied load for LLO is shown in Fig.1. It is observed that the Vickers hardness value increases with the applied load. Test load develops multiple cracks on the crystal surface due to the release of internal stress generated locally by indentation. It is observed from the measurement that the hardness value increases with increasing load.

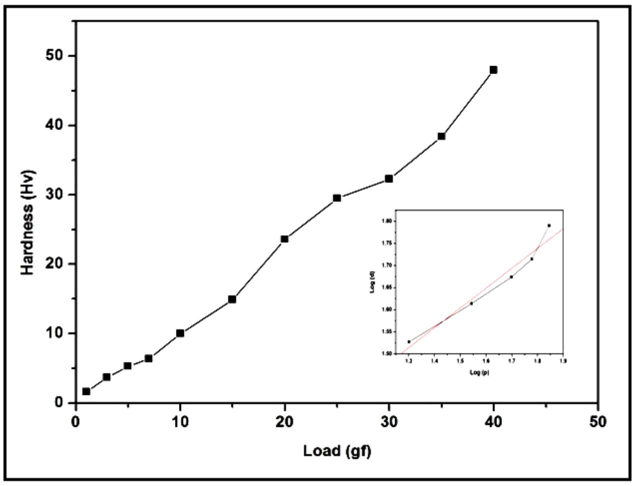

Fig. 1 shows the plot between applied load (P) and hardness number (Hv)

The value of hardness is found to increase with the increase of load for LLO crystal and the plot of log P versus log d yields a straight line and its slope gives the work hardening index n [13]. 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 2.04 and it is said to be soft material as mentioned by Onitsch [14]. From careful observations on various materials, Onitsch [14] and Hanneman [15] pointed out that, n lies between 1 and 1.6 for hard materials and it is more than 1.6 for soft materials. The work hardening coefficient plot inset in fig 1. The work hardening coefficient 'n' is found to be around 2.04 for LLO crystal. From the calculation we found LLO crystals belong to soft material category, its reveals the importance of device fabrication. The relation connecting the applied load and diagonal length'd' of the indenter is given by Meyer's law;

$$P = K_1 d^n \qquad (2)$$

where K_1 is the standard hardness value which can be found out. 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

$$P = K_2 (d + x)^2 \qquad (3)$$

Combining above two equations we get,

$$d^{n/2} = \left(\frac{K_2}{K_1}\right)^{1/2} d + \left(\frac{K_2}{K_1}\right) x \qquad (4)$$

The fracture toughness (K_C) for LLO crystal is given by

$$Kc = \frac{P}{\beta C^{3/2}} \qquad (5)$$

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 behavior is affected by another property called Brittle index (Bi). The Brittle index (Bi) for LLO crystal is given by

$$B_i = \frac{H_v}{K_C} \qquad (6)$$

From the hardness value, the yield strength (σ_v) of the material was found using the relation,

$$\sigma_V = \frac{Hv}{2}.9\ 1 - (n-2 \left[\frac{12.5(n-2)}{1-(n-2)}\right]^{n-2} \qquad (7)$$

and the first order elastic stiffness coefficient C_{11} for LLO crystal gives the idea about the tightness of bonding between neighboring atoms were calculated using Wooster's empirical relation

$$C_{11} = (H_v)^{7/4} \qquad (8)$$

and the high value of C_{11} indicates that the binding forces between the ions are quite strong [13] 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 LLO crystal

Parameters	**n**	**K_1 (Kgm^{-1})**	**K_2 (Kgm^{-1})**	**H_v ($Kgmm^{-2}$)**	**x**	**K_c ($Kgm^{-3/2}$)**	**B_i ($m^{-1/2}$)**	**σ_v (MPa)**	**C_{11} (10^{14} Pa)**
values	2.04	10.25	48.62	45		11.02 x 10^4	8 x 10^2	437.52	25.67

4. Conclusion

Good optical quality LLO crystals were grown by slow evaporation solution growth method. 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 LLO crystal is quite suitable for device fabrications.

Acknowledgement

The author thanks the Management and Principal of Sree Sastha Institute of Engineering and Technology, Chembarambakkam, Chennai-600123 for their continuous encouragement.

References

1. B. R. Lawn and E. R. Fuller, J. Mater. Sci. 9, 2016 (1975).
2. J. H. Westbrook, Report 58-RL-2033 of the G. E. Research Laboratory, USA, 1958.
3. R. Ramesh Babu, N. Vijayan, R. Goplakrishnan, and P. Ramasamy, Cryst. Res. Technol. 41, (2006).
4. Shaw MC (1973). The Science of Hardness Testing and its Research Application, Ed. By Westbrook J.H. and Condrad H, ASM. Ohio, pp. 1-11.
5. Westbrook JH, Conrad H (1971). The Science of Hardness testing and its Research Applications, American Society for Metals, Ohio.
6. Mott BW (1958). Hardness of Butter, Influence of Season and Manufacturing Method Micro indentation hardness testing, J. Dairy Sci. 41:360-368.
7. Xingtao KL, Fangfang WZ, Dongfeng X (2008). Electronegativity identification of novel super hard materials, Phys. Rev. Lett. 100:235504.
8. Ke YL, Dong FX (2009). Hardness of materials: studies at levels from atoms to crystals. Chinese Sci. Bull. 54:131-136.
9. Ke YL, Dong FX (2010). Hardness of group IVA and IVB nitrides. Physica Scripta, T139:014073.
10. Desai CC, Rai JL (1983). Microhardness studies of SnI2 and SnI4 single crystals. Bull. Mater. Sci. 5:453.
11. Stillwel CW (1938). Crystal Chemistry, McGraw Hill, New York.
12. Ashby NA (1951). The factor of hardness in metals. New Zealand Engineering. J. Nuclear Eng. 6:33-34.
13. Suresh Sagadevan and R. Varatharajan, international Journal of Physical Sciences, 8(39), 1892-1897 (2013).
14. E.M. Onitsch, Mikroskopie 2 (1947) 131.
15. M. Hanneman, Metall. Manchu. 23 (1941) 135.

*****