# Variable angle spectroscopic ellipsometry 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

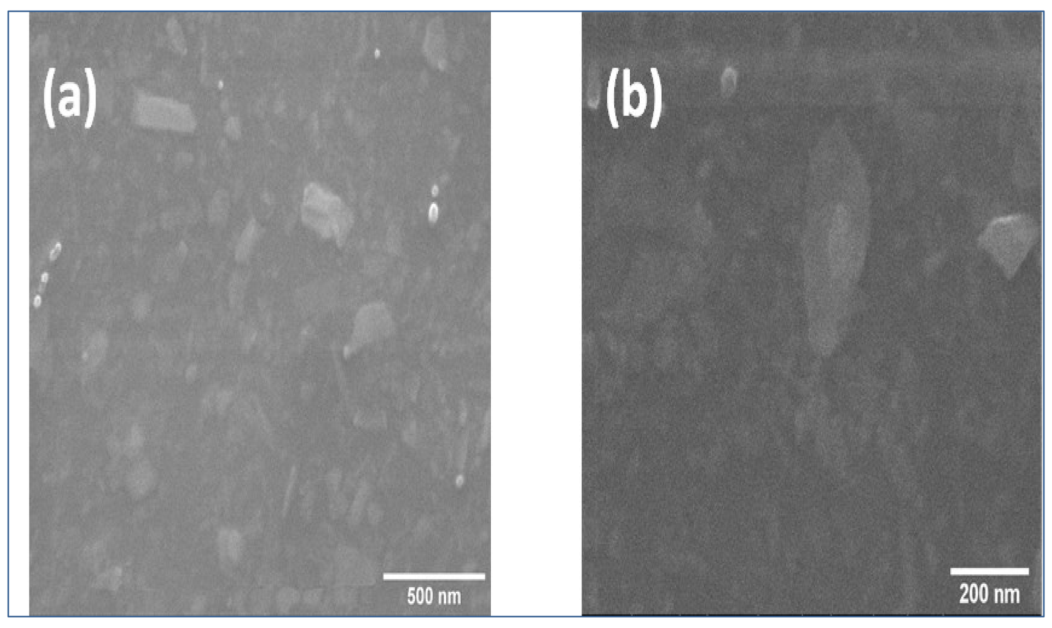


Fig.1: SEM image of spin-coated $MoS_2$ films onto $Si/SiO_2$ substrates (a) and its magnification (b).

- 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.

