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Studies on the mechanical properties of glycine lithium chloride NLO single crystal

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The microhardness study reveals the mechanical strength of the grown crystal. The Vicker's and Knoop hardness studies were performed to understand the mechanical behavior of the glycine lithium chloride crystals. The Vicker's and Knoop microhardness numbers (H_V and H_K) for the crystal were found for different loads. It is found that these numbers increase with an increase in the load. The Mayer's index *(n)* was found to be greater than 1.6 predicting a soft-material nature. The fracture toughness value (K_c), was determined from the measurements of the crack length. The brittleness indices (B_i) were found for the grown crystals. Using Wooster's empirical relation, the elastic stiffness constant (C_{11}) was calculated from the Vicker's hardness values at different loads. The Young's modulus was also calculated from Knoop microhardness values.

Key words: Microhardness number, Mayer's index, fracture toughness, brittleness indices, elastic stiffness coefficient, Young's modulus.

INTRODUCTION

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), 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 (Westbrook and Conrad, 1971). The hardness depends not only on the properties of the materials under test but also largely on the conditions of measurement. Microhardness tests have been applied to fine components of clock and instrument mechanisms, thin metal strip, foils, wires, metallic fibers, thin galvanic coatings, artificial oxide films, etc., as well as the thin surface layers of metals which change their properties as a result of mechanical treatments such as machining, rolling, friction and other effects. The microhardness method is widely used for studying the individual structural constituent elements of metallic alloys, minerals, glasses, enamels and artificial abrasives.

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 (Mott, 1958).

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Hardness is one of the important mechanical properties of the materials (Xingtao et al., 2008; Ke and Dong, 2009; Ke and Dong, 2010). It can be used as a suitable measure of the plastic properties and strength of a material (Desai and Rai, 1983). Stillwel (1938) defined hardness as resistance against lattice destruction, whereas Ashby (1951) 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.

In the present investigation, attention is focused on the mechanical properties of glycine lithium chloride single crystals such as Meyer's index number, brittle index and fracture toughness calculated from Vicker's microhardness number (H_V). The Young's modulus was calculated from the Knoop hardness test.

MATERIALS AND METHODS

Experimental procedure

Glycine lithium chloride single crystals were synthesized by dissolving glycine and lithium chloride in the molar ratio of 1:1 in distilled water. The solution was stirred continuously using a magnetic stirrer. The prepared solution was filtered and kept undisturbed at room temperature. The beaker was closed with a porously sealed cover and the solution in the beaker was allowed to evaporate. A few days later, tiny crystals were seen in the beaker. Among them, a defect free seed crystal was suspended in the mother solution, which was allowed to evaporate at room temperature. Large size single crystals were obtained due to collection of monomers at the seed crystal sites from the mother solution. The mechanical characterization of glycine lithium chloride crystals were made by Vickers microhardness and Knoop 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 10 s using Vickers and Knoop indenter attached to an incident ray research microscope (Mututoyo MH112, Japan).

Vicker's test

Vicker's test is said to be a more reliable method of hardness measurement. In order to get a similar geometrical impression under varying loads, Smith and Sandland (1923) have suggested that a pyramid be substituted for a ball. The Vickers hardness test method consists of indenting the test material with a diamond indenter, in the form of a right pyramid with a square base and an angle of 136° between opposite faces and subjected to a load of 1 to 100 kg (Figure 1). The base of the Vickers pyramid is a square and the depth of indentation corresponds to $1/7^{th}$ of the indentation diagonal. The longitudinal and transverse diagonals will be in the ratio of 7:1. The full load was normally applied for 10 to 15 s. The two diagonals of the indentation left in the surface of the material after the removal of the load were measured using a microscope, and their average was calculated. The area of the sloping surface of the indentation was calculated.

The Vicker's hardness is the quotient obtained by dividing the kg load by the square mm area of indentation.

$$H_V = \frac{2p\sin\frac{136}{2}}{d^2}$$

$$H_V = 1.8544P/d^2$$

where H_V = Vickers hardness number, P = load in kg, d = arithmetic mean of the two diagonals.

