

Growth and Characterization of α -MoO₃ thin films grown by spray pyrolysis technique

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Abstract. Molybdenum trioxide (MoO₃) is a substitute for the commonly used hole transport material PEDOT: PSS in organic photovoltaics (OPVs) because of its high stability and large carrier mobility and can be easily deposited through simple solution processed techniques. Here we report that spray deposition of MoO₃ thin films yielded a combination of three phases: monoclinic, hexagonal and orthorhombic at low temperatures and a pure orthorhombic phase (α -MoO₃) is obtained at 425°C is confirmed from the XRD measurements. Raman measurements confirmed the different vibration modes corresponding to MoO₃ nanostructures. Morphology and composition of the samples were studied through FESEM and EDAX measurements. FESEM images show an elongated structure of the MoO₃ nanostructures and EDAX confirms the presence of molybdenum and oxygen without the presence of any impurities. From UV-Vis transmission spectra, the band gap of the samples synthesized at different temperatures were found to be in the range of (2.84 – 3.15) eV. The fluorescent properties of the synthesized samples were studied from the room temperature photoluminescence (PL) measurements.

INTRODUCTION

Solar radiation is one of the most attractive and reliable renewable source of energy. The direct conversion of solar radiation into electricity reduced the environmental impacts and provided significant benefits over other conventional energy sources. The full exploitation of solar energy still remains a challenge due to the high cost required for this technology and employed materials such as silicon and their low conversion yield. In order to overcome these drawbacks scientists have carried out research on organic photovoltaic devices which can be prepared at low cost. Despite the low cost, they suffer from low power conversion efficiency compared to inorganic semiconducting solar cells which can be resolved by using various organic and inorganic buffer layers in organic solar cells (OSCs).¹ A typical organic solar cell structure includes a transparent electrode namely, ITO and a hole transport layer (HTL). Commonly used organic hole transport layers like PEDOT: PSS is hygroscopic in nature and cause etching of ITO electrode on glass.² Inorganic interfacial layers like MoO₃, V₂O₅, NiO etc have been employed as alternatives to PEDOT: PSS thus increasing the stability and performance of organic solar cells and these materials can be easily deposited through simple solution processed techniques.³ Among these, molybdenum trioxide (MoO₃) is found to be more stable on ITO surface and it facilitates effective charge transport between metal electrodes and active layer.⁴ These metal-oxide incorporated devices exhibit long life span and allow the fabrication of cost effective solar cells.

Molybdenum trioxide mainly crystallizes into three forms orthorhombic, hexagonal and monoclinic with later two forms being metastable. The orthorhombic form (α -MoO₃) is a promising oxide with structural anisotropy⁵ exhibiting a layered structure. Among the other transition metal oxides, MoO₃ exhibits interesting structural, chemical, electrical, and optical properties. It is a wide band gap semiconductor with potential applications in the fabrication of organic solar cells (OSCs).⁶ Precursors for the synthesis of MoO₃ can be easily dissolved in different