

## Surface and Interface of Catalysts

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Surface structure of catalytic materials can be well studied by means of the well-established surface science methods, usually in ultra-high vacuum. With spectroscopic method and imaging technique, the mechanism of a catalytic reaction at molecular level can be understood, evidenced by the Nobel Prize to Gerhard Ertl in 2007 for his pioneer contributions in study of surface of solid. However, the study of a *real* catalyst with surface science method is not straightforward as the industrial catalysts do not exhibit smooth surface of defined crystallographic orientation. Moreover, the real catalysts are characterized by their small size, spherical shape and the interaction with the support.

The emerging of aberration-corrected high-resolution electron microscope in the recent years makes it possible to study the surface and interface structure of industrial catalyst. The breakthrough of the resolution to sub-Å region and the complete removal of de-localization fringes on the periphery (Fig. 1) bring new knowledge on real catalyst that was not accessible without this technique. For instance, the presence of oxygen on surface and sub-surface of a Ag catalyst is predicted by Nobel Prize winner Ertl using spectroscopic methods, but could not be directly visualized until the advent of advanced, aberration-corrected TEM. Using this technique, it is found that even for a un-oxidized Ag catalyst, oxygen atoms are present on the edge and steps of the Ag surface, but not on the smooth termination of Ag (111) plane.

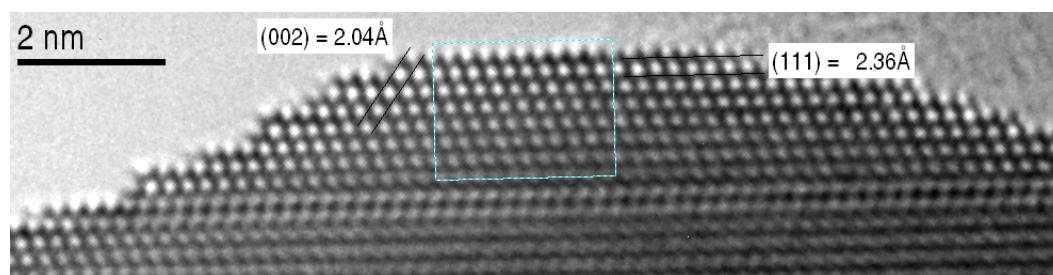


Fig. 1 High-resolution image of the surface profile of an industrial Ag/SiO<sub>2</sub> catalyst for hydrogenation of acrolein, taken on a Cs-corrected field-emission TEM. The image reveals the steps and kinks that may accommodate the oxygen species.

Examples of the identification of oxide species by aberration-corrected TEM and by DFT calculations, of the surface-modified carbon nanotubes for the dehydrogenation of *n*-butane will be presented.