When the mean diagonal of the indentation has been determined, the Vicker's hardness number can be calculated from the above formula. Several different loading settings give practically identical hardness numbers on uniform material, which is much better than the arbitrary changing of scale with the other hardness testing methods. The advantages of the Vicker's hardness test are that extremely accurate readings can be taken, and just one type of indenter is used for all types of metals and surface treatments.

Knoop hardness test

Knoop hardness can be treated as an alternative to the Vickers test, particularly for very thin layers, Fredrick Knoop developed a low-load test with a rhombohedral-shaped diamond indenter. The long diagonal is seven times (7.114 actually) as long as the short diagonal. With this indenter shape, elastic recovery can be held to a minimum. Knoop tests are mainly done at test forces of 10 to 1000 g (Figure 2); so, a high powered microscope is necessary to measure the indent size. Because of this, Knoop tests have mainly been known as microhardness tests. The magnifications required to measure Knoop indents dictate a highly polished test surface. To achieve this surface, the samples are normally mounted and metallurgically polished; therefore Knoop is almost always a destructive test.

The mechanical characterization of the glycine lithium chloride crystals was analyzed by the Vicker's and Knoop microhardness tests. Crystals with flat and smooth faces were chosen for the static indentation tests and the same crystal was mounted on the base of the microscope. The indentations were made gently by varying the loads from 10 to 100 g for a dwell period of 10 s using both the Vicker's diamond pyramid indenter and the Knoop indenter attached to an incident ray research microscope (Mitutoyo MH112, Japan). The intended impression of Vicker's was approximately square in shape. The shape of the impression is dependent on the structure, face and materials used. After unloading, the length of the two diagonals was measured by a calibrated micrometer attached to the eyepiece of the microscope. For each load, at least five well-defined indentations were considered and the average was taken as d. The Vicker's hardness was calculated using the standard formula

$$H_V = 1.8544P/d^2 \quad (1)$$

where P is the applied load in Kg, d in µm and H_V in Kg/mm^2. The Knoop indented impressions were approximately rhombohedral in shape. The average diagonal length (d) was considered for the calculation of the Knoop hardness number (H_K) using the relation

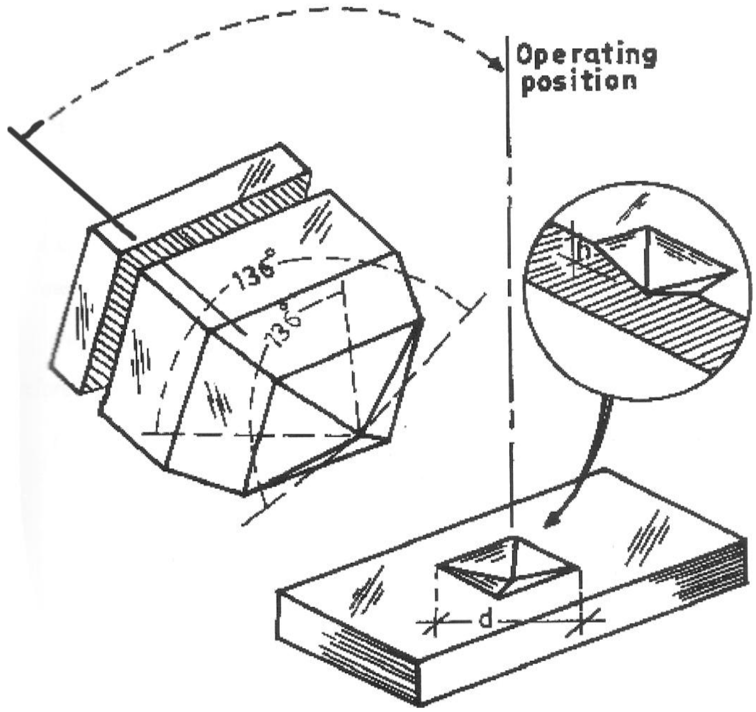

Figure 1. Vickers hardness test.

