Growth and Characterization Of Tantulam Selenide

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***Abstract*—**Layered structure (lamellar) solids of transition metal dichalcogenides MX2 (M=Mo,W,Nb,Ta, X=S,Se,Te) have been extensively studied partly because of their excellent lubricating properties and partly due to their photovoltaic properties. Undo extreme pressures fluid lubricants squeeze out from between metting surfaces, causing high friction and wear. With lamellar solids such as TMDCs, shearing takes place more easily when loads are high. So, lamellar solids are well suited to extreme pressure lubrication. As a part of programme of growing than single crystals, this paper presents the growth of TaSe2. The vapour transport technique using iodine as a transporting agent and EDAX and XRD studies gives confirmation also stoichiomatric and structural properties. The type, concentration of charge carriers and also the carrier mobility has been obtained by the Hall effect measurement at room temperature.

Keywords*-EDAX,XRD,Growth,Crystal.*

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I. INTRODUCTION

In recent years there has been a considerable interest in the study of the high pressure behaviour of solids because of academic, technology and geophysical reasons. The academic interest owes its origin to the fact at high pressure nature of the interatomic forces in matter change considerably. Single and few layer transition metal dichalcogenide Nano sheets WSe2, TaSe2 are prepared by mechanical exfoliation [1].Under normal conditions solids exhibit a particular crystal structure for which the total energy is minimum. However, on application of high pressure, the atomic arrangement in solid changes resulting in changes in interatomic distances and crystal structure. Electric and Optoelectronic properties and application of Vander Walls [2]. In this context it will be of great importance to study the Physical behaviour of lamellar solids like MX2 under extremely high pressure. Phonon and Thermal Properties of TaSe2 thin film. Phonon and Thermal Properties of TaSe2 thin film [Reference 3]. Moreover, TMDCs are found to decompose below their melting point and also are insoluble in water, hence the vapour transport technique is used for growing single crystals of TaSe2 using chemical vapour transport technique with Iodine as a transporting agent in order to get single crystals with maximum dimensions.

The crystal structure of TaSe2 is shown in Fig. 1. The crystal structure is monoclinic with the space group C2/m and unit cell dimensions are

a= 19.39 Å, b= 3.642 Å, c= 9.375 Å, β= 134°, 35 [1, 2]

II. GROWTH

The growth of Single Crystal of TaSe2 is divided in the following heads

A. Ampoule Cleaning

The best quality fused quartz tube was washed thoroughly with distilled water and heated with HF which reacts with silica to create roughness. It was again washed with distilled water which was followed by washing with hot mixture of conc.HCL and conc.HNO3 taken in equal proportion. It was again washed by distilled water to make the inner surface free from any residue of chemicals. Thus cleaned ampoule was kept in a SICO oven at 373 K and left over night to make it moisture free.

B. Compound Preparing

A 5gm mixture of Ta (99.95%) and Se (99.99%) was filled in the dried ampoule with Iodine of the quantity 5mg per cc of the ampoule volume was sealed in the thin capillaries and placed in the ampoule as a transporting agent. Then the ampoule was sealed at the pressure of 10-5 torr. The sealed ampoule was introduced into a two zone furnace at a constant reaction temperature to obtain the change of $TaSe_2$. The charge so prepared was rigorously shaken to ensure proper mixing of the constituents and kept in the furnace under appropriate condition to obtain single crystals of TaSe2. Table 1 shows the physical conditions used to grow single crystals of TaSe2.

