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Calculation of Mechanical Parameters of Thiourea Single crystals Grown by Inexpensive Slow Evaporation Technique

Minal N. Vansia[1], Kishor C. Poria[2]
[1]Assistant Proffesor,Shree Ramkrishna Institute of Computer Education and Applied Science, Surat- 395001,Gujarat –India.
[2]Vice-Chancellor, Hemchandracharya North Gujarat University,Patan -384265Gujarat –India.

Abstract: Single crystals of Thiourea(NH_2CSNH_2), an organic nonlinear optical material have been grown by simple and inexpensive slow evaporation technique at room temperature. The mechanical characterization of grown crystals were studied and their Vicker's Micro hardness number (Hv), Fracture toughness (Kc), Elastic stiffness constant (C_{11}) and yield strength (σ) were calculated. Standard hardness value K_1 and K_2 were calculated using Meyer's law and Kick's law.
Keywords: Thiourea single Crystals, Vicker's Microhardness, Fracture toughness, Elastic stiffness constant, yield strength. standard hardness.

I. INTRODUCTION

Mechanical strength of the materials plays a key role in the device fabrication. Vickers's hardness is one of the important deciding factor in selecting the processing (cutting, grinding, polishing) steps of bulk crystals in fabrication of devices based on crystals. In the view of device fabrication, calculations of mechanical parameters are very important. This can be done with the help of Vicker's micro hardness studies.

II. EXPERIMENTAL

For the present work the indentation were made using CLEMEX-HWMMT-X7. The Vickers diamond pyramidal indenter was used for indentation tests on the cleavage surfaces of single crystals of Thiourea grown by inexpensive evaporation technique. The thickness of the grown crystal were about 3 to 5 mm. Variation of Vicker's microhardness number with different loads for grown crystal are summarized in Table:1. The images of indentation marks on cleaned surfaces of grown crystals were shown in Figure:1

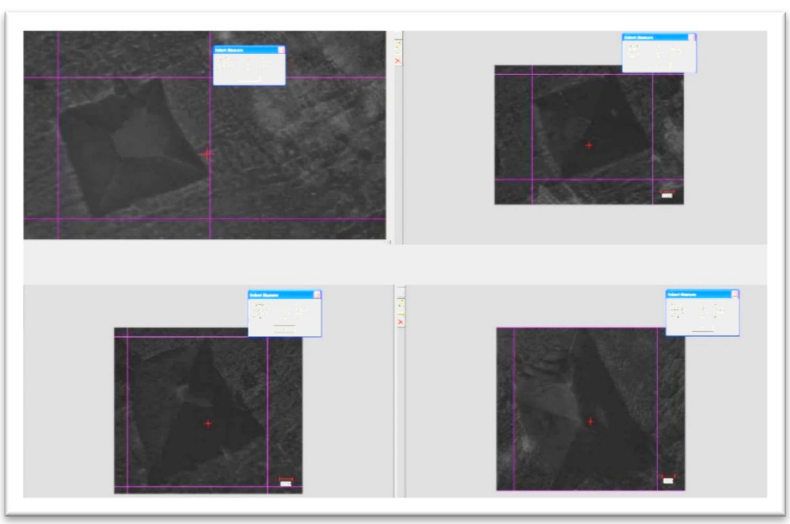

Figure:1: Images of indentation

load P(10^{-3}kg)	Hardness H_v(Kg/mm^2)	Average d(µm)	logP	log d
25	15	55.85	1.3979	1.7470
50	14	82.4	1.6989	1.9159
100	16	108.9	2.0000	2.0370
200	28	115.15	2.3010	2.0612

Table:1 Data for $P=K_1d^n$

III. MECHANICAL PARAMETERS

Hardness values are always measured from the surface. Thus, the observed hardness behavior is the summation of a number of effects involved in the materials response to the indentation pressure during loading, in the final measurement of the residual impression. The importance of microhardness study lies in the possibilities of making an indirect estimate of mechanical characteristics of materials such as yield strength and toughness having a specific correlation with the hardness.

IV. CALCULATION OF MAYER'S INDEX

The Mayer's index number was calculated from the Mayer's law, which relates the load and indentation diagonal length.

$P = kd^n$ ……………..(1)

$\log P = \log k + n \log d$ …..……………..(2)

Where k is the material constant and n is the Mayer's index (work-hardening coefficient). The above relation indicates that Hv should increase with the increase in P if n > 2 and decreases with P when n < 2.

The average value of Mayer's index n was determined from the plot of log P Vs. log d. in Figure:3, the slope of the plot of log p vs. log d will give the work hardening index (n) which is found to be 2.585. The Thiourea material is confirmed with large amount of mechanical strength which is suitable for device fabrication.

