Metal Oxygen Bond Anisotropy and Size Effects Scattering in $V_{1-x}M_xO_2$ (M = Nb, Mo)

Jacob F Phillips[1], Dr. Top B Rawot Chhetri[1], Dr. Matthew A Davenport[1], Dr. Tyra C Douglas[1], Logan M Whitt[1], Dr. Stephan Rosenkranz[2], Dr. Raymond Osborn[2], Dr. Matthew Krogstad[2], Dr. Jared M Allred[1]

[1]The University of Alabama, [2]Argonne National Laboratory

jfphillips@crimson.au.edu

The local structure of $V_{1-x}M_xO_2$ (M = Mo, Nb) was modeled by simulation of x-ray diffuse scattering from size effects. In VO_2, a metal to insulator transition (MIT) occurs at 340 K; this change in electronic properties is accompanied by a simultaneous structural transition from a rutile to a monoclinic (M1) structure type. It is not well agreed whether electronic correlations give rise to the structural transition in the MIT or if the structural transition produces the change in electronic properties. One way to investigate the relationship between structural and electronic properties in VO_2 is by doping with transition metals. The dopants considered in this study are Nb and Mo; Nb and Mo have similar atomic sizes, but Mo adds an extra electron per dopant atom to the system whereas Nb has the same valence as V. At low dopant fraction, both Nb-doped and Mo-doped VO_2 have a rutile average structure at high temperature, and both exhibit a temperature-induced electronic transition that coincides with a structural transition. However, their x-ray diffuse scattering patterns in the high temperature metallic phase differ greatly from one another; this indicates a difference in local structure for these dopant systems, despite sharing the same average structure. Since Nb and Mo have very similar ionic radii, it was postulated that differences in size effect scattering originate from differences in metal-oxygen bond length for the same metal octahedron, known as metal-oxygen bond anisotropy. It was determined that metal-oxygen size effects and metal-oxygen bond anisotropy contribute significantly to the observed x-ray diffuse scattering of both Mo-doped and Nb-doped VO_2; however, only Nb-doped VO_2 shows evident metal-metal size effects. Uncovering the nature of metal- metal interactions in Mo-doped VO_2 will require accounting for the contribution of correlated atomic displacements, known as atomic displacement parameter (ADP) correlations, to the local structure. Future studies will focus on optimizing the size effects model for $V_{1-x}M_xO_2$ at various compositions, assessing the composition and temperature dependence of the size effects scattering, and creating a combined ADP and size effect model for $V_{1-x}M_xO_2$.