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Physical characterization of spin-coated MoS_2 films

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Abstract

In the field of Transition Metal Dichalcogenides (TMDCs), molybdenum disulfide (MoS_2) has attracted an outstanding interest thanks to several applications. MoS_2 has potentialities not yet fully realized in solution-based applications. However, the lack of knowledge of the optical properties of MoS_2, especially in the infrared range, has significantly limited his use in many exciting photonic fields.

In this work, the broadband optical properties of MoS_2 films deposited by spin-coating onto Si/SiO_2 substrates were studied by means of Variable Angle Spectroscopic Ellipsometry (VASE).

The morphological and the structural properties of the samples were investigated by Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM) and Micro-Raman Spectroscopy.

Micro-Raman spectroscopy measurements reveal the presence of 2H-MoS_2 and 1T-MoS_2 phases. The optical properties of the films show a mid-gap state at~ 0.6 eV, not reported in an ellipsometry work before, induced by defects in the MoS_2 samples.

Methods and materials

- The commercial aqueous solution of MoS_2 dispersion 0.1-0.5 mg in H_2O, which was obtained by solution-based exfoliation methods, was bought from Sigma Aldrich.
- MoS_2 films were reproducibly prepared by spin-coating the solution onto Si/SiO_2 substrates (SiO_2 thickness of ∼ 2 nm). The results are reported on samples prepared at 6000 rpm spin coating speed and 60 s as deposition time.
- SEM analysis was accomplished with a FEI Quanta FEG 400 F7 eSEM microscope.
- Tapping mode AFM images were obtained in ambient conditions with a Multimode 8 equipped with a Nanoscope V controller (Bruker Instruments).
- Micro-Raman spectra were collected by using a Horiba-Jobin Yvon microprobe apparatus (spectral resolution ∼2 cm^{-1}).
- Spectra of the ellipsometric angles ψ and Δ were acquired using a V-Vase (Woollam Co.) ellipsometer in the [0.38 -3.5] eV photon energy range at 65°, 70°, 75° incident angles at room temperature.

