Thesis Title: Optical and Electrical Properties of Polycrystalline MoS_2 and its Application in Energy Harvesting

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Abstract

Layered transition metal dichalcogenides (TMDCs) has attracted wide attraction because of its exceptional layer dependent properties. The layered TMDCs covers a wide range of electronic materials, i.e. superconducting, semiconducting and insulating. Among TMDCs, MoS_2 has gained huge research interest because of its non-toxicity and high stability in ambient. Although, the layer dependent optical, and electrical properties of layered MoS_2 has been explored, but the properties of polycrystalline MoS_2 has been scarcely analysed. The present work focuses on the investigation of optical properties of polycrystalline MoS_2 and their application in photoelectrochemical water splitting and thermoelectric power generation.

The polycrystalline MoS_2 has been synthesised by the hydrothermal method, further thin films of polycrystalline MoS_2 is deposited on the quartz and SiO_2/Si substrate by spray coating of MoS_2 ink. The MoS_2 ink is prepared by dispersing MoS_2 powder in the ethanol under the vigorous mixing. The optical properties such as index of refraction and extinction coefficient has been analysed with the variable angle spectroscopic ellipsometry. Though the bandgap and bandedge positions of MoS_2 is suitable for photoanode in photoelectrochemical water splitting, but its low electrical conductivity limits its practical applications. In order to improve its electrical conductivity, a nanocomposite of secondary phase incorporated MoS_2 (Mo_2S_3/MoS_2) is synthesised. The incorporation of conducting secondary phase in MoS_2 matrix enhances its photo-current density in the photoelectrochemical water splitting enhances up to ~2 times. This

attribute to the lower in charge transfer resistance, analysed with EIS, and it reduced to ~4.76 kΩ for Mo_2S_3/MoS_2 nanocomposite as compared to ~7.31 kΩ for pristine MoS_2.

Moreover, the layered MoS_2 possess low thermal conductivity, which can be further useful for thermoelectric power generation. In the present work, a ∼70 times enhancement in the electrical conductivity is observed for the secondary phase (Mo_2S_3) incorporated MoS_2 nanocomposite sample. The barrier height between two adjacent grains is reduced from ~149 meV (MoS_2-MoS_2) to 72 meV (Mo_2S_3-MoS_2) for Mo_2S_3/MoS_2 nanocomposite sample, which further enhances the electrical conductivity and simultaneously enhances the Seebeck coefficient, due to low energy carrier filtering. The reduction in thermal conductivity of MoS_2 in the presence of Mo_2S_3 is due to more phonon scattering at the interfaces in Mo_2S_3–MoS_2 nanocomposite sample.