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ABSTRACTS

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Local atomic structure of rare-earth doped SrMoO4 phosphors by X-ray absorption spectroscopy

Dr Alexei Kuzmin[1], Dr Georgijs Bakradze[1], M.Sc. Inga Pudza[1], Dr. Andris Anspoks[1], Dr. Aleksandr Kalinko[2], Dr. Edmund Welter[2]
[1]Institute of Solid State Physics, University of Latvia, [2]Photon Science – Deutsches Elektronen-Synchrotron (DESY)

Rare-earth (RE) doped tungstates and molybdates with a chemical formula $AW(Mo)O_4$ have a long history of practical applications because of their unique luminescence properties. Although it is generally accepted that RE(III) ions substitute A(II) ions, only a few experimental proofs of the location of dopant ions in the $AW(Mo)O_4$ crystal structure can be found in the literature. The experimental difficulty arises from the low sensitivity of diffraction methods to low dopant concentration.

In this study, we performed X-ray absorption spectroscopy (XAS) measurements of RE-doped microcrystalline $SrMoO_4$ to investigate the local atomic structure around RE dopants as a function of the RE(III) ion size in the series: Nd(III), Eu(III), Ho(III), Er(III), Yb(III). XAS experiments were performed at the PETRA-III P65 beamline at the Sr and Mo K-edges and RE L_3-edges. The experimental EXAFS data were analyzed using the reverse Monte Carlo (RMC) simulations. The starting structural model was constructed based on the known crystallographic data obtained by diffraction. Atomic positions were relaxed to account for thermal disorder and static displacements till good agreement between the Morlet wavelets of the experimental and calculated EXAFS spectra was achieved. From the final atomic coordinates, a set of the partial radial distribution functions for different atomic pairs was obtained.

Experimental RE L_3-edge XANES spectra indicate that all RE ions exist in the oxidation state 3+ (small amounts of Eu(II) and Yb(II) were also detected). While the analysis of EXAFS spectra confirms that RE ions substitute the eight-fold coordinated strontium, the displacement of RE ions from the high-symmetry Wyckoff positions occupied by strontium was unambiguously evidenced by RMC simulations.

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