SEM and AFM measurements

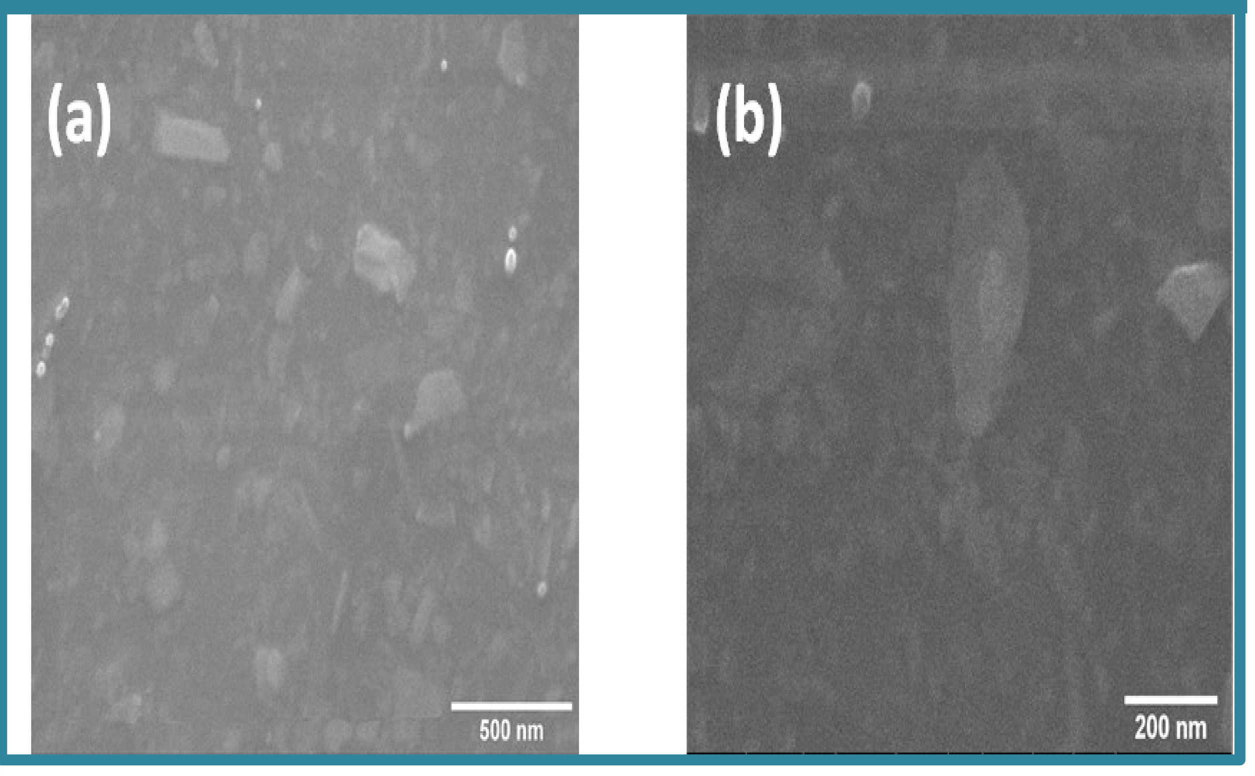

Fig.1: SEM image of spin-coated MoS_2 films onto Si/SiO_2 substrates (a) and its magnification (b).

- High resolution AFM imaging highlights the presence of a layered structure. The thickness of each layer is estimated to be (13±2) nm, as it is reported in the line profile.

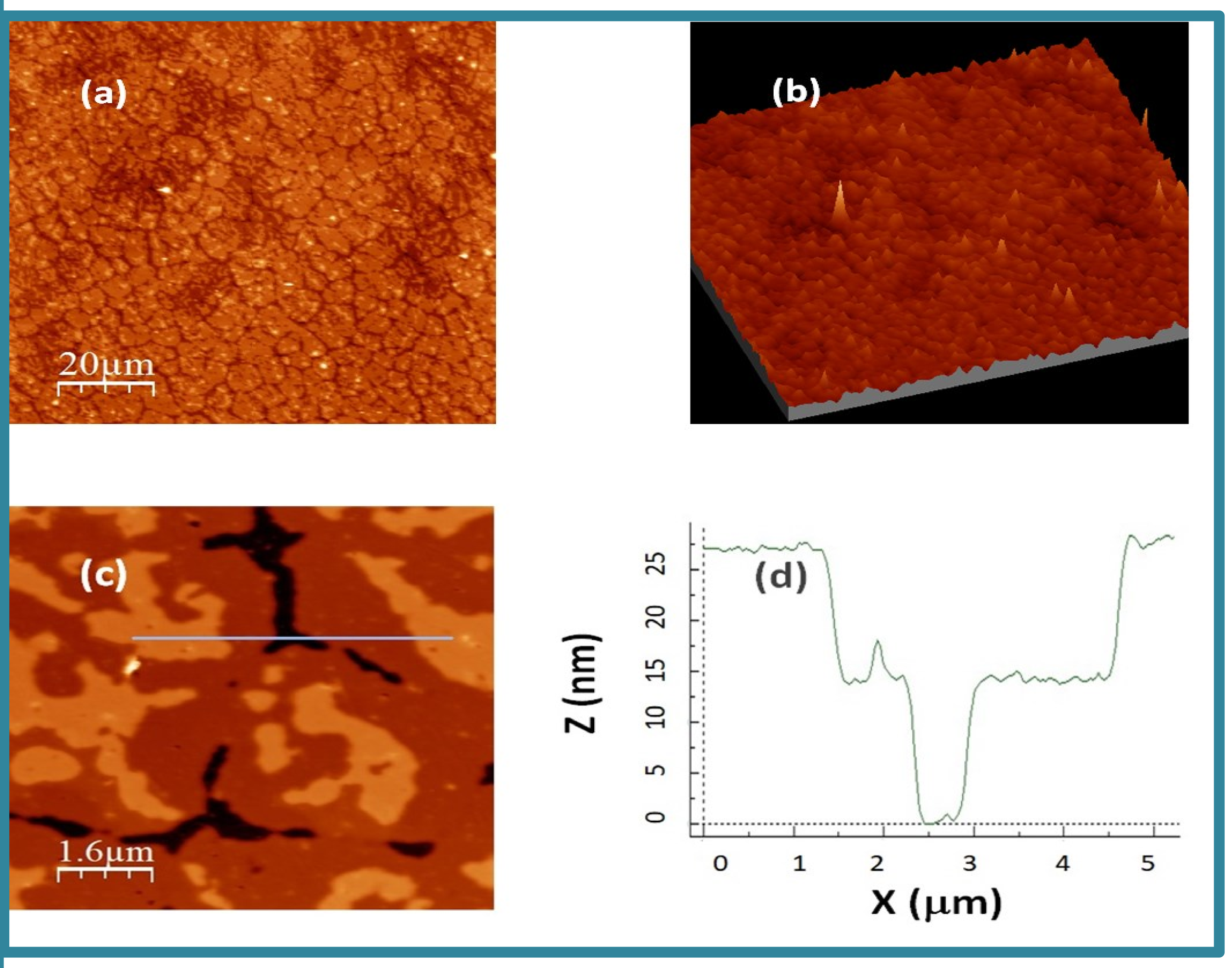

Fig.2: AFM surface images of spin-coated MoS_2 films onto Si/SiO_2 substrates acquired on a 100x100 mm^2 area in a 2D (a) and 3D (b) representation. Image acquired on an 8x8 mm^2 area (c) and profile along the cyan line (d).