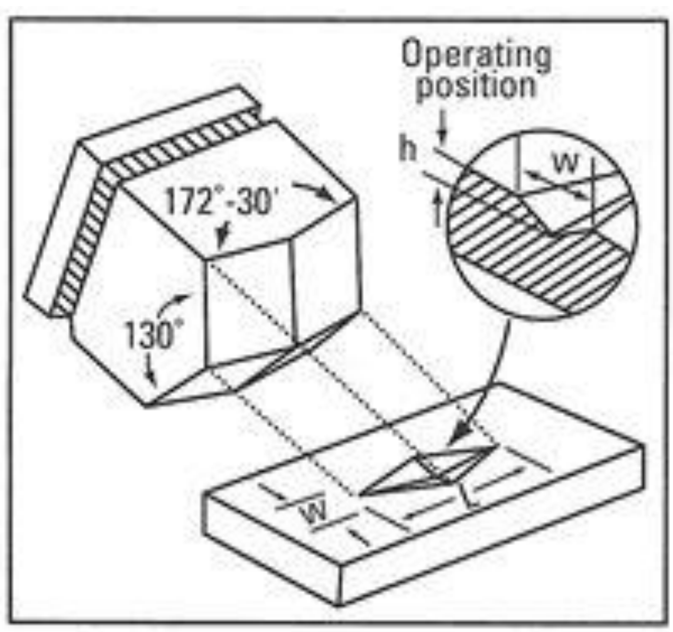

Figure 2. Knoop hardness test.

$$H_K = 14.229\, P / d^2 \quad (2)$$

where P is the applied load in Kg, d in µm and H_K is in kg/mm^2. Beyond 100 g of the applied load, crack initiation and fragmentation were observed. So the hardness test could not be extended beyond this load. The elastic stiffness constant (C_{11}) was calculated using Wooster's empirical relation as (Wooster, 1953).

$$C_{11} = H_V^{7/4} \quad (3)$$

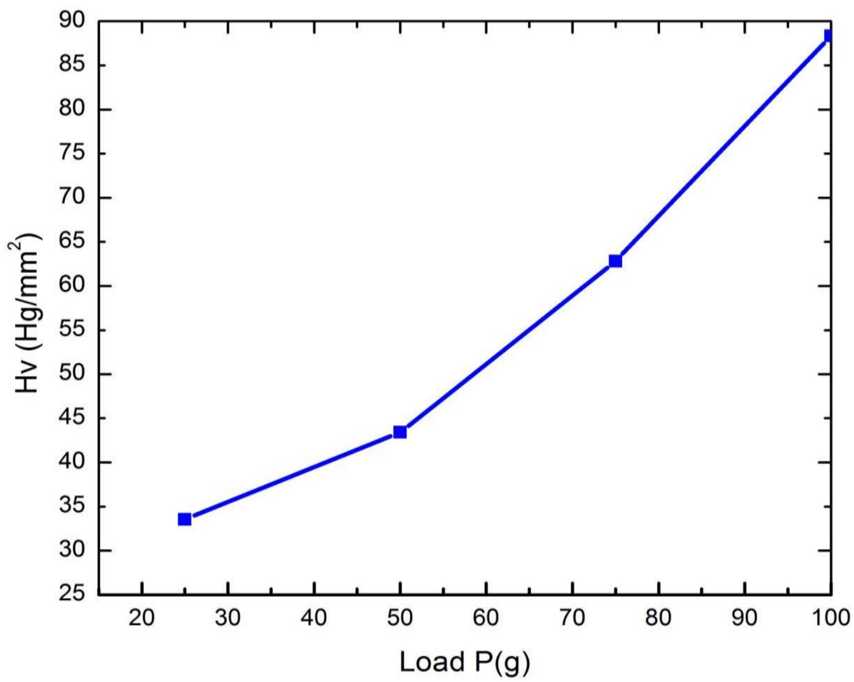

Figure 3. Variation of the microhardness number H_V with load.

