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DIRECT OBSERVATION OF CRYSTAL FIELD SPLITTING IN TUNGSTATES BY RESONANT X-RAY EMISSION SPECTROSCOPY

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Keywords

Resonant X-ray emission spectroscopy, Crystal-field splitting

Actuality and aim

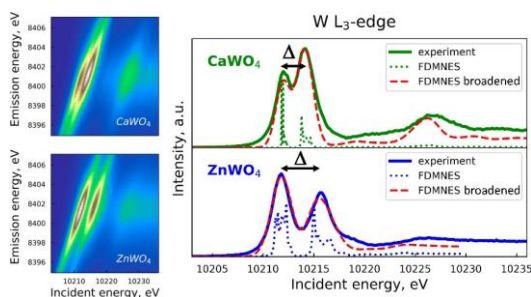
Resonant X-ray emission spectroscopy (RXES) is a photon-in photon-out X-ray technique providing information on the electronic states of metal with element selectivity and high energy resolution. It was successfully employed by us recently to study phase transitions in $\text{CuMo}_{1-x}\text{W}_x\text{O}_4$ solid solutions [1]. Here we demonstrate the sensitivity of the method to crystal field splitting in a series of AWO_4 ($A=\text{Mg, Ca, Zn, Cd, Sn, Pb}$) tungstates.

Methods

Polycrystalline tungstates were studied using the RXES technique by detecting $\text{W L}_{\beta 1}$ and $\text{L}_{\alpha 1}$ emission while scanning across the $\text{W L}_{2,3}$ -edges. The RXES map measurements were performed using von Hamos-type X-ray emission spectrometer at the HASYLAB DESY PETRA-III beamline P64 [2,3], and high-energy resolution fluorescence detected X-ray absorption near-edge structures (HERFD-XANES) were determined from the RXES maps. They were interpreted using the full-multiple-scattering XANES calculations using ab initio real-space FDMNES code [4].

Results

The RXES maps and corresponding HERFD-XANES spectra (see figure for $\text{Ca}(\text{Zn})\text{WO}_4$) reveal the structure of the unoccupied W 5d states and their splitting in the tetrahedral (1.3-2.0 eV) and octahedral (3.6-3.9 eV) crystal fields. The experimental results agree well with the calculations.



Experimental RXES maps and HERFD-XANES spectra for CaWO_4 and ZnWO_4 compared with the calculations.

Conclusions

Thus, RXES allows one to probe the splitting of the conduction band states in tungstates. The type of the splitting can be used as a fingerprint for different crystal lattices.

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