Micro-Raman spectroscopy measurements

- As it can be seen in Fig. 3 (a), the Raman modes E^1_{2g} and A_{1g} are present , which fall at about 380 cm^{-1} and 405 cm^{-1}, respectively [1]. Such findings indicate that Fig. 3 (a) has been collected on 2H-MoS_2.
- In Fig. 3 (b), in addition to the bands seen in Fig. 3 (a), the bands at about 290 cm^{-1} and 299 cm^{-1} are clearly detectable. In particular, the mode at 299 cm^{-1} is associated to 1T-MoS_2 [2], while the band at 290 cm^{-1} is assigned to the amorphous phase of MoS_2 [3]. These two modes are assigned to E_{1g}. The detectability of the E_{1g} mode, even in back scattering geometry, is ascribed to the disorder of the amorphous phase.

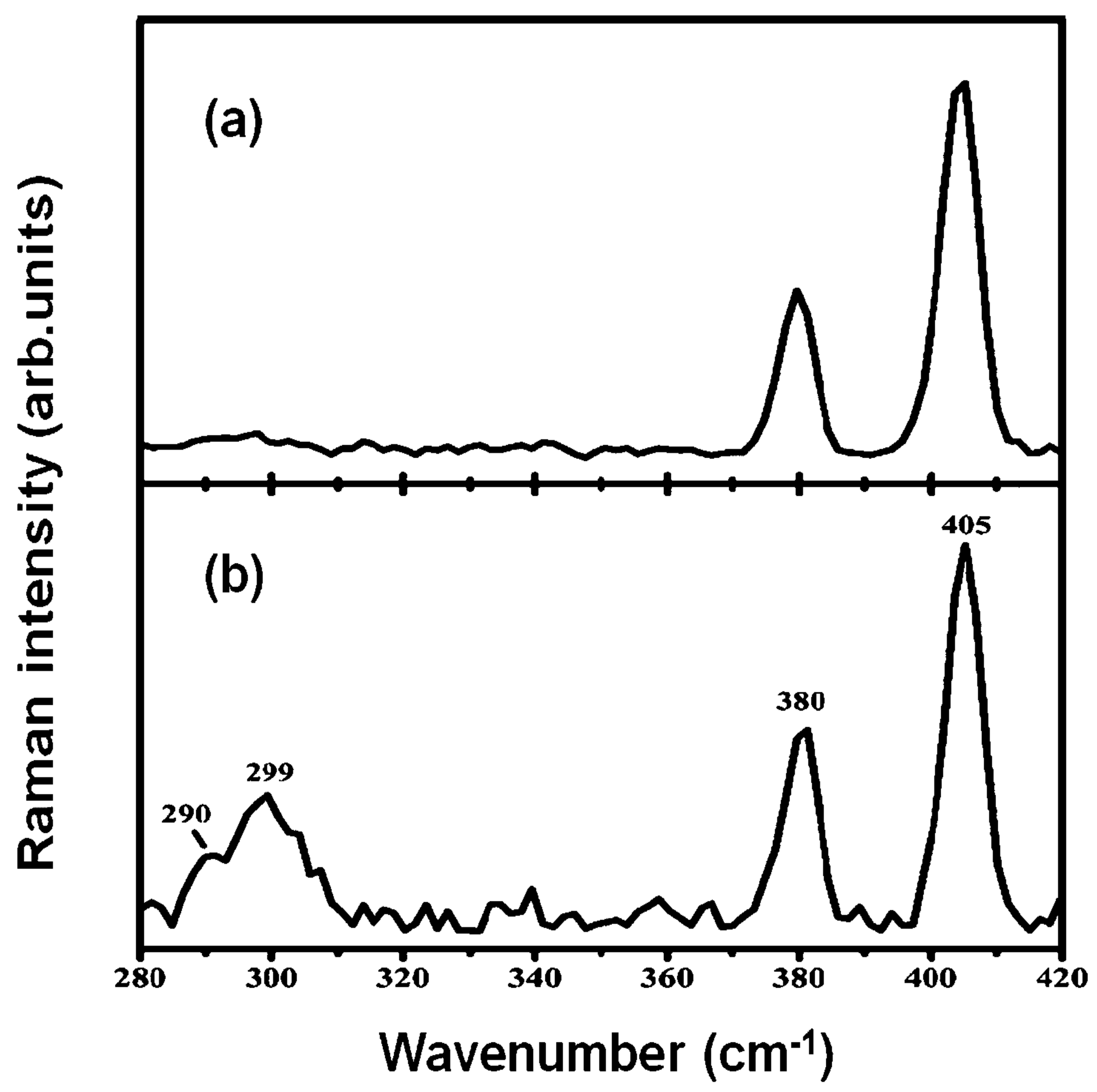

Fig. 3: Representative Micro-Raman spectra collected on MoS_2 films spin-coated onto Si/SiO_2 substrates; 2H-MoS_2 phase (a) and 1T-MoS_2 phase (b).

VASE measurements