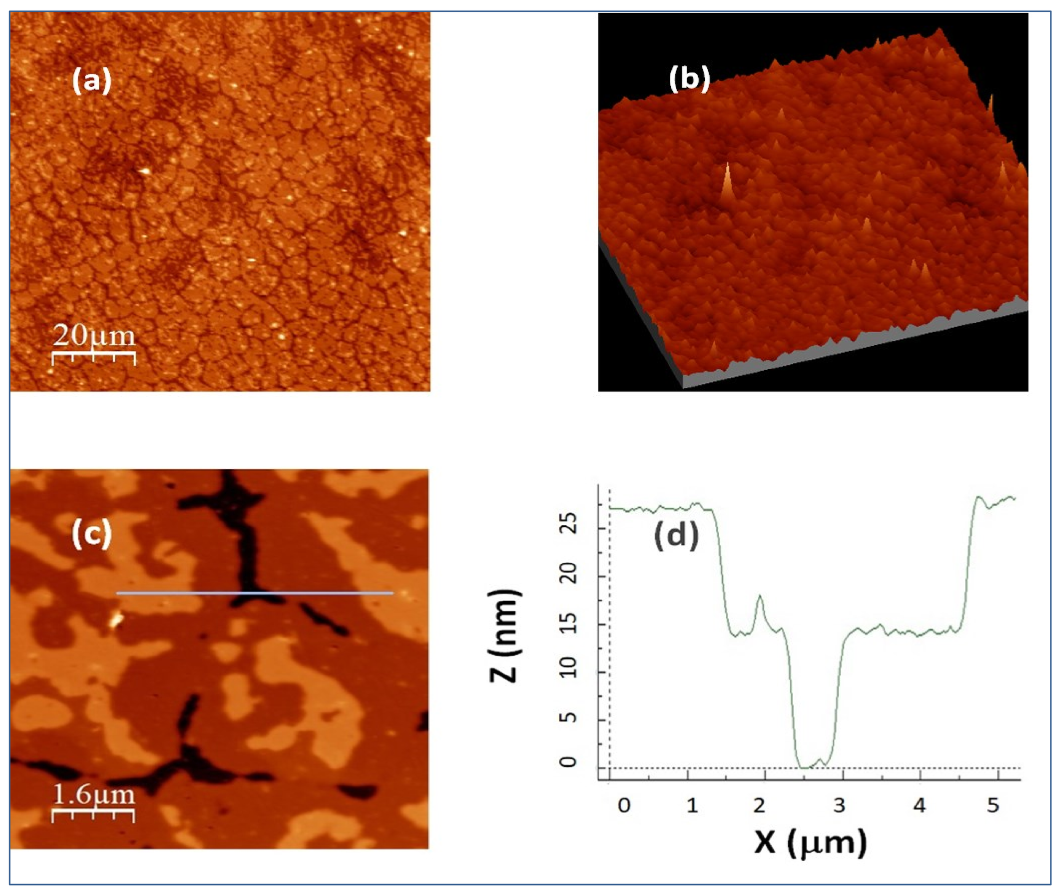


Fig.2: AFM surface images of spin-coated $MoS_2$ films onto $Si/SiO_2$ substrates acquired on a 100x100 $mm^2$ area in a 2D (a) and 3D (b) representation. Image acquired on an 8x8 $mm^2$ area (c) and profile along the cyan line (d).

## 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.

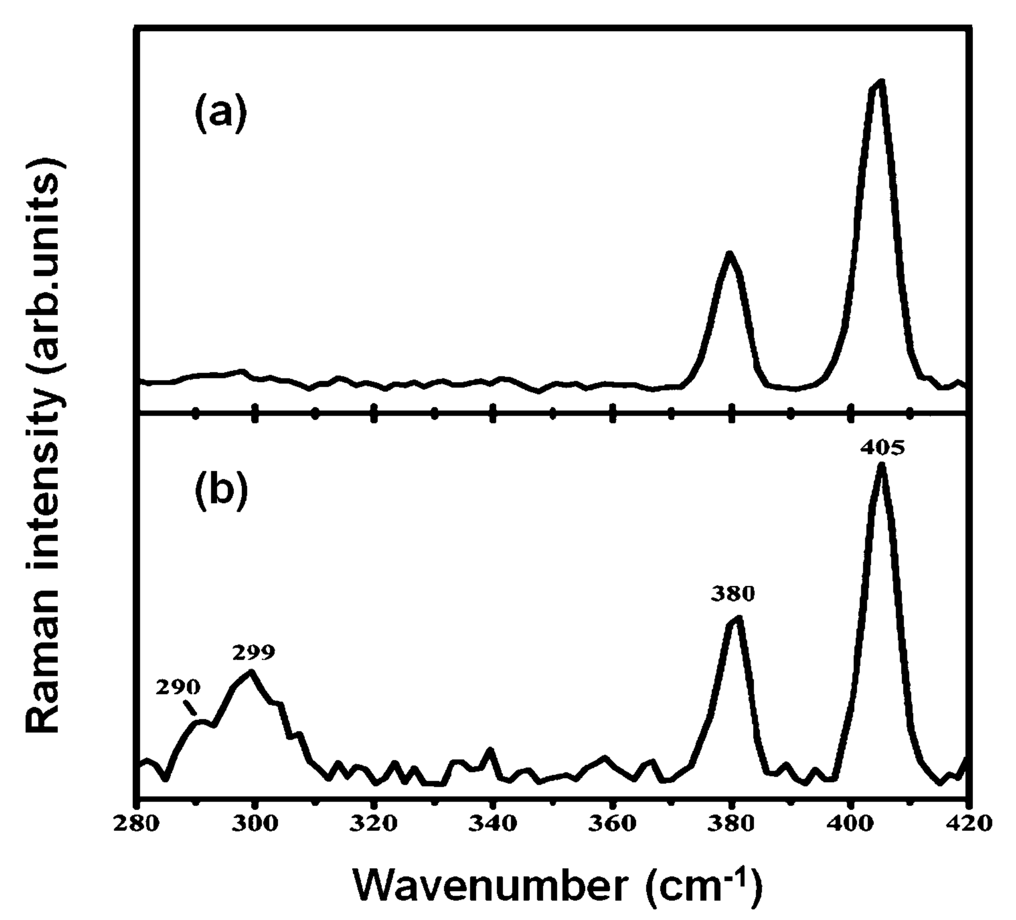


Fig. 3: Representative Micro-Raman spectra collected on $MoS_2$ films spin-coated onto $Si/SiO_2$ substrates; 2H-$MoS_2$ phase (a) and 1T-$MoS_2$ phase (b).

## 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].

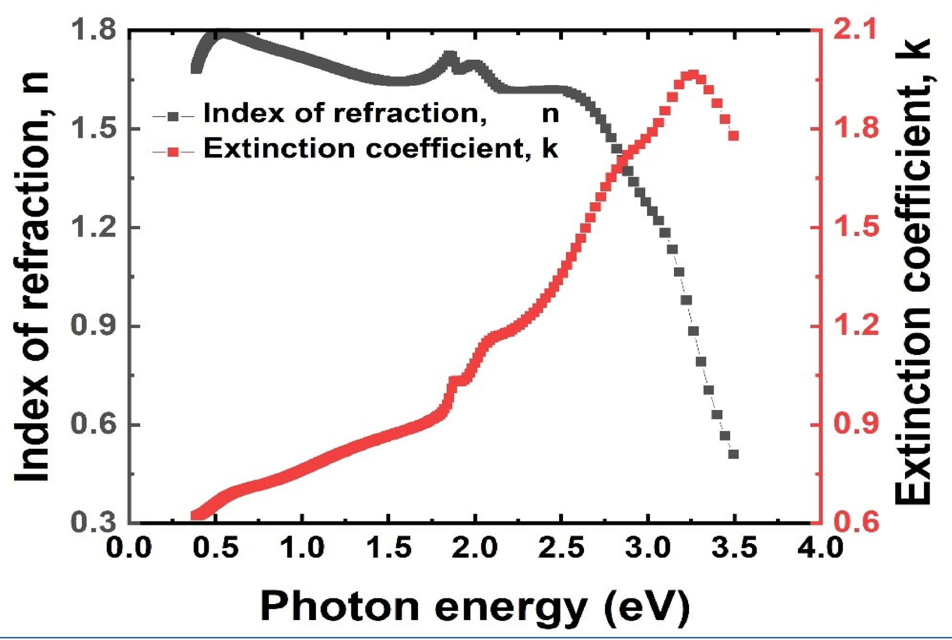


Fig. 4: Estimated dispersion laws of $MoS_2$ films spin-coated onto $Si/SiO_2$ substrates by VASE characterization.

## Conclusions

- $MoS_2$ films were prepared by spin-coating an aqueous solution onto $Si/SiO_2$ substrates ($SiO_2$ thickness of ~2 nm).
- The morphological and the structural properties of the samples were investigated by SEM, AFM and Micro-Raman Spectroscopy.
- Micro-Raman measurements reveal that there is the coexistence of both 2H-$MoS_2$ and 1T-$MoS_2$ phases, which could be useful for electrical applications.
- The optical properties of $MoS_2$ films were studied by VASE. Dielectric response of $MoS_2$ films was described with Lorentz dispersion model.
- The oscillator energy at ~0.6 eV may be related to a mid-gap state originating from intrinsic point defects that are present due to the disorder of the amorphous phase.

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