TABLE I. PHYSICAL CONDITIONS USED TO GROW SINGLE CRYSTAL OF $TaSe_2$

Compound preparation		**Growth Condition**			**Dimension of the ampoule**		Crystal size and appearance
Temperature	**Time**	**Temperature**		**Time**	**Diameter**	Length	1.5×4×0.04 mm^2 Black Opaque
		Hot Zone	**Cold Zone**				
500 °c	72 hrs	900 °c	850 °c	216 hrs	2.4 cm	25 cm	

TABLE II. INDEXING OF $TaSe_2$

d- spacing (Å)	(hkl)	Lattice Parameters
6.602	(200)	a= 19.24 Å
3.312	(002)	
3.221	(210)	b= 3.69 Å
3.221	$(\bar{2}10)$	c= 9.30 Å
2.200	(510)	
1.615	(420)	
1.615	$(\bar{4}20)$	

III. RESULTS

The shinning black opaque single crystal of $TaSe_2$ was obtained by CVT technique. The chemical composition of the grown sample has been well confirmed by carrying out EDAX analysis. Fig.2 shows the energy dispersive spectra of $TaSe_2$ single crystal. The atomic percentage of Ta and Se obtained with these spectra are 30.3% and 69.7% respectively which are slightly deviating from the required proportion of 26.69% and 73.31% respectively. In the present study, Phillips, X''Pert X-Ray diffractometer with Cu target has been used for obtaining the power diffraction pattern of $TaSe_2$. Fig.3 shows an X-Ray diffractogram of the crystal powder of TaSe2. The pattern consists of well-defined sharp diffraction lines, indicating good crystallinity of the specimen. Table 2 shows the indexing of the diffraction pattern. The calculated a, b and c parameters are

a = 19.24Å
b = 3.69Å
c = 9.30Å

The absorption spectrum taken from $TaSe_2$ single crystal in the form of thin flakes over the spectral range 700nm to 1450 nm is shown in Fig.4. Careful study of this spectrum reveals that an absorption edge is seen in the spectral range 850 nm to 900 nm.

Fig. 5 shows the spectral variation of $(\alpha h\nu)1/2$ vs $h\nu$. It represents indirect interband transition involving the emission or absorption of Phonons. The values of indirect band gap obtained from the intersection of the linear portion of the graph. In Fig.5 with the energy axis for zero absorption is 1.43eV.

For the determination of the direct bandgap, the spectral variation of $(\alpha h\nu)^2$ vs $h\nu$ as shown in Fig. 6 was studied. The value of direct bandgap obtained from the intercept of the straight line portion of the curve the $h\nu$ axis for zero absorption is 1.44eV.

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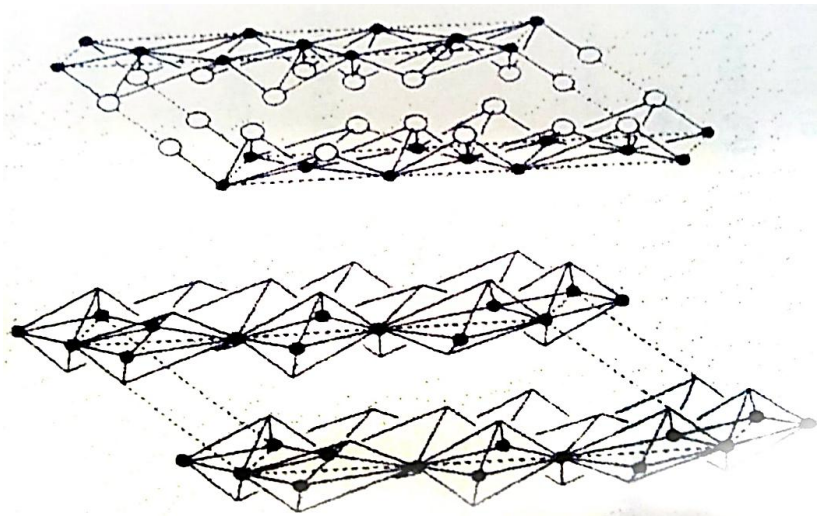

Figure 1. Crytal Structure of $TaSe_2$.

