Huifang Xu, Struct Chem Crystallogr Commun, 3:2
DOI: 10.21767/2470-9905-C1-002

2nd International Conference on

APPLIED CRYSTALLOGRAPHY

October 16-17, 2017 | Chicago, USA

Understanding interface and surface structures of nano-phases in natural Fe-oxyhydroxide and Fe-bearing olivine minerals

Huifang Xu, Seungyeol Lee and **Shiyun Jin**
University of Wisconsin-Madison, USA

Understanding interface structures, nano-precipitates, vacancies, impurities and adsorbed atoms on mineral surfaces are important to elucidate formation mechanism and reactions of minerals in the earth environments. Aberration-corrected Z-contrast imaging can provide chemical images with sub-Å resolution. Z-contrast images are HAADF images with atomic resolution. Multiple diffraction effects that appear in high-resolution transmission electron microscopic (HRTEM) images can be eliminated or minimized in Z-contrast images, because Z-contrast imaging uses non-coherent elastically scattered electrons at high scattering angle. We can obtain positions of atoms directly over a large range of thickness with Z-contrast to help distinguish columns of different atoms and their occupancies along the beam direction. Interface structures and crystal structures of nano-minerals and nano-precipitates can be solved by combining the Z-contrast imaging and ab *initio* calculation using density functional theory (DFT) methods. Vacancies, impurities, adsorbed heavy atoms can be also revealed directly. Vacancy ordering in Fe-bearing olivine and Fe-sulfides, adsorbed heavy metals (e.g., As, Au, U) on Fe-oxyhydroxide minerals are resolved clearly. Z-contrast images of the Fe-oxyhydroxides show ordered FeOOH proto-goethite nano-domains intergrown with nanophase goethite. The FeOOH nanophase is a precursor to the goethite. DFT calculations indicate that goethite is more stable than proto-goethite. Our results suggest that ordering between Fe and vacancies in octahedral sites result in the transformation from feroxyhyte to goethite through a proto-goethite intermediate phase. Combining Z-contrast images and TEM-EDS reveals that arsenate (AsO_4^{3-}) tetrahedra are preferentially adsorbed on the proto-goethite (001) surface.

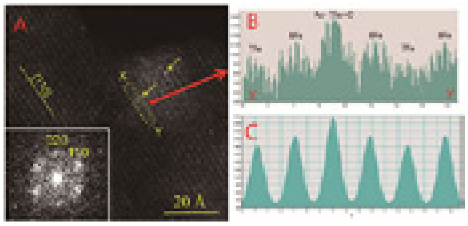

Figure-1: (A) a [001]-zone-axis Z-contrast image of proto-goethite, bright spots are positions of Fe atom columns. Very bright spots are adsorbed arsenic (As) atoms on the surface right above Fe; (B) the intensity profile of an outlined area from X to Y; (C) the intensity profile of simulated Z-contrast image showing the peak with As atom above an Fe atom column.

Biography

Huifang Xu has received his Bachelor's degree from Nanjing University and PhD degree from The John's Hopkins University in field of Mineralogy and Crystallography. He has completed his Postdoctoral studies at Arizona State University in area of Electron Crystallography. He is a Faculty Member in the Department of Geoscience and Materials Science Program at the University of Wisconsin-Madison. His research interests are studies of incommensurately modulated structures and nano-phase structures using e-beam imaging, X-ray diffraction and neutron scattering methods. He has published more than 100 papers in fields of mineralogy, crystallography and inorganic materials. He is an elected Fellow of Mineralogical Society of America.

hfxu@geology.wisc.com

Notes: