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Mechanical and dielectric nature of organic molecular anthracene single crystal

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Abstract - *High quality anthracene single crystals which is used as model organic molecular crystal used in the studies of solid-state properties has been grown by solvent evaporation method. The unit cell parameters of the grown crystals have been studied by single crystal X-ray diffraction analysis. Vicker's microhardness studies is carried out to investigate the mechanical properties like fracture toughness, brittleness index and elastic stiffness constant. Dielectric behaviour is studied for different frequency at various temperature and the results were discussed*

Key Words: Crystal growth, Single crystal X-ray diffraction, Mechanical, Dielectric studies

1. INTRODUCTION

Ramesh Babu et al. [1] reported that organic crystals shows remarkable opto-electronic properties due to delocalized electrons namely conjugated electron system possess various photoresponses such as photoconductive, photovoltaic and so on. Madhurambal et al., has already grown anthracene single crystals by using slow evaporation technique with various solvents namely acetone (C_3H_6O), benzene (C_6H_6), carbon tetrachloride (CCl_4), carbon bisulfide (CS_2) [2-3]. Anthracene is one of the organic single crstals with unique optical and electronic properties reported first in 1948 [4]. In the present investigation, we made an attempt to grow pure crystal by adopting solvent evaporation technique using chloroform as a solvent. This paper deals about the mechanical and dielectric properties of anthracene crystal

2. Material Synthesis

In our present study pure anthracene single crystals is grown by taking 50 ml of chloroform with measured quantity of anthracene powder (AR grade 99% pure) in a beaker and stirred continuously to yield saturated solution. The prepared solution was filtered using a sintered glass filter of 1μm porosity and the saturated solution is sealed with aluminium foil and the synthesized solution was kept in dark room without any mechanical disturbances. By repeated re-crystallization process good quality transparent single crystal is obtained within a period of 30 days. The photograph of the grown crystal is shown in Fig 1.

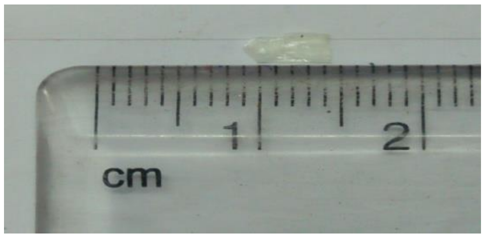

Fig 1: As grown anthracene crystal

3. Results and discussion

3.1 Single crystal XRD

Single crystal X-ray diffraction analysis for the grown crystal has been carried out to confirm the crystallinity and to identify the lattice parameters using ENRAF NONIUS CAD4 automatic X-ray diffractometer. The calculated lattice parameter values are a= 9.457 Å, b=6.045 Å, c=8.641 Å, α, γ = 90° and β=103.7° and the grown crystal is belong to monoclinic system with the space group $P2_1/a$ [2]. The XRD results are in good agreement with reported value and thus confirms the grown crystal.

3.2 Micro hardness study

Vickers microhardness number (VHN) was evaluated for anthracene crystal employing Futuretech FM-800 type E-series microhardness tester for various loads ranging from 1-100 g. The value of H_v is calculated using the relation

$$H_v = 1.8544\ P/d^2 \qquad (1)$$

where P is the applied load in g, d is the diagonal length in mm and H_v in kg/mm². The variation of H_v with the applied load is shown in Fig 2. Fig 3 shows a plot of log P vs log d yields a straight line and the slope gives the work hardening coefficient 'n'. According to Onitsch [4], the work hardening coefficient 'n' should lie between 1 and 1.6 for harder materials and if the value of n is above 1.6 it comes under softer materials. The value of n is 2.62 for anthracene crystal and concludes the grown crystal belongs to soft category. The Mayer's index number was calculated from Mayer's law, which relates load and indentation diagonal length. According to Meyer's relation

The a

$$P=K_1\, d^n \quad (2)$$

where K_1 is the standard hardness value which can be found out from the plot of P versus d^n.

As the material take some time to revert to the elastic mode after every indentation, a correction 'n' is applied to the d value.

Kick's law is related as $P=K_2\,(d+x)^2$ (3)

The above equation (2) and (3)

$$d^{n/2}=(K_2/K_1)^{1/2}d + (K_2/K_1)^{1/2}x \quad (4)$$

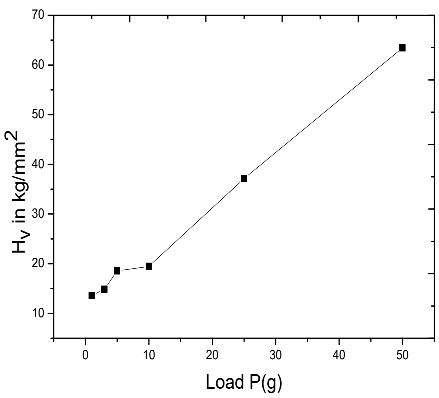

Fig 2: Variation of H_v vs load P

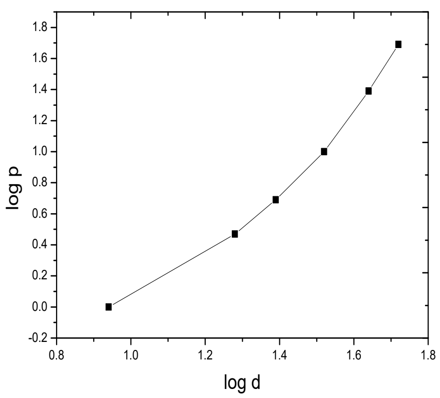

Fig 3: Variation of log P vs log d

The slope of $d^{n/2}$ versus d yield $(K_2/K_1)^{1/2}$ and the intercept is a measure of x. The fracture toughness K_c is given by