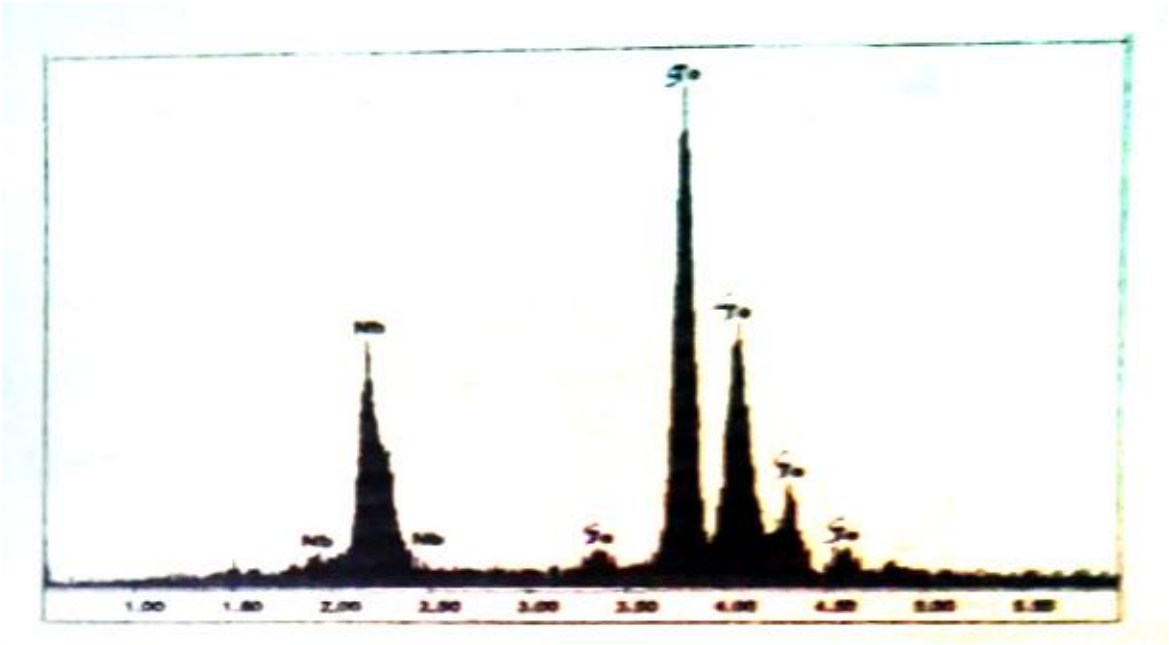

Figure 2. Energy Dispersive Spectra.

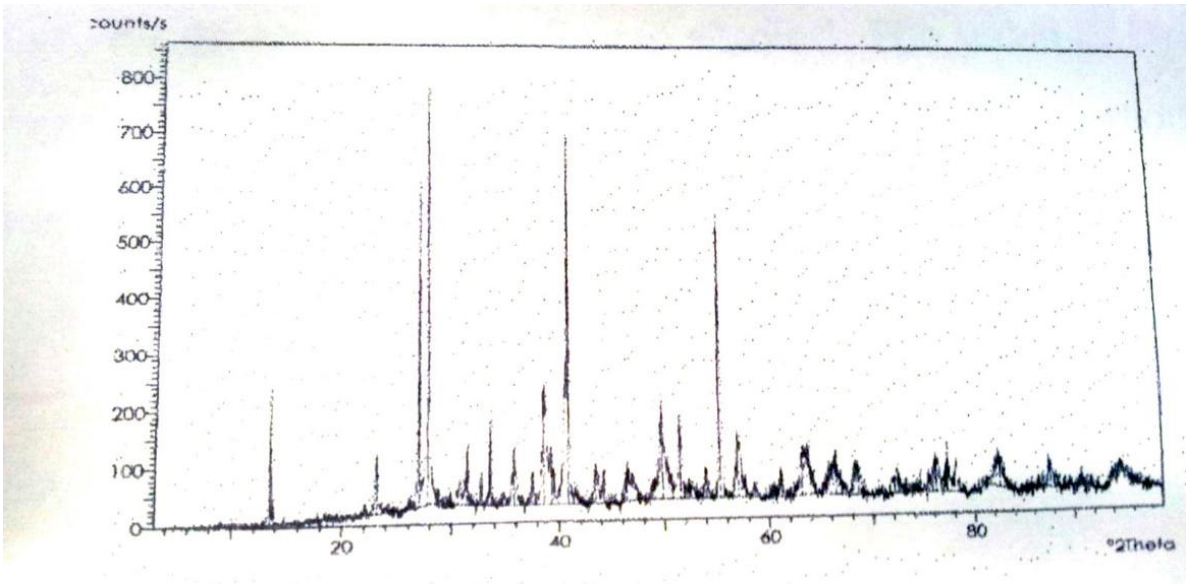

Figure 3. X-ray Diffractogram.

