Journal of Basic and Applied Engineering Research
p-ISSN: 2350-0077; e-ISSN: 2350-0255; Volume 2, Issue 19; October-December, 2015, pp. 1669-1672

http://www.krishisanskriti.org/Publication.html

Investigation of Optical Properties of MoS_2 Derivative with Tungsten

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Abstract—*Semiconductor dichalcogenide materials have been growing interests in science and technologies during last decade. The tuneable direct band gap of such materials gives rise to potential applications in applied optoelectronics and photonics. In this report we investigated optical properties of Sulphide of Molybdenum and its derivative with Tungsten using UV-Vis spectroscopy, Raman spectroscopy and Photoluminescence (PL) spectroscopy. Formation of MoS_2 with inhomogeneous crystallite dimensions was confirmed by XRD pattern. Distinguished pattern of XRD for the derivative were observed. From Kubelka Munk plot of UV-Vis spectra the materials were showed to be large band gap semiconductors. Raman peaks at 384.95cm^{-1} (E^1_{2g}) and 406.12cm^{-1}(A_{1g}) were found for MoS_2 sample. Large shift in Raman peaks were observed in case of the derivative sample with Mo:W=1:3 molar ratio confirmed by EDX. PL spectra revealed the strong blue emission as depicted in UV-Vis spectra.*

Keywords*: semiconductor, dichalcogenide, derivative, Kubelka Munk Plot, photoluminescence.*

1. INTRODUCTION

Due to the presence of finite energy band gaps, semiconductor materials have been widely used in electronics, optoelectronics and industrial applications. Transition-metal-dichalcogenide (TMD) materials have graphene like X-M-X layered crystal structure, with a general formula MX_2 (M= Mo, W, V, Nb, Ta, Ti, Zr, Hf and X= S, Se, Te), exhibiting semiconductor behavior **[**1]. TMDs represent an intriguing family of materials with prospects for a broad range of unique properties and applications [2-4]. Among the large group of non-planar inorganic graphene-analogous layered TMD materials, MoS_2 and WS_2 are the two most widely studied materials in recent years. Both MoS_2 and WS_2 sheets have intrinsic band gaps depending on their thickness. Bulk MoS_2 is an indirect-band-gap semiconductor while monolayer MoS_2 is a direct-band-gap semiconductor with larger band gap energy (~2eV) [5, 6]. Synthesis of layered MoS_2/graphene (MoS_2/G) composites, use of MoS_2/TiO_2 nanocomposites in PV cell, application of ITO-MoS_2-Au stacked structure in PV cells have been reported in recent years [7, 4]. In this report nano derivatives of MoS_2 with W having Mo:W molar ratio 1:3 had been synthesized. The details of the synthesis process were explained by Rao and his group [8] in three different ways. We have used the solid state reaction between Molybdic Acid and Tungstic Acid with excess Thiourea as sulfur source for material synthesis. Structure and compositions of the samples were characterized by XRD and EDX. The optical properties were investigated using UV-Visible spectroscopy, Raman spectroscopy and Photoluminescence spectroscopy (PL) and compared with MoS_2.

2. EXPERIMENTAL

The synthesis of MoS_2 and Derivative of MoS_2 with tungsten was done using the reaction described by Rao et al. **[**8]. Commercially available Molybdic acid {RANKEM (M0240)}, Tungstic acid {Himedia (RM6308-100G)} and Thiourea { RANKEM (T0050) } were used for the solid state reaction in N_2 gas environment at 500°C. This was done in a tube furnace modified for N_2 environment. The raw chemicals were first powdered using mortar and pestle and then the powdered chemicals were mixed with proper molar ratios. These chemicals were placed inside the furnace and heated at 500°C in N_2 environment and products were obtained as shown in figure1.

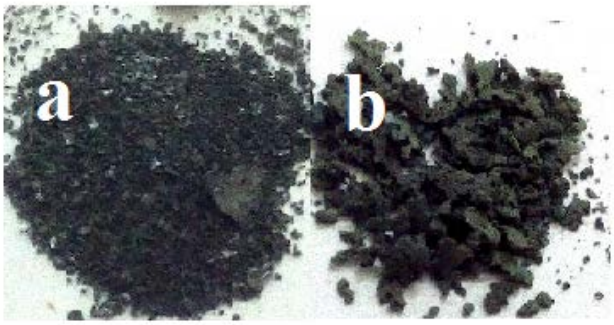

Fig. 1: a. MoS_2 sample, b. Mo-W-S sample

The black product were powdered and cleaned several times with distilled water for characterization.

