Surface Charge Redistribution in SOFC Materials

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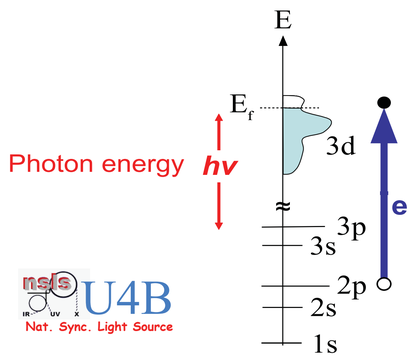
The electronic structure of V-doped, Y-doped, and Mo-doped $SrTiO_3$ (0-10 % atomic doping) has been studied using polarization dependent X-ray absorption spectroscopy (XAS). The Y is determined to substitute for the A-site Sr as Y^{3+} and that charge neutrality is maintained by the introduction of oxygen vacancies (the Sr remaining as Sr^{2+} and the Ti as Ti^{4+}). Placing these films under electrical potentials in reducing and oxidizing environments, we find that the electronic structure of the elements used for doping remain unchanged, although the Ti remains as Ti^{4+}, the intensity of the Ti L_2 and L_3 X-ray absorption features (branching ratio) varies in response to the electrochemical environment allowing us to quantify the surface charge redistribution and oxygen vacancy concentration.

Samples were generated and characterized at Montana State University. XAS experiments were conducted at the National Synchrotron Light Source and the Advanced Light Source.

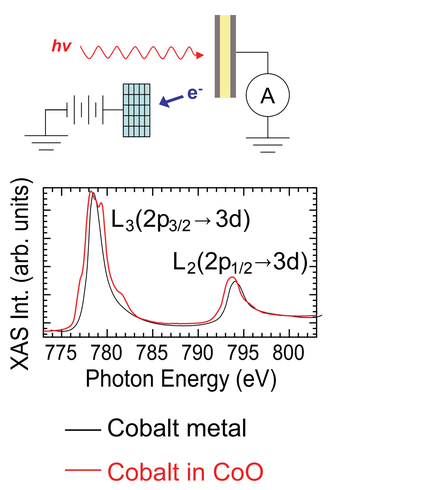
X-ray Absorption Technique

Element Specific Spectroscopy



Using synchrotron radiation allows us to tune the photon energy to match the absorption edge of specific elements. This allows us to probe the chemical and structural state of the element of our choice in a sample, including elements in burried layers of a multilayer sample. The probing depth can also be varied using various detection techniques such as total electron yield or fluorescence.

X-ray Absorption Spectroscopy

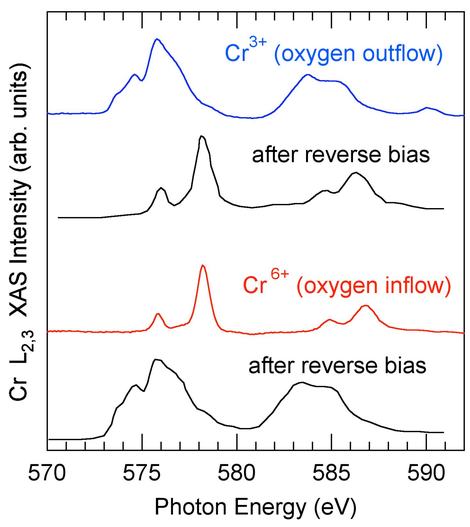


X-Ray Absorption Spectroscopy provides element specific chemical and structural sample information, as illustrated for cobalt in the spectra above.

Sample Preparation

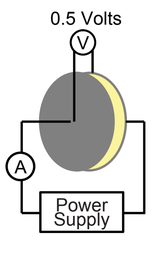
Motivation

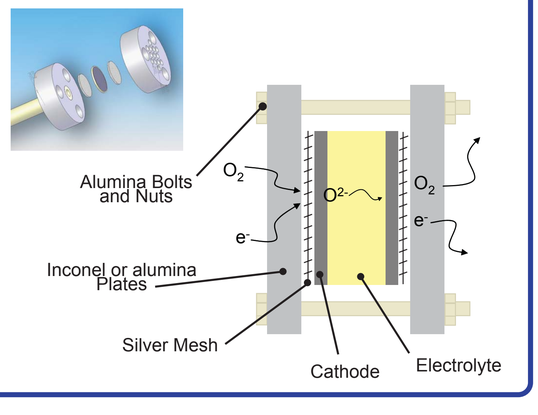
Cr valence is found to change with bias and oxygen ion flow, reversibly changing from Cr^{3+} to Cr^{6+}.



Sample Testing

Samples are sandwiched between plates with silver (or gold) mesh contacts. Inconel plates can be used to provide built-in Cr contamination. Alumina plates provide a clean environment to test other operating parameters such as oxygen partial pressure or moisture content.





