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Exploring fundamental aspects of the structural organization in weberite-type tantalate oxides using neutron total scattering technique.

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The total scattering technique provides key information about the periodic long-range structure and local atomic correlations, essential to unravel underlying defects and structural disorder. Understanding how complex oxides disorder is critically important for many energy-related applications that require materials operating in harsh environments (high pressure, temperature, and radiation fields).
We used neutron total scattering and X-ray diffraction to study a series of weberite-type tantalate oxides (RE3TaO7, RE= rare earth). Weberite-type oxides are structurally related to fluorite and their chemical flexibility and ability to incorporate atomic substitutions can produce systems relevant for nuclear waste management, atomic transport, or magnetic applications. Modeling of neutron total scattering data across all material's length scales demonstrated that short-range correlations differ from the respective long-range atomic organizations: The Q-space analysis revealed three different long-range symmetries, whereas r-space correlations displayed a continuous behavior across the entire compositional series, even extending to the fully disordered defect-fluorite structure. This can be explained by the change in different tilt systems and polyhedra distortions that increase continuously with cation size mismatch. The long-range structures are the configurational average of the local sub-nanodomains; the existence of phase transformations across phase boundaries between three structural families is related to a change in the tilt system in one case and the crossing of a critical distortion level in the other. This complex multiscale disordering behavior can explain the different properties of these systems and, in particular, their varying amorphization resistance to ion irradiation.

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