3. CHARACTERIZATION

The XRD pattern of the as-prepared samples were obtained using RIGAKU MINIFLEX Difractometer with Cu-Kα radiation (λ= 1.5405 Å). EDX of the sample was obtained using JEOL JSM-6390LV Scanning Electron Microscope. The UV-Vis spectra of all as prepared samples for absorption were obtained using UV-Visible absorption spectrometer (UV 2450, SHIMADZU CORPORATION) available in our department. Raman spectra were obtained using Lab Ram HR Laser Micro Raman System. PL was done in F-2700 FL Spectrophotometer.

3.1 XRD

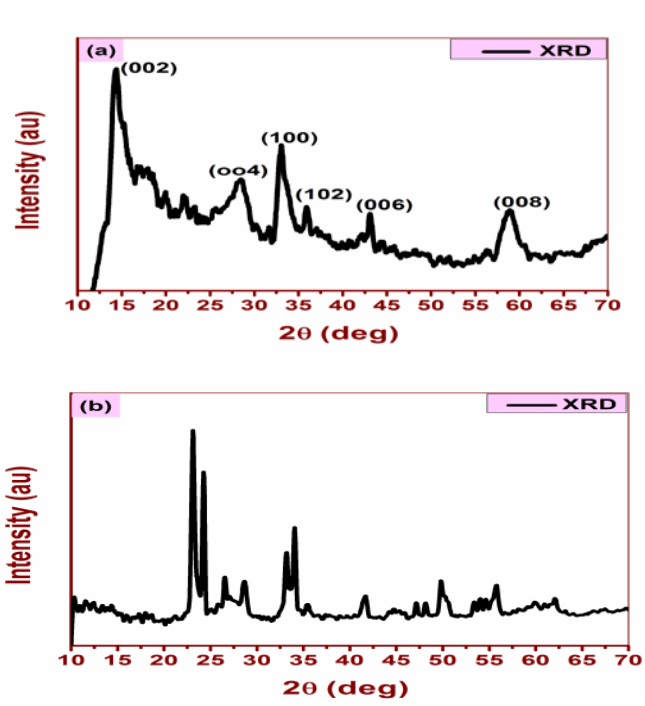

Fig. 2: XRD of (a) MoS_2, (b) Mo-W-S samples.

3.1.1 Williamson-Hall plot

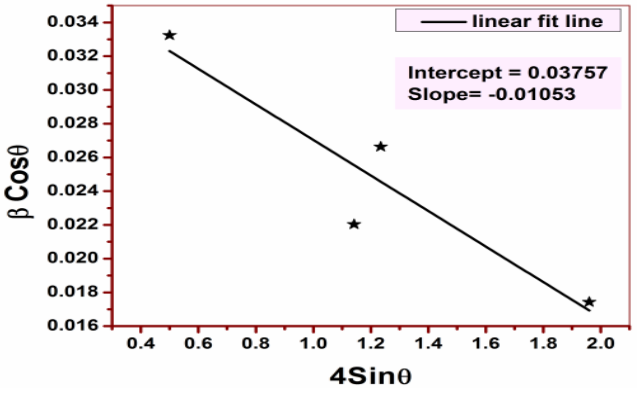

Fig. 3: Williamson–Hall plot of MoS_2 sample.

3.2 EDX

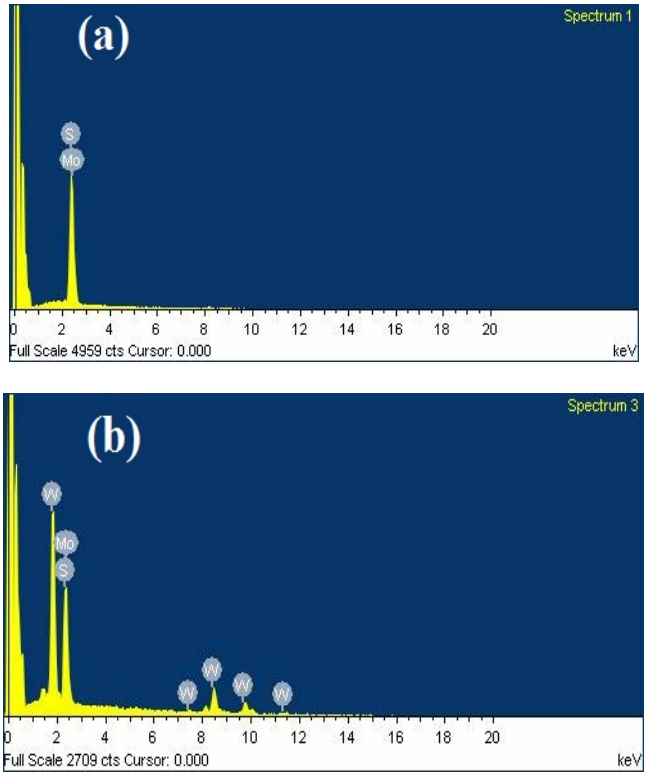

Fig. 4: EDX of (a) MoS_2, (b) Mo-W-S samples.

