

## Insights into the structure of MoS<sub>2</sub>/WS<sub>2</sub> nanomaterial catalysts as revealed by aberration corrected STEM

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Molybdenum disulfide/Tungsten disulphide (MoS<sub>2</sub>/WS<sub>2</sub>) is a compound very useful for its properties; it is used as lubricant, catalyst in hydrodesulfuration, in hydrogen fuel storage, etc. As part of the 2nd Joint Congress of the Portuguese and Spanish Microscopy Societies the present work reports about the different types of MoS<sub>2</sub>/WS<sub>2</sub> nanomaterials which have been investigated by using aberration corrected STEM namely: (1) MoS<sub>2</sub> nanotubes (2) MoS<sub>2</sub> hexagonal nanoplates, (3) rippled or helical MoS<sub>2</sub> nanowires, (4) Co-doped MoS<sub>2</sub>/WS<sub>2</sub> nanowires and (5) fullerene-like WS<sub>2</sub> nanoparticles [1-6].

Aberration-corrected electron microscopy (STEM-HAADF) has been used to understand the capping, nature and structure of the MoS<sub>2</sub> nanotubes. Thus the 3R rhombohedral stacking sequence was identified in this study [1]. In another study MoS<sub>2</sub> nanoplates having a size of 20–30 nm were investigated using aberration corrected STEM. Thus detailed insight into the structure of these nanoplates was obtained in great detail in this study and they were subsequently used in catalysis: namely the hydrodesulphurization reaction of dibenzothiophene [2]. The structure of MoS<sub>2</sub> nanowire catalysts (supported on Al<sub>2</sub>O<sub>3</sub> substrates) was investigated to provide detailed information of its shape and structure. HAADF (High Angle Annular Dark Field) - STEM images shows very clearly that the catalyst is formed by elongated chains with a twisted and helical structure (Figure 1). Based on the HAADF-STEM images, three atomic models were built to illustrate the different morphologies found in the MoS<sub>2</sub> catalyst [3]. A very significant increase in their activity can be achieved by adding Co or Ni as a promoter. Thus aberration corrected STEM (scanning transmission electron microscopy) has been used to characterize Co doped MoS<sub>2</sub>/WS<sub>2</sub> nanowire catalysts (supported on Al<sub>2</sub>O<sub>3</sub> substrates). The high-resolution imaging reveals clearly the location of Co in the individual nanowire catalysts (Figure 2). Based on the HAADF-STEM images, two models for the Co-Mo-S and Co-W-S catalysts were built to illustrate the different morphologies found in the catalysts [4,5]. In addition IF-WS<sub>2</sub> nanoparticles have been investigated by using aberration corrected scanning transmission electron microscopy (C<sub>s</sub>-STEM) whereby the new 1T type of stacking, common in MoS<sub>2</sub> but never seen before in the case of the IF-WS<sub>2</sub> nanoparticles was identified [6].

### References

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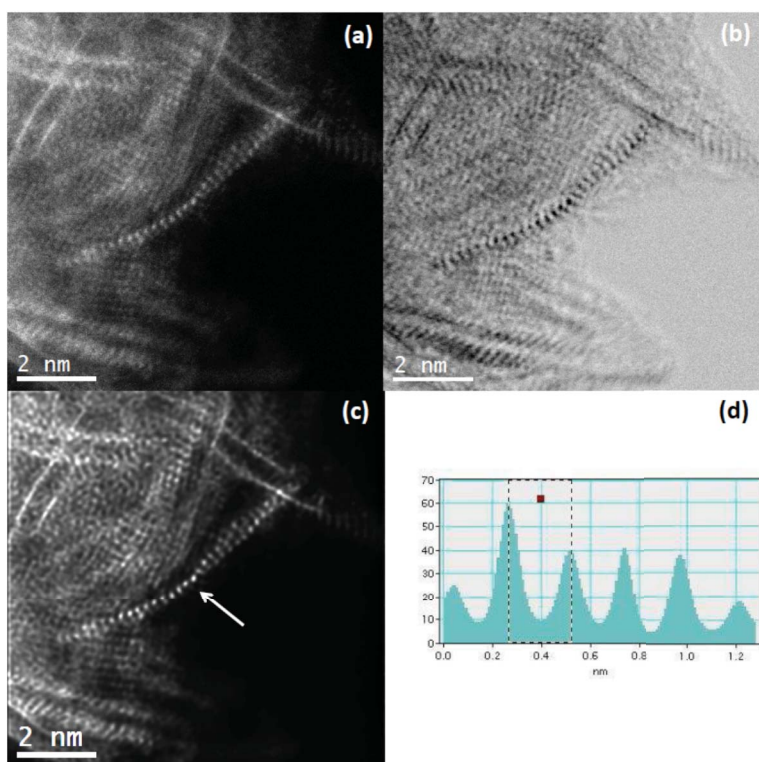


