

Single-atom sensitive imaging of two-dimensional MoS₂ nanoparticles

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The anisotropic, layered structure of graphite is encountered in a variety of complex compound materials such as the transition metal disulfides MS₂ (M=Mo, W). These compounds consist of S-M-S layers with covalent intralayer bonds and with a weak van der Waals interlayer interaction. Like graphene, such S-M-S layers have within the last two decades been found to form numerous of nanoscale polymorphs (including fullerene-like structures, nanotubes/wires and platelets), each with unique physico-chemical properties significantly different from the corresponding bulk materials [1]. Here, we focus on planar, single-layer MoS₂ nanoparticles, which is of broad, current interest as catalyst for the industrial oil refining, hydrogen evolution and photo-oxidation.

It is well-known that the catalytic reactivity of MoS₂ is associated with the edges of its 2-dimensional S-Mo-S layers. Detailed edge structure information is thus essential in order to understand the nature of the catalytic active sites [2]. Previously, unprecedented insight into the atomic structure of single-layer MoS₂ nanoparticles prepared under ultra high-vacuum conditions on planar model substrates have been obtained from scanning tunneling microscopy (STM) and from density functional theory (DFT) calculations [2]. However, the information from the model systems is difficult to relate to catalyst particles synthesized by industrial-style methods because the precise structure and distribution of the edge sites are sensitive to the preparation conditions, edge-attached promoter atoms, and interactions with support media [2]. For long, it has therefore been a key goal to obtain high-resolution electron microscopy images of industrial-style, supported MoS₂ catalysts, viewed in the (001) projection, but the lack of sufficient contrast and resolution has prevented such images to be obtained [3].

Recent advances in high-resolution transmission electron microscopy (HRTEM) have now made it possible to obtain images of unsupported graphene-type structures with single-atom sensitivity [4]. In this contribution, we demonstrate how this HRTEM approach also provides atomically resolved information of MoS₂ nanoparticles dispersed on a high-surface-area graphite support [5]. Figure 1 shows the HRTEM reconstructed phase image of a hexagonal MoS₂ nanocrystal supported on a few graphene-layers thick flake. A detailed contrast analysis of the image provides an unambiguous identification of the single- and double-layer domains in the MoS₂ nanocrystal and thus information about the types and concentration of the edge sites. It will be discussed how this atomic-scale information about the industrial-style catalysts may be related to catalytic reactivity and assist new, improved structure-functionality relationships to be established.

References

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Figures

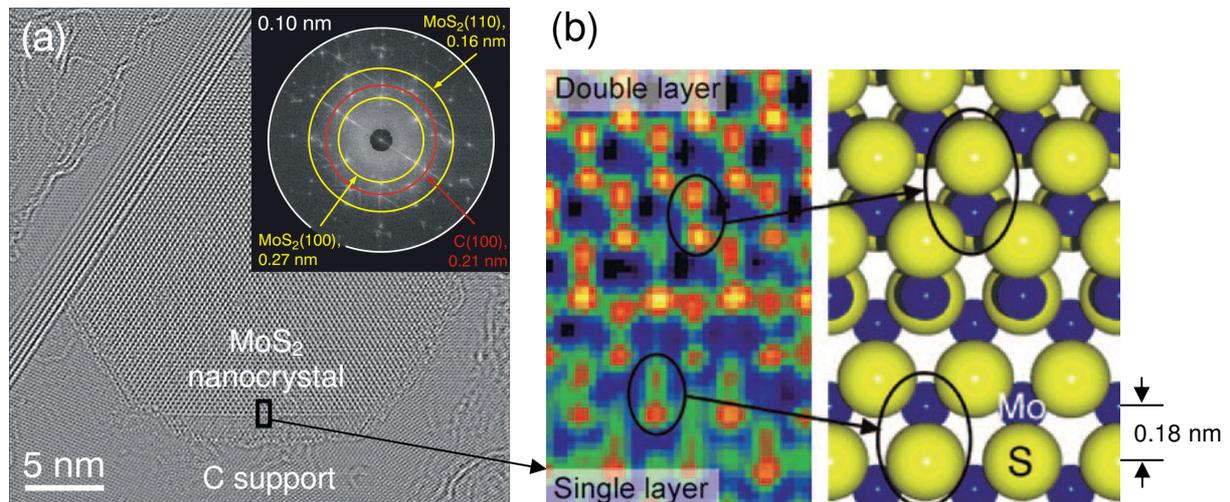


Figure 1: (a) Reconstructed aberration corrected HRTEM phase image of a MoS₂ nanocatalyst supported on graphite recorded in MoS₂ (001) projection as revealed from the Fourier transform (inset). (b) Close-up of region near the edge of the MoS₂ particle illustrating the atomic arrangement of single- and double layer MoS₂ structure [5].