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Probing Long- and Short-Range Disorder in Y2Ti2-xHfxO7 by Diffraction and Spectroscopy

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We have studied the long-range average and short-range local structures in Y2Ti2-xHfxO7 (x = 0-2.0) using diffraction and spectroscopy techniques respectively. Both neutron and synchrotron X-ray powder diffraction data show a clear phase transition of the average structure from ordered pyrochlore to disordered defect-fluorite at x ~ 1.6; the long-range anion disorder appears to develop gradually throughout the entire pyrochlore region in contrast to the rapid loss of cation ordering from x = 1.4 to 1.6. The commonly observed two-phase region around the pyrochlore / defect-fluorite phase boundary is absent in this system demonstrating high sample quality. X-ray absorption near-edge structure (XANES) results at the Y L2-, Ti K- and L3,2-, Hf L3- and O K-edges indicate a gradual local structural evolution across the whole compositional range; the Y coordination number (CN) decreases and the CN around Ti and Hf increases with increasing Hf content (x). The spectroscopic results suggest that the local disorder occurs long before the pyrochlore to defect-fluorite phase boundary as determined by diffraction, and this disorder evolves continuously from short- to medium- and eventually to long-range detectable by diffraction. This study highlights the complex disordering process in pyrochlore oxides, and the importance of a multi-technique approach to tackle disorder over different length scales and in the anion and cation sublattices respectively. The results are important in the context of potential applications of these oxides such as ionic conductors and radiation-resistant nuclear waste forms.

Keywords or phrases (comma separated)

Pyrochlore, defect-fluorite, order to disorder transition, diffraction, XANES

Are you a student?

No

Do you wish to take part in</br>the Student Poster Slam?

No

Are you an ECR? (<5 yrs</br>since PhD/Masters)

No

What is your gender?

Female

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