Figure 1. MoS<sub>2</sub> catalysts supported on Al<sub>2</sub>O<sub>3</sub>: a) HAADF-STEM image and b) BF-STEM image of the MoS<sub>2</sub> catalysts, c) Filtered HAADF-STEM image of the MoS<sub>2</sub> catalyst, d) The line profile corresponding to the interatomic distances of the Mo–Mo atoms (bright atom contrast), distances of 2.7 Å between the atoms. The white arrow shows the S atoms that make up the S–Mo–S chevron.

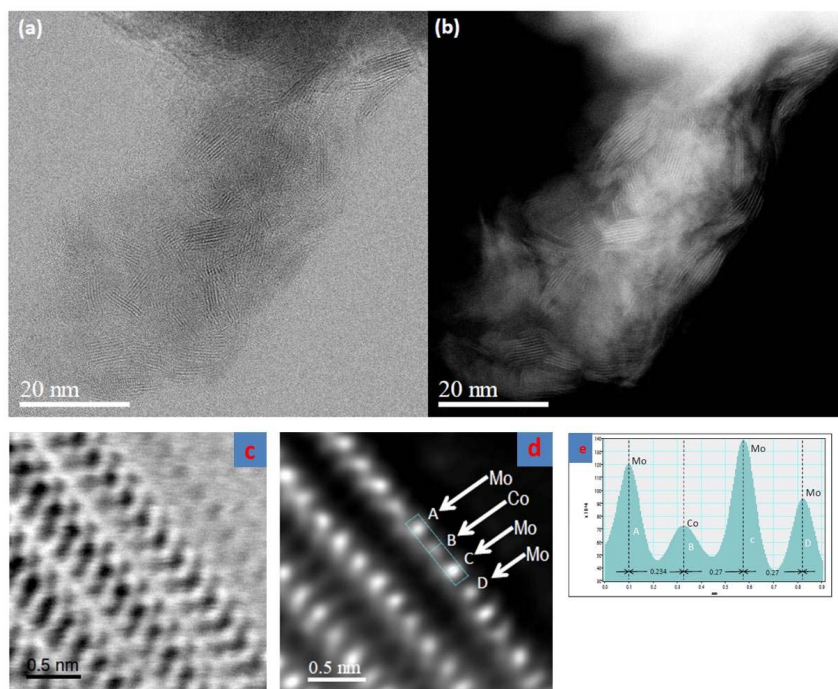


Figure 2. (a) and (b) show the low magnification BF-STEM and HAADF-STEM images of the Co-doped MoS<sub>2</sub> nanowire catalysts, (c) and (d), Ultra high magnification BF-STEM and HAADF-STEM images of the Co-doped MoS<sub>2</sub> nanowire catalysts (unsupported catalyst), and (e) corresponding line profiles (the spacing between the Mo-Co-Mo-Mo atoms, atoms A-B-C-D). The Co atoms have a lesser intensity in comparison to the Mo atoms as a consequence of the difference in their respective atomic numbers.