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AN INVESTIGATION ON THE MORPHOLOGICAL EFFECT ON THE ELECTRO-OPTICAL PROPERTIES OF MoS_2 FLAKES AS A COUNTER ELECTRODE FOR Pt-FREE DYE-SENSITIZED SOLAR CELLS

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Abstract: The effective reduction and regeneration triiodide/iodide (I_3^-/I^-) redox couple are important for an efficient Dye Sensitized Solar Cell (DSSC) that is ruled by the properties of the counter electrode (CE). Among the non-noble metal electro catalysts, transition metal dichalcogenide, molybdenum disulphide has been identified as a low cost and efficient platinum free potential counter electrode material for Dye Sensitized Solar Cells (DSSCs). The present work reports, the morphological effect of MoS_2 nanoflakes via convenient hydrothermal method. The physical and chemical properties of the as-synthesized samples were characterized using different analytical tools. From the morphological studies, it is observed that the nano flakes have a layered planar structure with smooth surfaces which benefit the enhancement of electrochemical activity. The UV-diffuse reflectance spectrum confirms the band structure transition due to the quantum confinement effect of MoS_2. The photoconductivity studies revealed that there is a linear increase of current in the dark and visible light-illuminated MoS_2 nanoflakes with increase in the applied field. Thus, the improved photoconductive and interesting behavior of MoS_2 nanoflakes validates it as a promising counter electrode for DSSCs.

Keywords: DSSCs, MoS_2, Nanoflakes, Counter electrode, Transition metal dichalcogenide.

1. Introduction:

Counter electrode, a key component in DSSCs, is mainly used as a catalyst to reduce the oxidized species of the redox couple, in Dye-Sensitized Solar Cells [1]. Generally, platinum is the most preferred counter electrode material for DSSCs because of its best electro catalytic activity towards I_{3-} reduction [2, 3]. However, platinum is not suitable for mass production owing to its high cost. Therefore, much effort has been taken to replace and explore platinum free materials as counter electrodes in DSSCs [4]. Among the inorganic materials such as transition metal sulphides, nitrides, [5] and oxides, transition metal sulphides are gaining much interest as counter electrode in DSSCs [6]. MoS_2, molybdenum disulphide is one of the transition metal dichalcogenide with layered structure naturally occurring as molybdenite [7]. Among the various morphologies explored previously, nanoflakes have much scope that might revolutionize solar energy conversion upto 30% which is almost twice that of the present day's conversion. In the present work, we elucidate the formation of nanoflakes MoS_2 by a solution-based hydrothermal method.

2. Experimental Procedure

The preparation process involved the dissolution of ammonium heptamolybdate tetrahydrate in deionized water. Then Thiourea and cetyl trimethylammonium bromide were added to deionized water in two separate beakers. Then the mixture was poured into the solution of ammonium heptamolybdate tetrahydrate and was mixed thoroughly by stirring. The as-obtained solution mixture was then transferred to a stainless steel Teflon liner autoclave for hydrothermal treatment. The greenish black colored precipitates were washed and collected by filtration.

3. Characterization

The UV–Vis absorption spectrum of the sample was recorded in the wavelength range of 200 to 800 nm (Perkin Elmer UV Win Lab 6.0.3.0730 / 1.61.00 Lambda 650). Morphologies of the as-synthesized nanoparticles were observed using FEI quanta 200 FEG Field Emission Scanning Electron Microscopy (FESEM). The Field-dependent dark and photoconductivity studies were carried out using Keithley picoammeter 6485. The experimental setup for the measurement of field-dependent dark and photoconductivity is as used by Ponniah and Xavier [8]

4. Results and Discussion

4.1 Morphological and Elemental Analysis

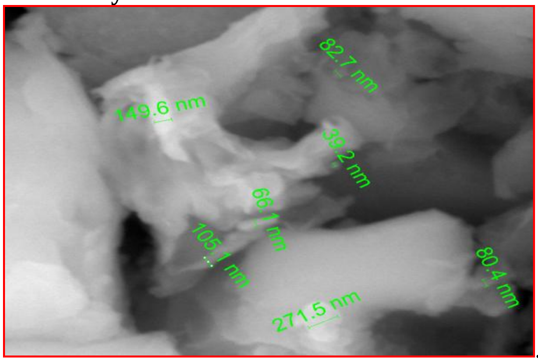
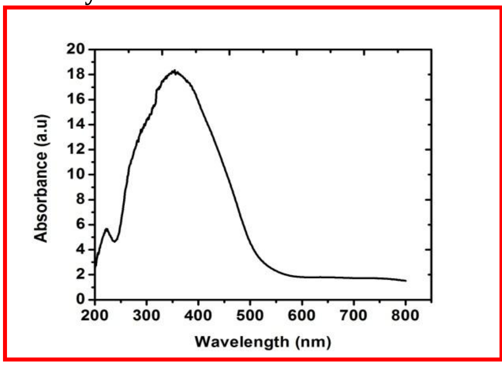


Fig.2 SEM micrograph of MoS_2 nanoflakes.