$$K_c=P/\beta c^{3/2} \quad (5)$$

The another property which affects the mechanical behavior is Brittleness index is given by

$$B_i = \frac{H_v}{K_c} \quad (6)$$

where c is the crack length measured from the centre of the indentation mark to crack tip. P is the applied load and geometrical constant β=7 for Vickers indenter

Table 1: Various hardness parameter of grown anthracene crystal

Various hardness parameter	Anthracene crystal
n	2.62
K_1 (kg mm^{-1})	4.91 x 10^{-3}
K_2 (kg mm^{-1})	3.646
K_c (MN m$^{-3/2}$)	0.02380
H_v (kg m m^{-2})	68.235
B_i (m$^{-1/2}$)	2562.67

3.3 Dielectric study

The dielectric loss and dielectric constant of anthracene crystals were studied at different temperatures (313, 343, 373, 403 and 433 K) using HIOKI 3532 LCR HITESTER in the frequency region 50 Hz to 5 MHz. The plot of dielectric constant and loss versus log f at various temperatures is shown in Fig 4 & 5 respectively. The net polarization of crystal is increased which increases its dielectric constant. The dielectric constant is higher at lower frequency because of presence of all four polarizations, namely electronic, ionic, orientation and space-charge and it decreases gradually at higher frequency. The value of dielectric loss is low due to lesser defect concentration and increase in the crystalline perfection.

AC Conductivity study

The AC conductivity of anthracene crstal is calculated using the following relation

$$\text{where } \sigma_{ac}=2\pi f\epsilon_0\,\epsilon'\tan\delta \quad (7)$$

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where f is the frequency in hertz. Fig 6 shows the plot of ac conductivity with respect to log frequency for anthracene crystal.

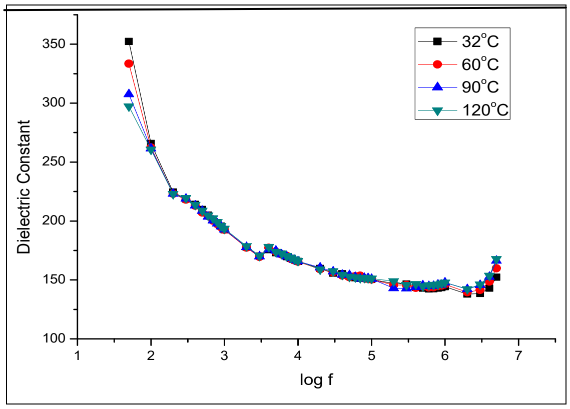

Fig 4: Dielectric constant vs log f

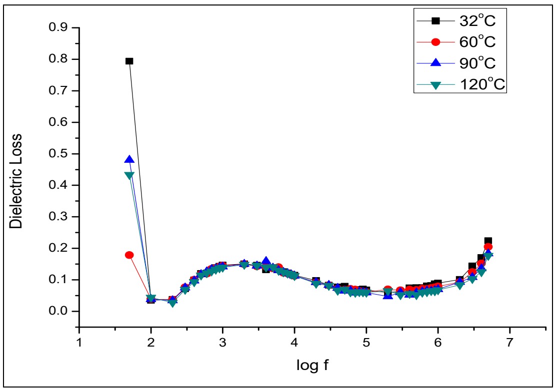

Fig 5: Dielectric loss vs log f

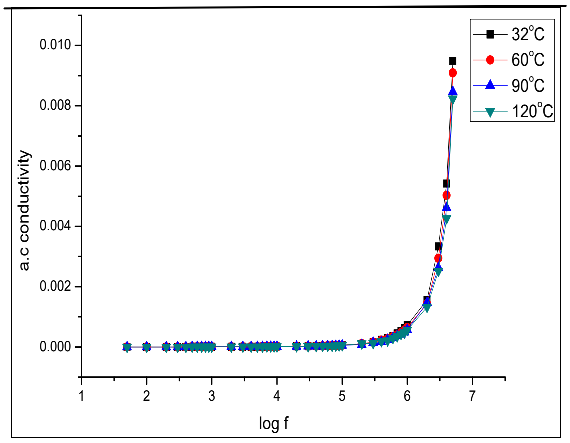

Fig 6: Plot of ac conductivity vs log f

4. Conclusion

Optically good quality single crystal of anthracene was grown by solvent evaporation method and the crystals were characterized by XRD to determine the space group and lattice parameters. Vickers micro hardness study reveals that the value of hardness number H_v increases with increase in load and the work hardening coefficient for pure crystal was calculated as 2.62. Dielectric loss and dielectric constant was found for the grown crystal

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