MoS_2 oxidation: from single $(MoO_3)_x$ clusters to MoO_3/MoO_x layers

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Layered semiconductor MoS_2 as a representative of the transition metal dichalcogenides (TMDs) family has been used in (opto)electronic and energy-harvesting devices due to its fascinating properties. Recently, surface oxidation has been introduced to manipulate its electrical properties [1]. This presentation concentrates on some aspects of MoS_2 oxidation and oxidative etching producing single $(MoO_3)_x$ clusters as well as MoO_3/MoO_x layers.

Heating the MoS_2 samples in the etching regime (370 °C) resulted in formation of sub-nm oxide clusters. Comparison between height profiles obtained by atomic force microscopy (AFM) imaging and density functional theory simulations on the sub-nm Mo_xO_y fragments onto a MoS_2 monolayer suggested that these clusters are mainly MoO_3 monomers and dimers at the sulfur vacancies (Fig. 1a). A combination of several surface science methods such as Raman measurements, energy and wavelength dispersive X-ray spectroscopies as well as X-ray absorption near edge structure data confirmed the MoO_3 nature of such clusters. These results show that oxidative etching and removal of Mo atoms at the atomic level follow predominantly via formation of single MoO_3 molecules [2]. Moreover, the ability of Kelvin-probe force microscopy (KPFM) in air for the detection of sub-nm oxide clusters (Fig. 1b and c) has been extended toward Mo oxide layers atop MoS_2 crystals and other substrates [3].

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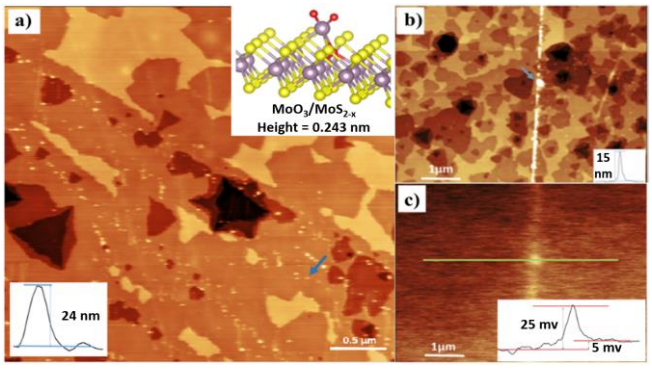

Fig. 1. (a) High-resolution non-contact (NC-) AFM image of an etched MoS_2 flake. The upper inset shows a simulated structure and calculated height of a MoO_3 monomer at a sulfur vacancy in MoS_2 monolayer. The lower inset shows the height of a sub-nm cluster depicted by blue arrow. (b) NC-AFM topography and (c) corresponding contact potential difference (CPD) obtained by KPFM. The inset in (b) shows the height profile of a cluster depicted by blue arrow. The inset in (c) shows the CPD profile along the green line [2].

[1] R. Szoszkiewicz, Materials, 20, 5979 (2021).
[2] S. Sovizi, S. Tosoni, R. Szoszkiewicz, Nanoscale Advances, 21, 4517 (2022).
[3] S. Sovizi, R. Szoszkiewicz et al., in preparation