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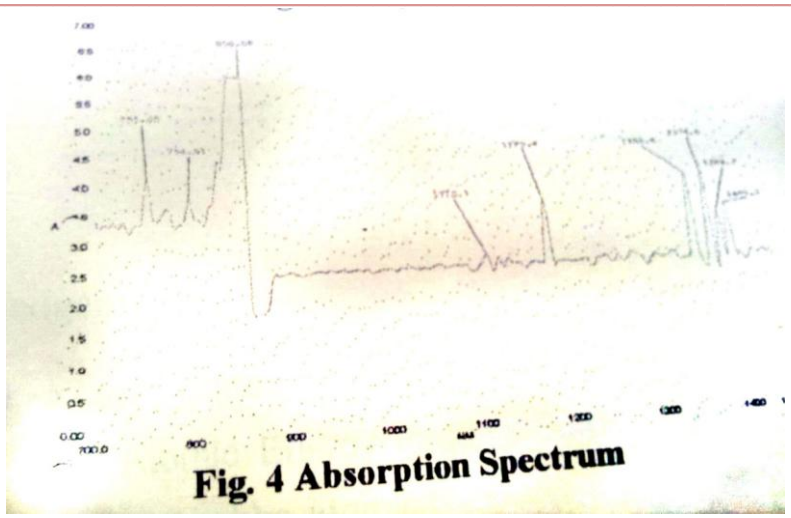
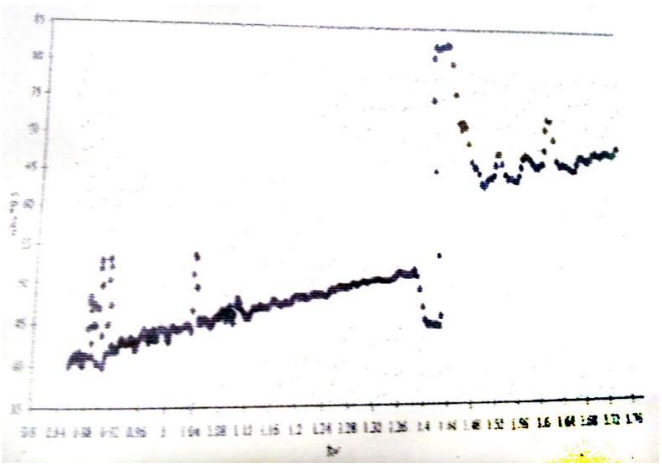


Figure 4. Absorption Spectrum.



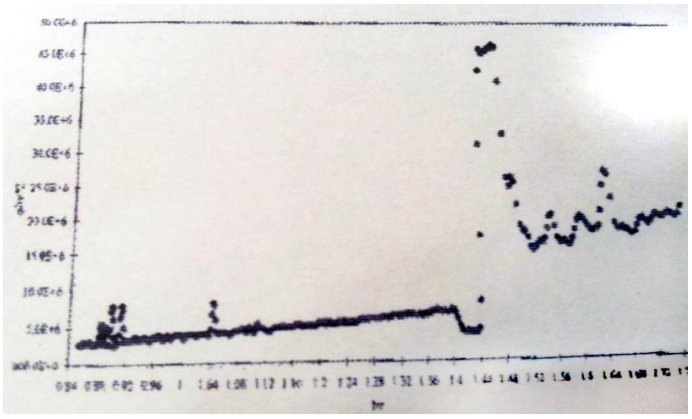


Figure 5. Spectral variation of $(\alpha h\nu)^{1/2}$ vs $h\nu$.