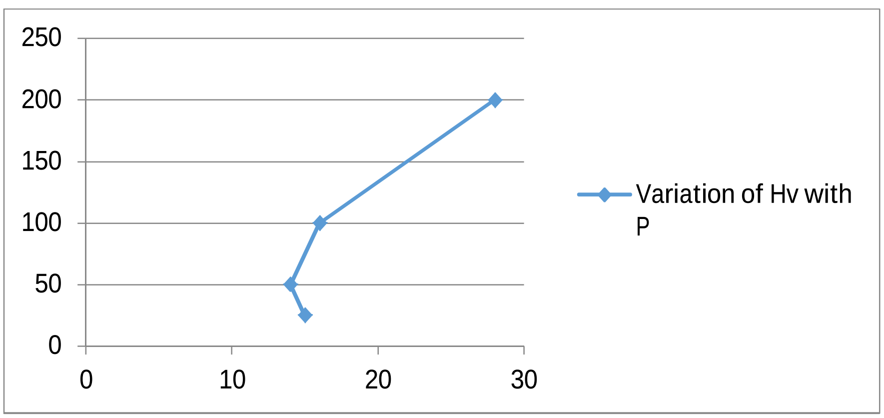

Figure:2: Plot of P→H

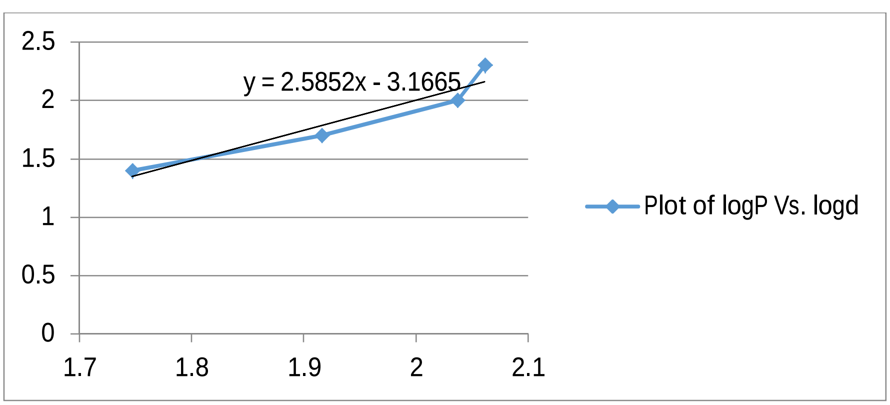

Figure: 3: Plot of logP→ logd

load P (10^{-3}kg)	Hardness H_v(Kg/mm^2)	Yield strength $\sigma_y = (Hv/3)(0.1)^{n-2}$	Elastic stiffness $C_{11}=H_v^{7/4}$	Fracture toughness $K_c=P/[\beta C]^{3/2}$
25	15	3.9002	114.3298	0.0032
50	14	3.6402	101.3267	0.0036
100	16	4.1602	128.0000	0.0047
200	28	7.2804	340.8211	0.0087

Table:2: Calculated Hardness parameters

According to Meyer's relation

$P = K_1.d^{\,n}$ ……………………. (3)

Where K_1 is the standard hardness value. After every indentation the material takes some time to revert to elastic mode. So a correction x is applied to the d value.

According to Kick's law

$P = K_2\,(d + X)^2$ …………………. (4)

From equations (3) and (4)

$d^{n/2} = (K_2/K_1)^{1/2}\, d + (K_2/K_1)\, X$ ……………….(5)

The variation of $d^{n/2}$ with d gives K_2/K_1 and the intercept is the measure of X. Using the relations (2), (3), (4) and (5) the hardness parameters such as n, K_1, K_2 and X were calculated and presented in the Table .

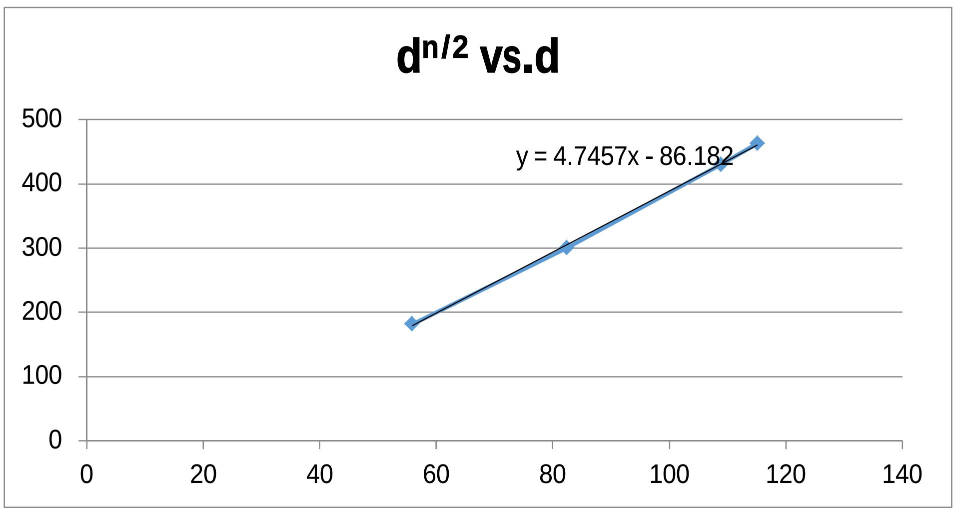

Figure: 3: $d^{n/2}$ vs.d

Parameters	values
Meyer index n	2.585
K_1($\times 10^{12}$ kg/m^2)	3.166
K_2($\times 10^{6}$ Kg/m^2)	7.111
X(µm)	3.827