3.3 UV-Vis spectroscopy

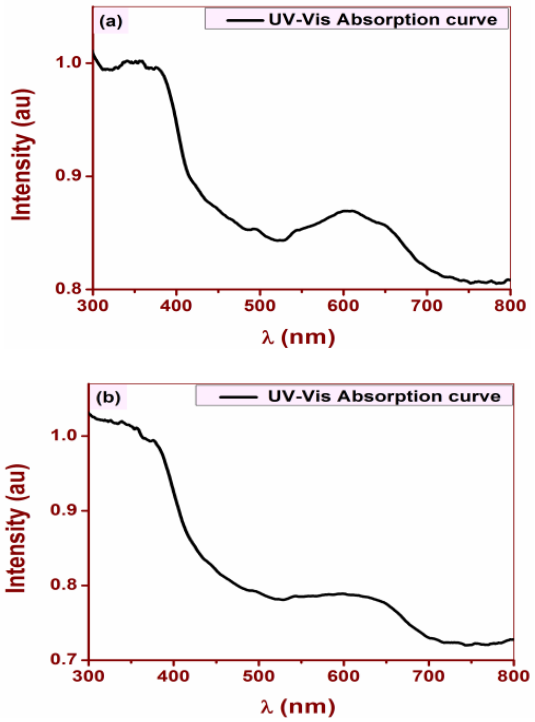

Fig. 5: UV-Vis spectra of (a) MoS_2, (b) Mo-W-S samples.

3.3.1 Kubelka Munk plot

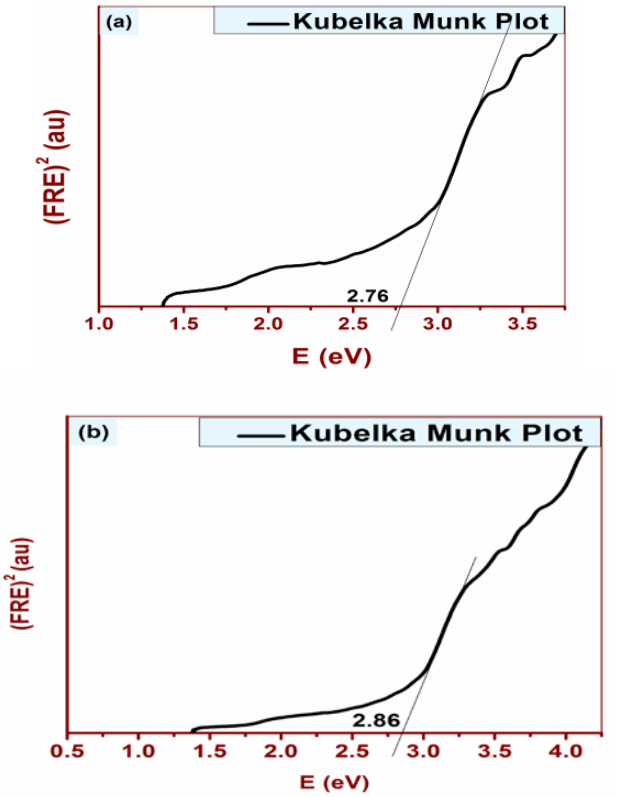

Fig. 6: Kubelka Munk plot of (a) MoS_2, (b) Mo-W-S samples.

3.4 Raman Spectroscopy

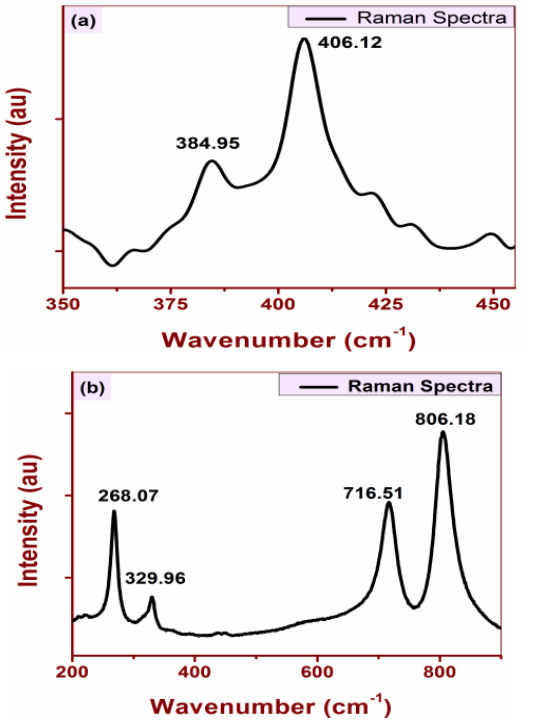

Fig. 7: Raman spectra of (a) MoS_2, (b) Mo-W-S samples.

