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Spectroscopic and Structural Properties of Yb^{3+}-Doped and Undoped 2D-MoS_2 Thin Films for Optoelectronic and Photonic Device Applications

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Molybdenum disulphide (MoS_2) has layered structure and is classed as a transition metal-disulphide (TMD) material. Recently it has drawn significant attention for exploring optoelectronic and photonic properties on sub-nanometre scale, with a potential for accessing quantum interactions [1]. The electronic structure and stoichiometry of TMDs make them distinguishable from the metallic graphene, as the TMDs depict a clear bandgap, as in compound semiconductors [2], which is quite attractive for device engineering and applications in photovoltaic, energy storage, and bandgap engineered light-sources [3]. In this research, the fabrication of undoped and Yb^{3+}-ion doped MoS_2 nanometre (nm)-scale thin films are discussed using femto-second pulsed laser deposition (fs-PLD) and the structural and spectroscopic properties of fs-PLD are compared with liquid-phase epitaxy grown undoped MoS_2 films. Such a comparative analysis may offer materials fabrication platform in future for engineering optoelectronic and photonic devices on silica glass and silicon platforms.

The structural characterisations of two types of MoS_2 thin films were analysed using Raman (in Fig. 1a), FTIR, UV-visible, and X-ray photoelectron spectroscopic, atomic force and transmission electron microscopic techniques (Fig.1b). The electronic structure of molybdenum disulfide (MoS_2) was analysed through the first priciples calculations using density functional theory (DFT) using CASTEP code. Fig.1c shows the band structure of bulk and monolayer MoS_2. DFT is known to significantly underestimate the band gap in materials, We have, therefore, used a recent computationally intensive hybrid functional (HSE06) code, which is able to predict the band gap accurately. Bulk MoS_2 was geometry optimised (dispersion corrected TS-PBE functional) giving a=3.159 Å (-0.1%) and c=12.071 Å (-1.8%). A monolayer of MoS_2 was modelled using a supercell with an interplanar (vacuum) distance of 15 Å to avoid interactions between adjacent sheets. DFT calculations accurately predict the expected increase in the band gap from bulk MoS_2 (1.26 eV indirect) to monolayer MoS_2 (1.99 eV indirect, ~2.2 eV direct). Indirect bandgap of monolayer MoS_2 lies between point Γ to Γ-K in first Brillouin zone, while the direct band gap lies in point –K. The indirect to direct bandgap transition observed in MoS_2 when shifted from bulk to monolayer is due to the quantum confinement effects [4].

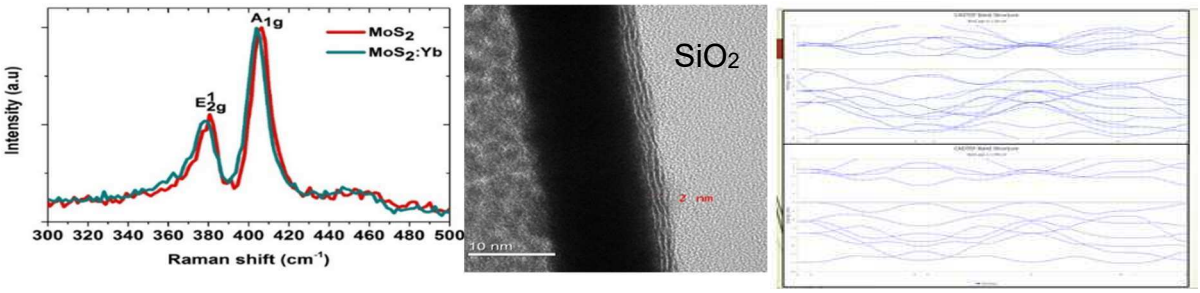

Figure 1. a) Raman spectroscopic data for Yb^{3+}-doped and undoped MoS_2, b) a TEM image of 2 nm thick cross-section of MoS_2 deposited on silica substrate via fs-PLD, c) electronic band structure diagram for bulk and monolayer MoS_2.

We have also investigated the nonlinear optical properties of doped and undoped MoS_2 films using open aperture Z-scan technique, which utilised a 532 nm laser source (frequency doubled YAG) with 7 ns pulse duration and 10Hz repetition rate. In case of Yb^{3+} doped films, the enhancement in saturable absorption (SA) at room temperature was observed, which may be utilized for applications in nano-scale photonic devices such as passive mode locking and optical switching. The results presented herein provide an important fundamental insight into the nonlinear optical response and are of crucial importance in designing and engineering novel multifunctional rare-earth doped 2D materials, which may be controlled and optimized during fabrication for device engineering.

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References:

[1]. F. Bonaccorso, Z. Sun, T. Hasan, A. C. Ferrari, "Graphene photonics and optoelectronics" Nature Photonics 4, 611-622 (2010).
[2]. S. Manzeli, D. Ovchinnikov, D. Pasquier, O. V. Yazyev, A. Kis, "2D transition metal dichalcogenides" Nat. Rev. Mat. 2, 17033 (2017).
[3]. Kin Fak Mak, Jie Shan, "Photonics and optoelectronics of 2D semiconductor transition metal dichalcogenides", Nature Photonics, 10, 216-226 (2016).
[4]. M. Chhowalla, H. S. Shun, G. Eda, L. J. Li, K. P. Loh, H. Zhang. "The chemistry of two-dimensional transition metal dichalcogenides nanosheets" Nature Chemistry 5, 263-275 (2013).