Table:2: Calculated Standerd Hardness Values

V. CONCLUSION

Vicker's microhardness measurement reveals the soft nature of the crystal and shows reverse ISE. The mechanical parameters like fracture toughness (K_c), elastic stiffness constant (C_{11}), yield strength (σ_v), standard hardness K_1 and K_2 were calculated and summarized in table.

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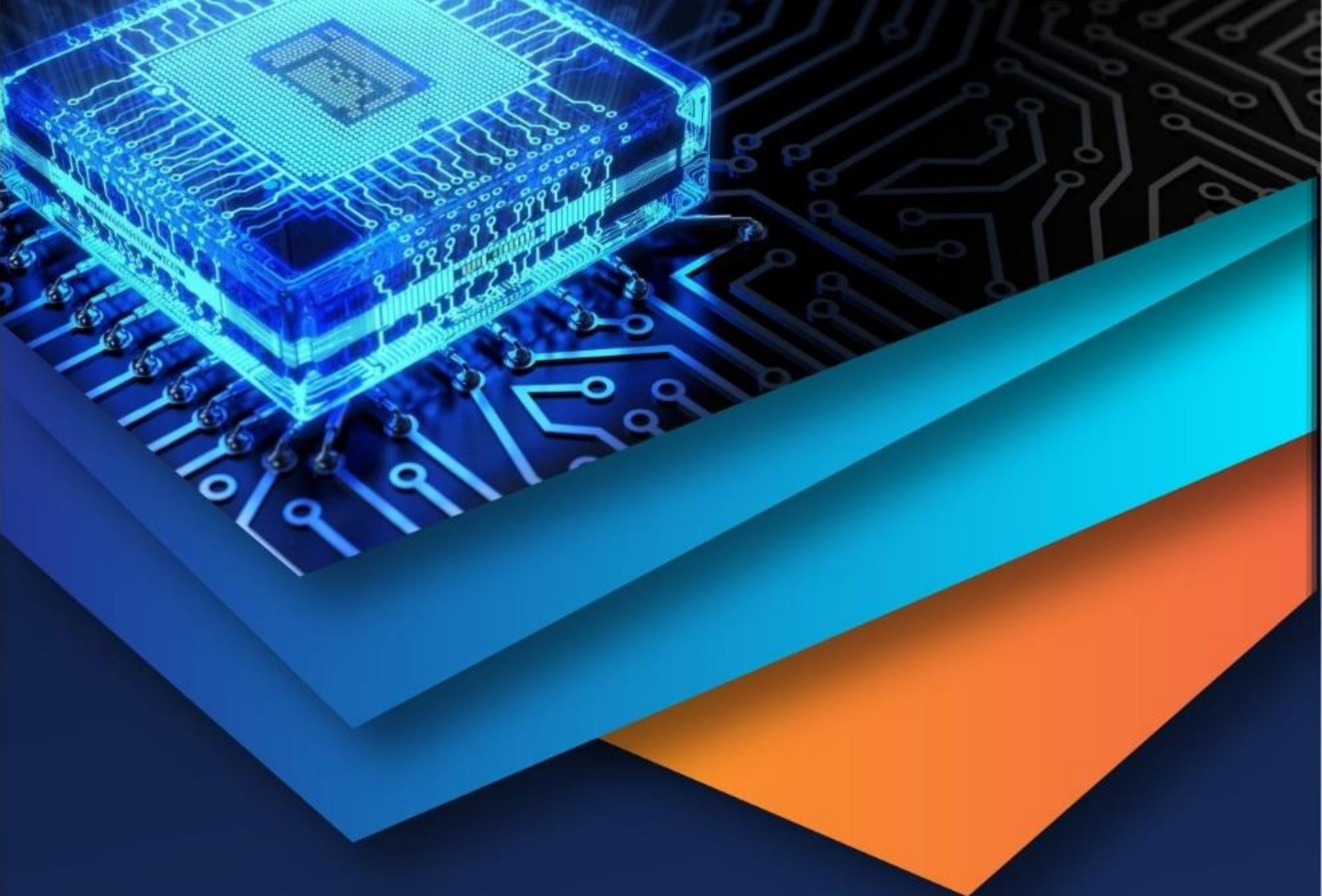

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