From the SEM micrograph (Fig.2) it is observed that the as-synthesized MoS_2 nanoflakes are formed with smooth surfaces and the thickness ranges from 39-271nm [9]. The nanoflakes have a layered planar structure due to the well-known Van der Wall interactions and the centre of gravity that facilitates the nanoflakes to align themselves as layers [10].

4.2 Optical Analysis



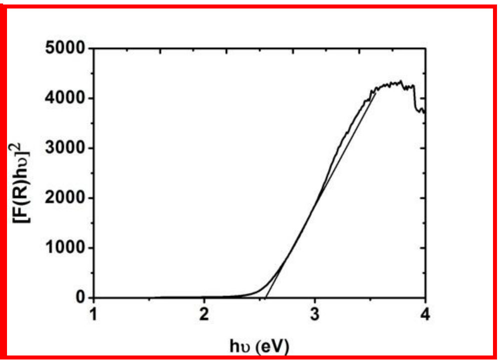


Fig. 3a UV-Vis absorption spectrum **Fig.3b Kubelka-Munk function versus photon energy**

UV-Vis absorption spectrum (Fig. 3a) shows that the MoS_2 nanoflakes have a strong optical absorption peak at 395nm which is almost nearer to the visible region, and hence, the absorption tends to decrease exponentially as the wavelength increases. This decrease in the absorption indicates the increase in band gap (2.6eV) compared to its bulk counterpart (1.29eV). From the optical absorption edge, the band gap calculated using Kubelka-Munk function (Fig. 3c) was estimated to be approximately 2.6eV. Compared to 1.29eV of bulk, a blue shift of 1.31eV in the band gap was observed for the MoS_2 nanoflakes which could be ascribed to the quantum confinement effect originated from the structural modification of MoS_2 nanoparticles to nanoflakes [11]. This property of MoS_2 portrays it to be a good candidate for photovoltaic and photo catalytic applications, due to its strong absorption in the solar spectral range [12].

4.3 Photoconductivity Studies

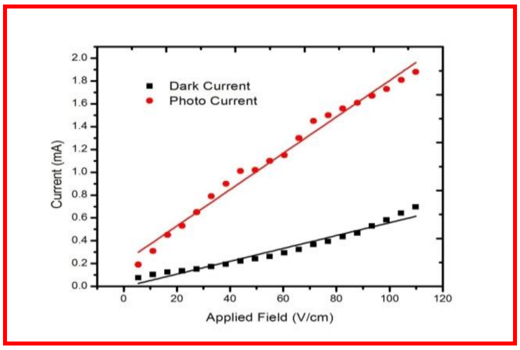


Fig.4 Field dependent conductivity plots of MoS_2 nanoflakes

In Fig.4 the plots indicate that with increase in the applied field there is a linear increase of current in the dark and visible light-illuminated MoS_2 depicting the ohmic nature [13]. It is also observed that the photocurrent is found to be significantly greater than the dark current by about ~ 4 folds for a fixed field of 50 V/cm. The improved photoconductive nature of MoS_2 nanoflakes besides promoting them as a promising counter electrode material for DSSCs also paves way for the potential use of novel nanostructures in high-performance opto-electronic devices.

5. Conclusions

The structure and morphology analysis of MoS_2 nano flakes synthesized through hydrothermal process has been carried out to probe the electro-optical properties of MoS_2 nano flakes. The optical analysis established the band structure transition due to the quantum confinement effect of MoS_2. The morphological studies revealed that MoS_2 nanoflakes have a layered planar structure with smooth surfaces which benefits the enhancement of electrochemical activity and the thickness ranging from 39-271nm. Electro-optical studies revealed that the photocurrent is found to be significantly greater than the dark current. Thus the improved photoconductive and interesting behaviors of MoS_2 nanoflakes can pave way for the potential uses of novel nanostructures in high-performance optoelectronic devices.

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