Type of presentation: Poster

IT-2-P-2016 Surface Science of Metal Oxides by High-resolution TEM

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Surfaces of metal oxides are of crucial importance for a variety of technological applications such as heterogeneous catalysis, thin film growth, gas sensing, and corrosion prevention [1]. Due to the complexities of oxides in crystal structure and electronic structure, however, the surface science of oxides lags far behind that of metals or semiconductors. Conventional surface-science techniques, typically scanning tunneling microscopy (STM) and low energy electron diffraction (LEED), are usually limited to surfaces of single crystals with relatively simple structures. Metal oxides are usually good insulators, either band insulators or Mott insulators, making them not suitable for STM, LEED, and most of spectroscopic methods using low energy electrons as probes. On the other hand, the complex atomic structures of oxides results in too many structural parameters to be determined by spectroscopy or diffraction methods. Recent developments in high-resolution transmission electron microscopy (TEM) provide us opportunities to overcome the above difficulties. With the realization of aberration-correction, the point resolution of TEM has been improved into the milestone 1 Angstrom scale. In addition, the correction of the spherical aberration has almost eliminated the contrast delocalization in high-resolution images. Therefore, high resolution TEM becomes an even more powerful tool than before for materials research at a truly atomic-scale. Here, we will present our recent works on atomic and electronic structure of oxide surfaces [2-4]. We will show that the structure and dynamics of oxide surfaces can be directly imaged and measured at the sub-angstrom scale with an accuracy of picometers, comparable to that obtained by conventional surface science techniques on single crystals. Special attention will be on line defects at the surfaces of MgO and Fe2O3.

References:

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Acknowledgement: This work was supported by National Basic Research Program of China (2011CB606406), NSFC (51071092, 51371102, 11374174, 51390471, 51390475), and Program for New Century Excellent Talents in University. This work used the resources of the Beijing National Center for Electron Microscopy and Shanghai Supercomputer Center.

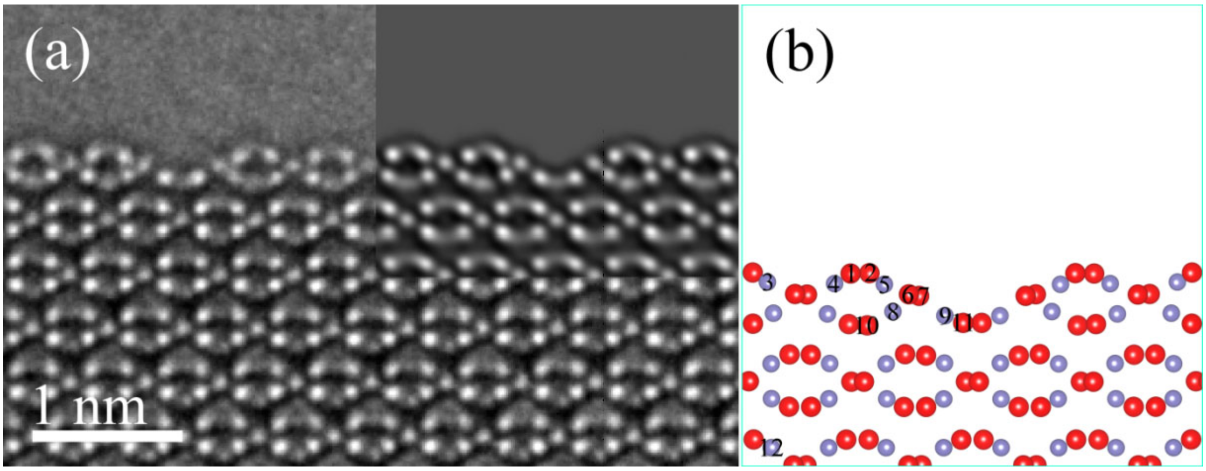

Fig. 1: (a) HRTEM image of the α-Fe_2O_3 (-1102) surface defect viewed in the [1-101] direction. The inset shows the simulated image of the relaxed structure by DFT calculations (b).