RESULTS AND DISCUSSION

Vicker's microhardness test

Figure 3 shows the variation of H_V as a function of applied loads, ranging from 25 to 100 g. It is clear from the figure that H_V increases with an increase in the load. The Mayer's index number was calculated from the Mayer's law, which relates the load and indentation diagonal length.

$$P = kd^n \quad (4)$$

$$\log P = \log k + n \log d \quad (5)$$

where *k* is the material constant and *n* is the Mayer's index (or work-hardening coefficient). The above relation indicates that H_V should increase with the increase in P if n > 2 and decrease with P when n < 2. The '*n*' value was determined from the plot of log P *vs* log d, as shown in Figure 4. The slope of the plot of log P versus log d will give the work hardening index (n) which is found to be 3.50. The material glycine lithium chloride is confirmed with large amount of mechanical strength which is better for device fabrications. According to Onitsch (1950) the value of '*n*' is less than 2 for hard materials and more than 2 for soft ones. Thus, glycine lithium chloride crystals belong to the soft-material category. Since glycine lithium chloride is having moderately higher value of hardness number, the material is found to be suitable for device fabrications.

The elastic stiffness constant (C_{11}) was calculated by Wooster's empirical relation. The calculated stiffness constant for different loads was tabulated (Table 1). The crack length is measured from the centre of indentation mark to the crack end. Here, the crack length (*l*) is the average of two crack lengths for each indentation. Resistance to fracture indicates the toughness of material (Jain et al., 1994). The fracture mechanics of the indentation process gives an equilibrium relation for a well-developed crack extending under the centre loading condition;

$$K_c = \frac{P}{\beta_0 l^{3/2}}, l \geq \frac{d}{2} \quad (6)$$

where β_0 is the indenter constant, equal to 7 for the Vicker's diamond pyramid indenter (Lawn and Marshal, 1979) and other symbols have their usual meanings. For the glycine lithium chloride crystal, the value of K_c is found to be 2.84×10^4 Kg $m^{-3/2}$, 3.15×10^4 Kg $m^{-3/2}$, 15.16×10^4 Kg $m^{-3/2}$ and 27.69×10^4 Kg $m^{-3/2}$ at 25, 50, 75 and 100 g respectively.

Brittleness is another property, which affects the mechanical behaviour of a material, and is expressed in terms of the brittleness index (B_i) as.

$$B_i = \frac{H_V}{K_c} \quad (7)$$

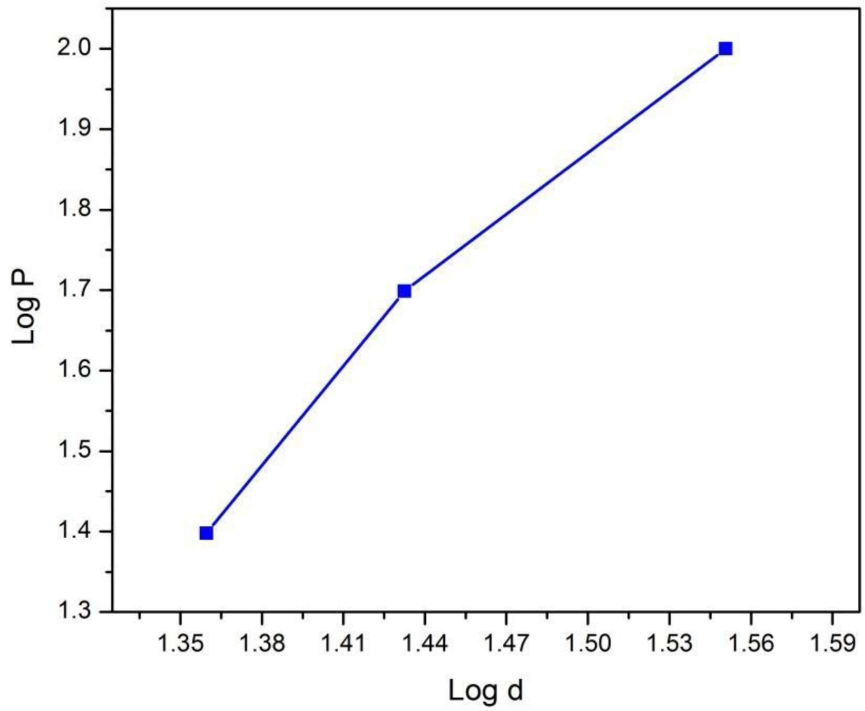

Figure 4. log P vs. log d.

Table 1. Elastic stiffness constant of glycine lithium chloride.