- The dielectric response of MoS_2 films on Si/SiO_2 substrates was described using a combination of seven Lorentz oscillators [4].
- The oscillator energies at 1.87 eV, 2.05 eV, 2.81 eV and 3.1 eV are related with the A- , B-, C -,D-exciton peaks, respectively.
- The oscillator at 2.4 eV could be related to second excited states of the excitons forming A-peak while the oscillator energy at ∼1.78 eV could be assigned to the energy of defect-induced photoluminescence.
- The oscillator at ∼ 0.6 eV could be related to the fact that the presence of crystalline defects in MoS_2 samples, such as sulfur vacancies, may induce localized mid-gap states that have the potential to modify the electronic structure of the systems [5].
- The obtained MoS_2 films have a lower index of refraction in comparison to previous studies [6].

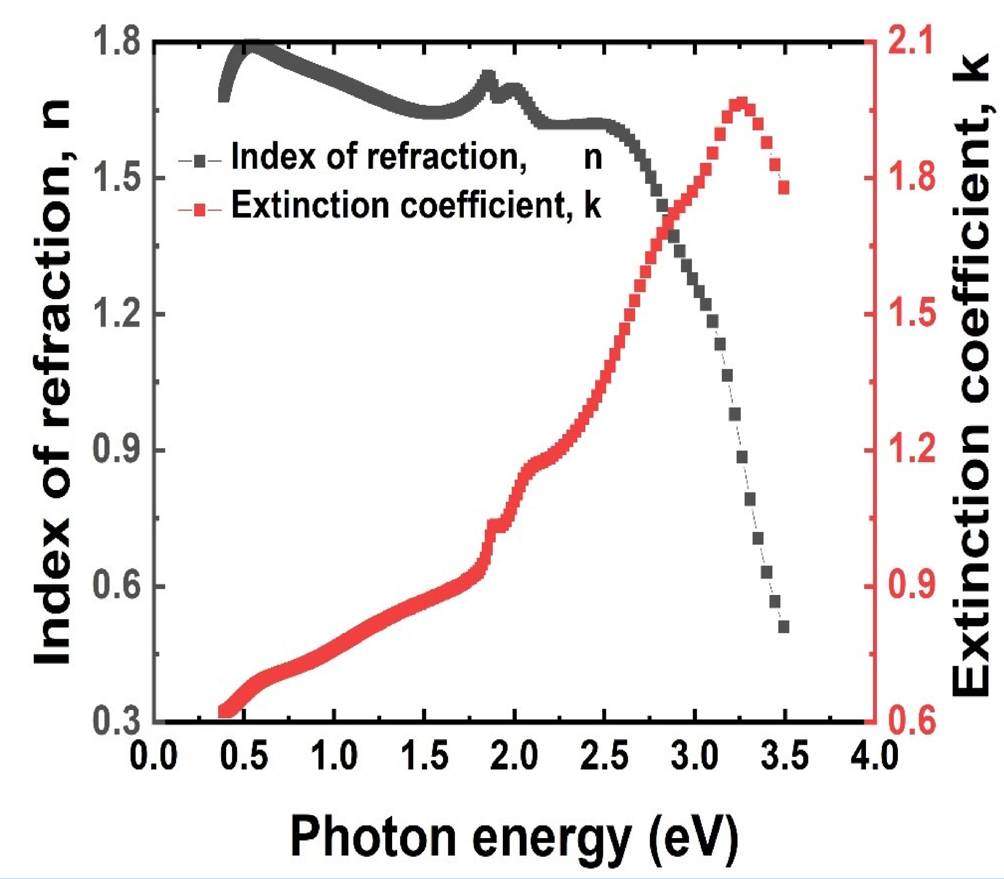

Fig. 4: Estimated dispersion laws of MoS_2 films spin-coated onto Si/SiO_2 substrates by VASE characterization.

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