XAS Results

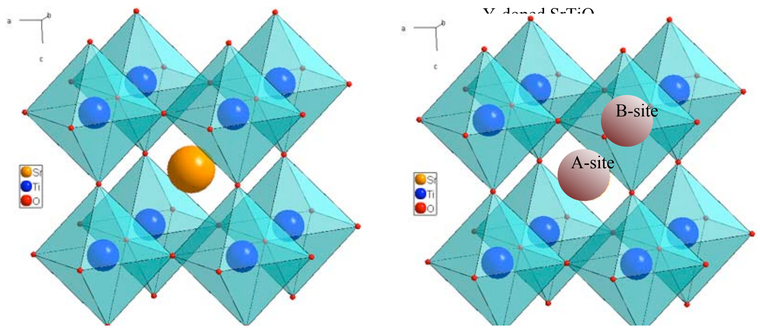
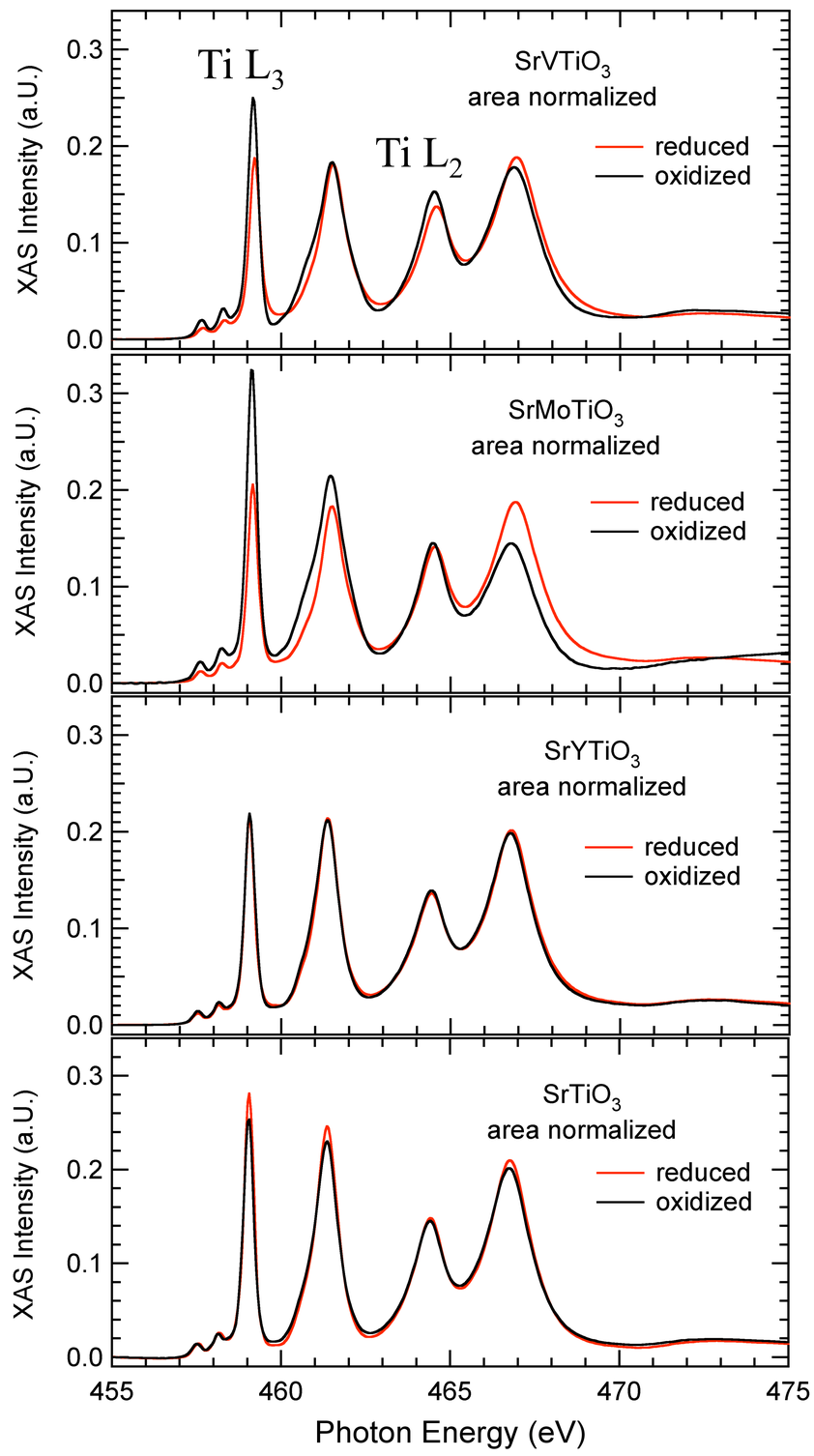


Image from webelements.com



Conclusions

1. By comparing the XAS spectra of the Sr, Ti, and O as well as the dopants V, Mo, and Y, to reference powders and theoretical calculations, we can identify the dopant valence. We confirm that Y is in the Y^{3+} valence and find that it substitutes for Sr in the A-site. V and Mo are still being analyzed.

2. Comparing the Ti L_3 and L_2 edges separately, we can quantify the changes in O vacancy concentration under oxidizing and reducing conditions. We find that oxidation and reduction of Y-doped STO does not alter the surface oxygen vacancies but does for V and Mo.

Acknowledgments

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