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Determination of Ce Oxidation State in $SrHfO_3$:Ce Perovskites by XANES

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A new class of scintillating materials $MHfO_3$:Ce (M = Ba, Sr, Ca) with ABO_3 perovskite crystal structure for high-energy nuclear medical applications has been recently discovered [1]. A low level of Ce^{3+} was found to be an efficient dopant for the desirable luminescent properties of the material. Due to the partial oxygen pressure used in synthesis, some Ce^{3+} can be oxidized and become Ce^{4+}, which is not a luminescent emitter. This may consequently have an adverse effect on the scintillator performance. The luminescent properties also depend on the Ce cation location in crystal lattice, which is being investigated by single-crystal X-ray diffraction on $SrHfO_3$ [2]. While optical measurement may be indicative for the presence of Ce^{4+} at a particular crystal lattice site, the determination of overall Ce oxidation state and the percentage of Ce^{4+} is important to controlling the synthesis condition and optimizing the material performance.

In this study, Ce oxidation state in $BaHfO_3$ and $SrHfO_3$ was analyzed by Ce XANES in fluorescence mode. Because Ba L emission lines overlap with Ce L emission lines, for BaHfO3, the measurements were performed at the Ce K-edge and the oxidation state was derived from the edge shift. For $SrHfO_3$, on the hand, the measurements were carried out at the Ce L3-edge using CeF_3 and CeO_2 as respective standard for Ce^{3+} and Ce^{4+} (figure 1). In Ce^{3+} dominated materials, numerical simulation shows that the white line intensity decreases linearly with increasing Ce^{4+} content, and thus the white line peak height was used to estimate Ce^{4+} content. This approach was found to be more sensitive than the linear combination method based on two reference spectra.

Reference:

[1] S. L. Dole, and S. Venkataramani, U.S. Patent #5124072
[2] S. M. Loureiro, Y. Gao, G. Wu & S. Venkataramani, in preparation.

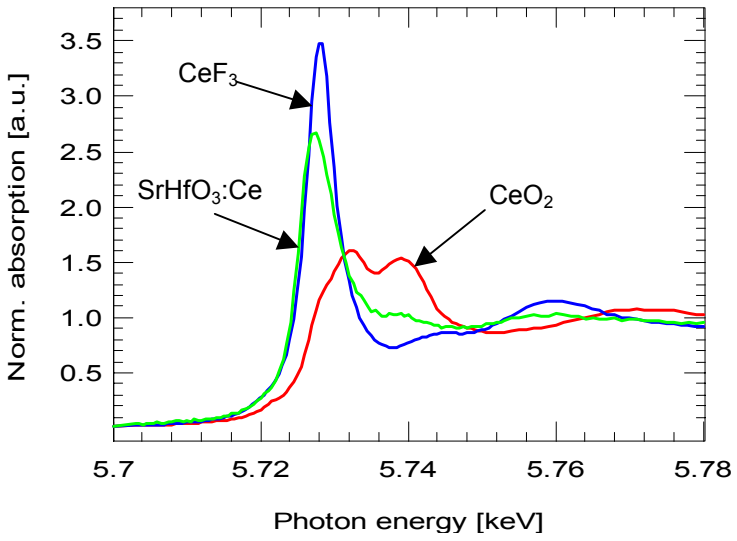

Figure 1. XANES from Ce L3-edge showing the characteristic Ce^{3+} and Ce^{4+} spectra and a spectrum from a $SrHfO_3$:Ce sample with 67% Ce^{3+}.