3.5 PL Spectroscopy

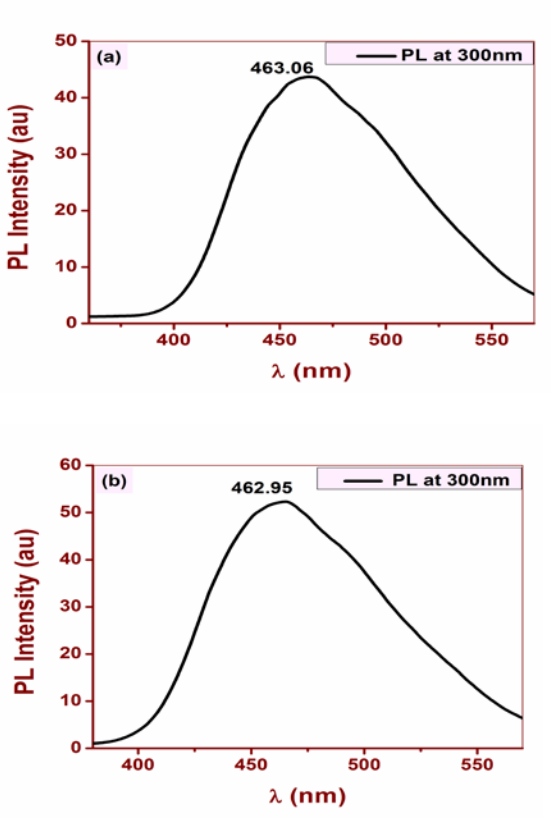

Fig. 8: PL of (a) MoS_2, (b) Mo-W-S samples.

4. RESULTS AND DISCUSSION

4.1 XRD

Comparing with 1999 JCPDS no. 75-1539, it was observed that the XRD pattern of Fig. 2(a) resembled with MoS_2 with hexagonal crystal system. The pattern 2(b) was quite different from 2(b) which indicated formation of material with different crystalline structure. The Williamson-Hall plot in Fig. 3 [10] for MoS_2 samples predicted the crystallites to be of dimension approximately 4nm. Using Scherrer's formula [**9]**

$$L = \frac{k\lambda}{\beta \cos\theta} \qquad 1$$

where λ, β, θ were wavelength of X-ray (1.5405 Å), full width at half maxima (F.W.H.M.) (in radian) of XRD peak, and corresponding Bragg's angle respectively and k was a constant equal to 0.9, the crystallite size of Mo-W-S samples were found to be approximately 23nm. The broad peaks in Fig. 2(a) showed the formation of smaller crystallite of MoS_2 while sharp peaks in Fig. 2(b) showed the formation of larger crystallites in case of Mo-W-S sample.

4.2 EDX

The EDX pattern confirmed the composition of Mo and S in Fig. 4(a) and Mo, W and S in Fig. 4(b) with Mo:W molar ratio 1:3.

4.3 UV-Vis spectroscopy

The UV-Vis absorption spectra are shown in Fig. 5. From Kubelka Munk plot in Fig. 6 we found that the optical band gap energy of MoS_2 sample and Mo-W-S sample were approximately 2.76eV and 2.88eV.

4.4 Raman Spectroscopy

The Raman spectra for as synthesized samples are shown in Fig. 7. Characteristic peaks at 384.95 and 406.12 were obtained for MoS_2 sample for E^1_{2g} and A_{1g} mode of vibration. The Raman peaks for Mo-W-S samples were significantly different from MoS_2 sample.

4.5 PL

The PL peak in Fig. 8 for MoS_2 sample was obtained at 463.06nm and that for Mo-W-S sample at 462.95nm. The Band gap energy corresponding to these PL peaks resembled with the band gap energies obtained from Kubelka Munk plot. The broadening of the peaks indicated the presence of defect states in the material as well as thermal excitation.

5. CONCLUSIONS

Optical emission properties and chemical composition of Semiconductor *dichalcogenide materials* were studied. MoS_2 derivative with Tungsten having Mo-W molar ratio 1:3 was found to be large band gap semiconductor which could be a promising material for power electronics devices. Also strong blue PL emission near 463nm indicated the material's good applicability in luminescence devices. Further detailed morphology study of the derivatives is needed.

6. ACKNOWLEDGEMENT

The authors gratefully acknowledge the help of SAIC and dept. of Physics Tezpur University.

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