Supplementary material (ESI) for Journal of Materials Chemistry

Supplementary Information

X-ray absorption fine structure (XAFS) spectroscopy measurements at the Eu L-III absorption edge were made on the SAMMs material and a Eu_2O_3 standard at the Materials Research Collaborative Research Team (MRCAT) beamline at the Advanced Photon Source.[1] Measurements of SAMMs material were made in the fluorescence mode and measurements of the Eu_2O_3 standard were made in the transmission mode. For these experiments, the undulator gap was tapered ($\Delta E \sim 1$ keV) and scanned while a double crystal silicon [111] monochromator was used to select the x-ray energy. Higher order harmonics were removed with a harmonic rejection mirror. The I_0 ion chamber was filled with a nitrogen/helium (10/90) gas mixture. The transmission and fluorescence ion chambers were filled with free flowing Ar at atmospheric pressure. Linearity test [2] were performed on both samples and indicated less than 0.3% nonlinearity in the experimental setup for a 50% attenuation of the incident x-ray beam intensity. All measurements were repeated three times and the resulting $\chi(k)$ data were averaged. The MacXAFS analysis software (*version 4.0*) [3] was used in this study.

The top data plot of figure (X) illustrates the quality of the averaged k^3 – weighted data for the SAMMs material. The middle plot of figure (X) illustrates the results of the Fourier transform (ΔK=1.6–10.6 $Å^{-1}$, dk=1.25 $Å^{-1}$) of the k^3 – weighted data. A single shell, single scattering model was used to fit the Fourier filtered first shell data (ΔR=1.12-2.65 Å) of the Eu_2O_3 standard with the theoretical *FEFF7* code [4]. The input parameters required to reproduce the Fourier filtered Eu_2O_3 standard data (E_0=-2 eV, $S0^2$=0.9) were used to fit similarly Fourier filtered (ΔR=1.02-2.55 Å) SAMMs data. Results of the fit of the Eu_2O_3 standard data indicated a Eu-O coordination number of 6 ± 1, a radial distance

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of 2.33 ± 0.015 Å, and an XAFS Debye-Waller term of 0.0124 ± 0.0025 $Å^{-2}$. These results are in agreement with a previous study [5]. The bottom plot of Figure A illustrates the quality of fit of the Fourier filtered Eu L-III XAFS data from the SAMMs material. Results of the fitting analysis indicate an average Eu-O coordination number of 8 ± 1.2, a Eu-O radial distance of 2.40 ± 0.015 Å, and an XAFS Debye-Waller term of 0.0145 ± 0.0025 $Å^{-2}$. These results are consistent with the Eu ion being octacoordinate, in either a square prism or square antiprism coordination environment.

Cited Literature

1. C. U. Segre, N. E. Leyarovska, L. D. Chapman, W. M. Lavender, P. W. Plag, A. S. King, A. J. Kropf, B. A. Bunker, K. M. Kemner, P. Dutta, R. S. Duran, and J. Kaduk, *Synchrotron Radiation Instrumentation: Eleventh U.S. National Conference*, edited by P. Pianetta, et al., pg. 419-422, American Institute of Physics, New York, 2000.

2. K. M. Kemner, J. Kropf, and B. A. Bunker, *Rev. Sci. Instrum* **65**, 3667-3669 (1994).

3. C. E. Bouldin, W. T. Elam and L. Furenlid, Physica B, **208&209**, 190-192 (1995).

4. S. I. Zabinski, J. J. Rehr, A. Ankudinov, R. C. Albers, and M. J. Eller, *Phys. Rev. B* **52**, 2995-3009 (1995).

5. U. Shimizugawa, N. Umesaki, J. Qiu, and K. Hirao, *J. Synchrotron Rad.* **6**, 624-626 (1999).

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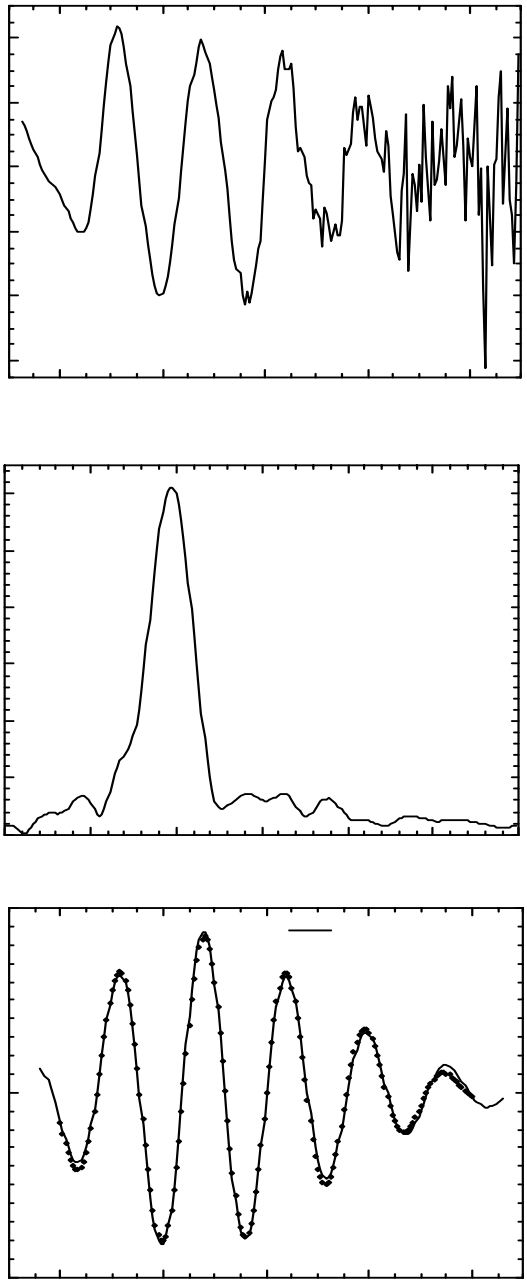

Figure A. Eu L-III XAFS results indicating the quality of the k^3-weighted $\chi(k)$ data (top), the Fourier transform of the k^3-weighted $\chi(k)$ data (middle), and the quality of the theoretical fit to the Fourier filtered first shell data (bottom).

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