Load P (g)	H_V (Kg/mm^2)	C_{11} x 10^{14} Pa
25	33.55	4.67
50	43.40	7.33
75	62.80	14.00
100	88.35	25.46

The calculated values of B_i are found as 13.07 × 10^4 m$^{-1/2}$, 13.78 10^4 m$^{-1/2}$, 4.14 × 10^4 m$^{-1/2}$ and 3.19 × 10^4 m$^{-1/2}$ at 25 g, 50 , 75 and 100 g respectively.

Knoop microhardness test

Knoop hardness (H_K) was plotted against loads (P). The plot is shown in Figure 5. From this measurement, it is found that as the load increases the Knoop microhardness number also increases. From the Knoop microhardness measurements, the Young's modulus (E) of the crystal was calculated using the relation (Pal and Kar, 2005).

$$E = 0.45H_K / (0.1406 - b/a) \quad (8)$$

where H_K is the Knoop microhardness value at a particular load, and 'b' and 'a' are the shorter and longer Knoop indentation diagonals respectively. The calculated Young's Modulus is 1.53 ×10^{10} Nm^{-2}.

Conclusion

The Vicker's and Knoop microhardness studies were carried out on the grown glycine lithium chloride single crystal. The Vickers and Knoop hardness numbers were calculated for the glycine lithium chloride single crystal, by the application of load and the hardness numbers were found to increase with an increase in the load. The value of the Mayer's index number is found as 3.50, which proves that glycine lithium chloride falls in the soft-material category. The calculation of the stiffness constant (C_{11}) reveals that the binding force between the ions is quite strong. The Young's modulus was calculated from the diagonal lengths of the Knoop indentation.

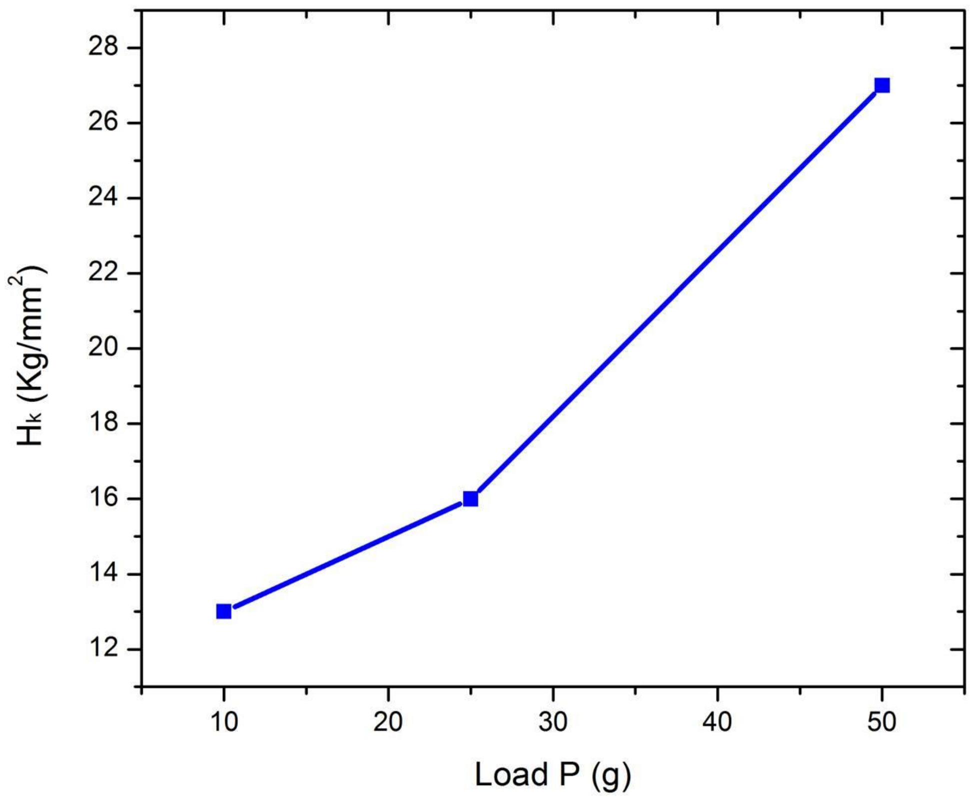

Figure 5. Variation of the Knoop microhardness with load.

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