Interface study of silver nano-particles using an image Cs-corrected TEM

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Imaging the interface and surface structure with atomic details is a dream of materials scientists. Usually, this is the task of high-resolution TEM that could, in principle, provide atomic structure of the studied sample if oriented in a crystallographic direction. However, delocalization effects due to the lens aberration are harming the quality of atomic images of interface/surfaces because of the cross talk between the single atomic columns. Hence a deeper understanding of atomic distance relaxation effects, surface reconstruction, surface defects like terrace edge or kink atoms and additional surface layers on nano-particles needs TEM with Cs-corrected optics.
The contrast delocalization depends on the spherical aberration C_s and the defocus Z of the objective lens. It can be quantified by the radius of the point-spread function [1]:

$$R = \max\left|\frac{\partial \chi}{\partial \vec{g}}\right|, \text{ where } g = [0, g_{max}] \text{ is the spatial frequency and } \chi(\vec{g}) = \frac{1}{2}Z\lambda g^2 + \frac{1}{4}C_s\lambda^3 g^4 \text{ is the}$$

aberration function with λ the wave length of the imaging electrons. In TEM equipped with an image C_s-corrector (CETCOR from CEOS) [2,3] the contrast delocalization can be dramatically reduced or even completely canceled when $C_s = 0$ at Gaussian defocus. The phase shift introduced by a weak phase object contributes to the contrast distribution if an additional phase shift is added in the imaging process [4, 5]. At the same time the optics should transfer all spatial frequencies up to the information limit of the TEM with a singlet phase contrast pass band. By choosing the optimal spherical aberration and defocus the contrast delocalization is well below 0.1nm.
By using image Cs corrected TEM with Cs tuned to the optimal phase contrast pass band, the surface structure of Ag nano-particles prepared by incipient wetness techniques (Ag-IW) and by precipitation of silica gel (Ag-P) [6], respectively, has been studied on a Tecnai TF20 S-TWIN. The high resolution images of a Ag-IW particle in Fig. 1 and 2 reveal clearly the Ag atomic termination of the particle surface, while the Ag-P particle (Fig. 1, right) shows a disordered surface structure. The difference in surface structure is the reason why the two catalysts show different performance in the hydrogenation reaction of acrolein [7].

References

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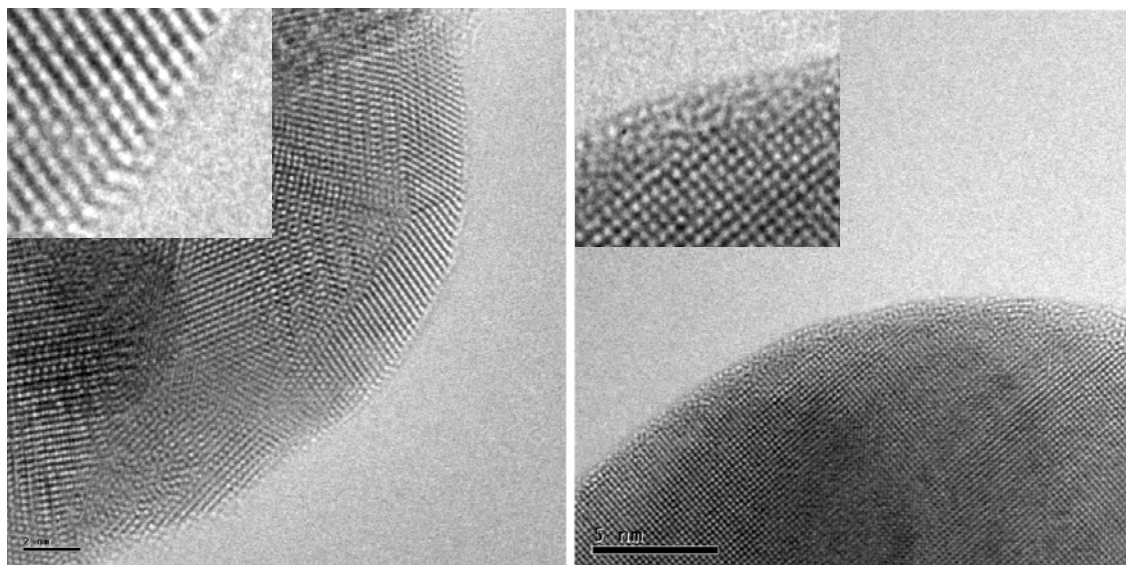
Fig.1. Cs-corrected HR-TEM image of a Ag-IW silver particle terminated by silver atoms (left) and a Ag-P silver particle terminated by an disordered surface layer (right).
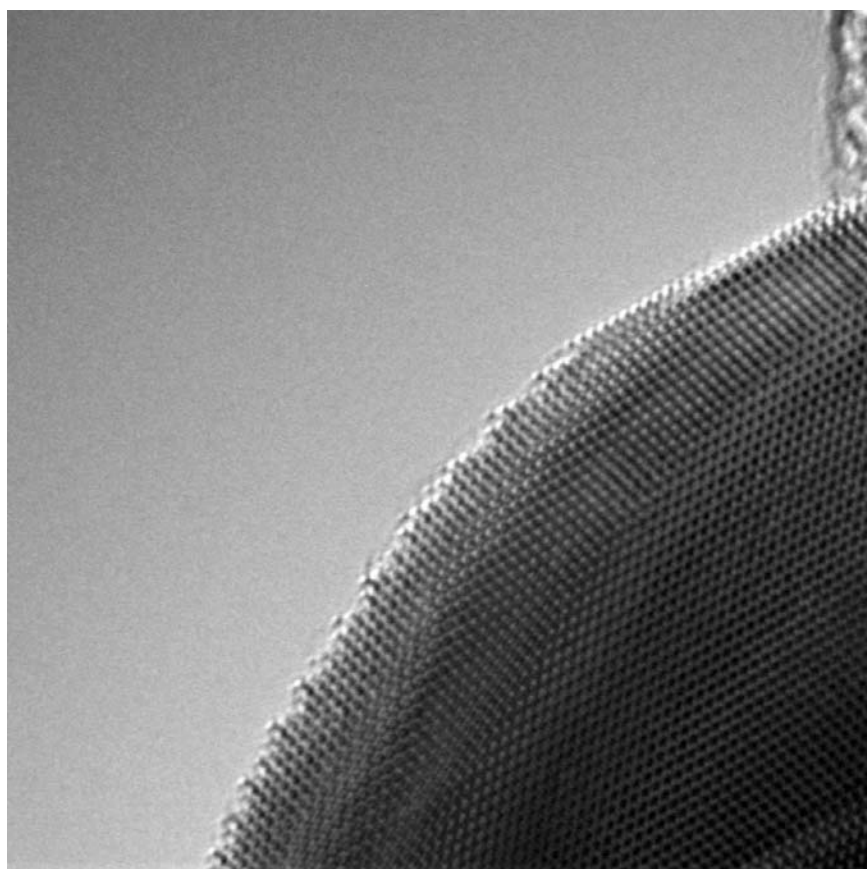

Fig. 2. Cs-corrected HR-TEM image of silver particle (Ag-IW). The termination with minimum surface energy leads to the smooth atomic arrangement (upper part of the particle). Kink and edged atoms (habitus planes) have to be accommodated to keep the overall morphology of the particle - being spherical- to minimize the total surface energy.