XAS characterization of nano-chromite particles precipitated on magnetite-biochar composites

Ning Chen, Canadian Light Source, ning.chen@lightsource,ca
Md Samrat Alam, University of Alberta, mdsamrat@ualberta.ca;
Daniel S. Alessi, University of Alberta, alessi@ualberta.ca

Biochar has drawn extensive attention as a low-cost, effective material to increase soil fertility, carbon sequestration and in the treatment of wastewater. Among its many uses, biochar can be used as a substrate to produce composites with iron minerals and microbes that may be used to enhance the immobilization of potentially toxic metals from the environment. In this study, we report on the removal of aqueous chromate (Cr(VI)) species by magnetite-biochar (M-BC) composites. To do so, magnetite was chemically precipitated on the surface of the biochar to make M-BC composites, and batch experiments were then carried out with M-BC to reduce Cr(VI) to Cr(III).

The Cr K-edge XAFS data were collected at the HXMA beamline at the Canadian Light Source to determine the Cr speciation and coordination at M-BC composite surfaces. During the experiment, a double crystal Si(111) monochromator was used to provide the monochromatic X-ray for the experiment. The beamline was configured in its focused mode with Rh mirrors (collimating and focusing mirrors) in the X-ray beam path. The experiment was performed in fluorescence mode by using a Canberra 32 element Ge array detector.

By using Cr K edge XAS data, the existence of chromite nanoparticles on the M-BC composites was first identified by theoretical XANES modeling [1]. Guided by the "contrast" of the whiteline dual-peak fine structure experimentally resolved from the Cr K edge XANES, the XANES modeling further revealed the dimension range for the chromite nanoparticles carried by M-BC composites. This XANES result is further supported by the R space curve fitting for the corresponding Cr K edge EXAFS data. The theatrical calculation for the amplitude and phase for the scattering paths was performed by using Feff7 [2], which guided the R space curve fitting. Both of FDMNES and FEFF modeling were based on the chromite crystallographic data from [3].

We found that the result from XANES modeling and EXAFS R space curve fitting are consistent with each other. FDMNES calculations successfully reproduced the experimental XANES of the sample system and identified XANES features that can be used as ~~indicators~~ finger print feature to estimate~~for specific~~ the dimension of the chromite cluster sizes at the nanoscale. This XANES theoretical modeling and R space curve fitting combined element-specific local structure approach may have significant application, specifically in environmental systems containing amorphous and crystalline Cr species at nano- to sub-nano molecular scales.

[1] Joly, Y., 2001, Phys. Rev. B 63, 125120-125129.
[2] Rehr, J. J. and Albers, R.C., 2000, Rev. Modern Phys. 72: 621-654.
[3] Lenaz, D., Skogby, H., Princivalle, F.,and Halenius, U., Phys. Chem. Miner. 31: 633-642.