Characterization of 2D α-MoO_3 microcrystals deposited by pulsed laser deposition based process

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INTRODUCTION

2D-Transition Metal oxides (TMOs), although less studied than the well-known 2D transition metal dichalcogenides(2D-TMCs) are appealing due to some specific advantages. Like the TMCs they are semiconductors, however they are less contaminant and offer a large potential for tuning their electro-optical properties by varying their stoichiometry. In particular, MoO_3 is transparent and shows a wide bandgap (>3 eV) and a high dielectric constant k ~ 500.

Additionally, orthorhombic α-MoO_3 possesses the well-known layered crystal structure of MoO_3 which offers the possibility to create two dimensional (2D) morphologies (de Castro et al., 2020). In this context, 2D MoO_3 has shown extraordinary properties such as anisotropic polariton propagation (Ma et al, 2019) and is an ideal material for electronic applications for high power electronics and short wavelength optoelectronics.

DEPOSITION AND CRYSTALLIZATION

Currently, most of the work in 2D-semiconductors is still made using small flakes obtained from mechanically cleaved single crystals, however there is no doubt that it will be advantageous to deposit large 2D-strucutres as this will have tremendous impact both for the manipulation and integration of these materials (Kim et al, 2019).

In context we show the successful preparation of nanometer thick thin films formed by 2D MoO_3 crystals by a pulsed laser deposition-based process that starts with the deposition in vacuum from a MoO_3 target of dense, amorphous and continuous substoichimetric MoO_{3-X} layers. Subsequently, the films are annealed in air up to 300ºC while *in-situ* following the evolution of their optical properties in the UV-VIS wavelength region by spectroscopic ellipsometry.

CHARACTERIZATION

When the temperature reaches 250ºC, a clear change in the optical properties starts which is related to the films crystallization. Analysis of the optical properties shows how the initially absorbing films with a metallic-like behavior after the annealing become transparent in the NIR and VIS regions, and shows a band gap >3 eV. This optical change is related to the formation of large rectangular micron size α-MoO_3 single crystals with a thickness of the order 10 nm, easily observable by optical microscopy. A full characterization of the morphology, structure and stoichiometry has been confirmed by X-ray diffraction analysis, Raman spectroscopy (Fig. 1), atomic force microscopy (AFM) and transmission electron microscopy. We will show the distinct features of the measured dielectric constant of the 2D MoO_3 microcrystals and compare them to that of the bulk in terms of defects and lattice stress. Finally, we analyze the implications for different optoelectronic applications.

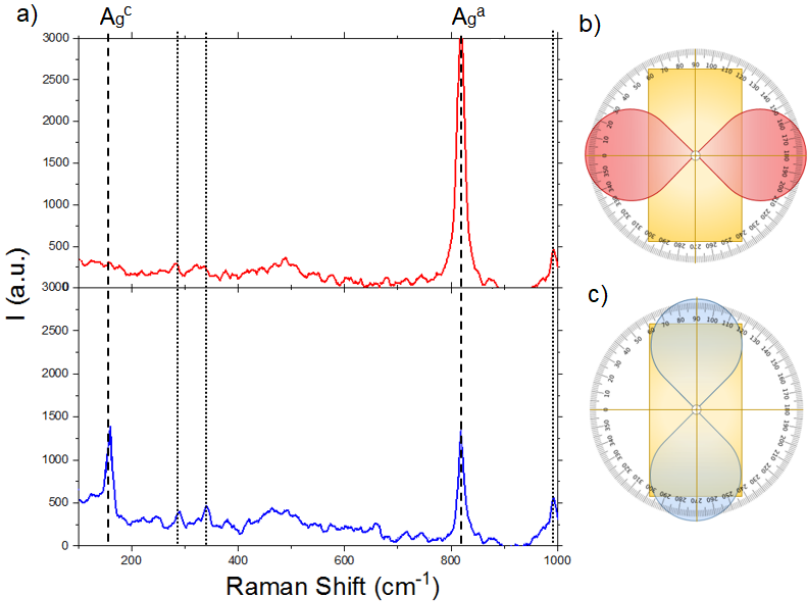

Fig 1*. Changes in the Raman spectrum of MoO$_3$ monocrystal due to the position of the crystal with respect to polarization (a). Scheme of polarization perpendicular to the long side of the crystal (b). Scheme of polarization parallel to the long side of the crystal (c).*

REFERENCES

de Castro Silva, I., Reinaldo, A. C., Sigoli, F. A., Mazali, I. O. (2020): Raman spectroscopy-in situ characterization of reversibly intercalated oxygen vacancies in α-MoO 3. RSC Advances, **10(31)**, 18512-18518.

Ma, W., Alonso-González, P., Li, S., Nikitin, A., Yuan, J., Martín-Sánchez, J., Taboada-Gutiérrez, J., Amenabar, I., Li, P., Vélez, S., Tollan, C., Dai, Z., Zhang, Y., Sriram, S., Kalantar-Zadeh, K., Lee, Shuit T., Hillenbrand, R., Bao, Q. (2019): In-plane anisotropic and ultra-low-loss polaritons in a natural van der Waals crystal. Nature, **562**, 557–562.

Kim, J., Dash, J., Kwon, J., Hyun, C., Kim, H., Ji, E., Lee, G. (2019): Van der Waals epitaxial growth of single crystal α-MoO$_3$ layers on layered materials growth templates. *2D* Mater, **6**, 015016.