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Resonant X-ray emission spectroscopy to reveal coordination of W ions in $CuMo_{1-x}W_xO_4$ thermochromic materials

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Abstract

X-ray absorption spectroscopy (XAS) is widely used to probe the local structure of materials, but there are cases where this method provides limited information due to the natural broadening of the core state (~4.5 eV for the W L_3-edge). Resonant X-ray emission spectroscopy (RXES) allows one to detect indirectly (through the second-order process) XAS-analogues spectra but with much higher resolution (<1 eV).
In this study, XAS and RXES were used to study a variation of the local atomic and electronic structure in polycrystalline $CuMo_{1-x}W_xO_4$ ($0.04 \leq x \leq 1.00$) solid solutions across the thermochromic phase transition as a function of temperature (from 10 to 300 K) and sample composition.
We demonstrated [1] that the analysis of the RXES plane at the W L_3-edge provides useful bulk sensitive information on the coordination of tungsten atoms and allows one to determine the crystal-field splitting parameter Δ for the 5d(W) states. Furthermore, this information can be extracted from the RXES plane using two different approaches: by analysing the high-energy resolution through fluorescence detected X-ray absorption near-edge structure (HERFD-XANES) and off-resonant X-ray emission spectra.
RXES method is well suited for in-situ measurements and was used here to determine the hysteresis behaviour of the structural phase transition between α and γ phases in thermochromic $CuMo_{1-x}W_xO_4$ solid solutions on cooling and heating, even at low ($x < 0.10$) tungsten content.

Keywords: $CuMo_{1-x}W_xO_4$, crystal-field splitting, RXES, HERFD-XANES

(1) Pudza, I., Kalinko A., Cintins, A., Kuzmin, A., Study of the thermochromic phase transition in $CuMo_{1-x}W_xO_4$ solid solutions at the W L_3-edge by resonant X-ray emission spectroscopy, Acta Mater. 2021, 205, 116581. https://doi.org/10.1016/j.actamat.2020.116581.

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