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Neutron Total Scattering and X-ray Diffraction Analysis of Radiation Effects in A_3BO_7 Weberite-type Complex Oxides

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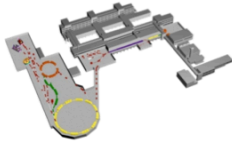
Motivation

- Nuclear technology requires materials which maintain structural stability in harsh radiation fields
- Irradiation-induced structural disorder in weberite-type (A_3BO_7) oxides is not studied

Methods

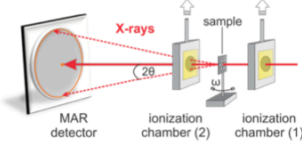
Swift Heavy Ion Irradiation at GSI

- 2.2 GeV ^{197}Au (electronic energy loss)
- Fluence: $5 \times 10^{12} - 8 \times 10^{12} \text{ cm}^{-2}$



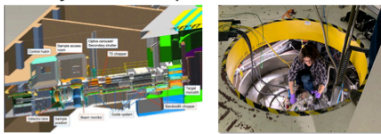
X-ray Diffraction at APS

- High-resolution, intense light sources



Neutron Total Scattering at NOMAD

- High-resolution, neutron total scattering with access to both diffraction and pair distribution analysis techniques



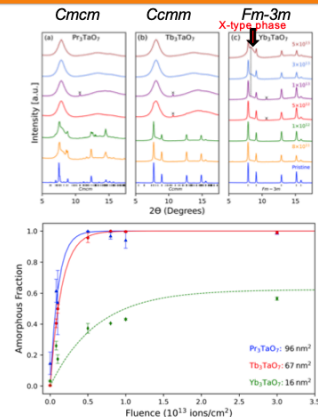
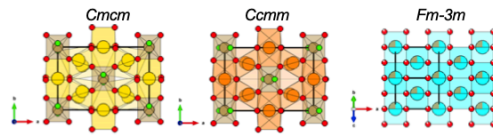
J. Neufeind, M. et al., Nucl. Instruments Methods Phys. Res. Sect. B Beam Interact. with Mater. Atoms, vol. 287, pp. 68-75, 2012.
 E. C. O'Quinn et al., J. Mater. Sci., vol. 53, no. 19, pp. 13400-13410, 2018.

Materials

- $A_3\text{TaO}_7$ ($A = \text{Pr, Tb, Dy, Y, Yb}$)
- Tuning the structure by changing the A-site cation
- 2 different tilt systems ($Cmcm$, $Ccmm/C222_1$) and 1 disordered structure ($Fm-3m$)

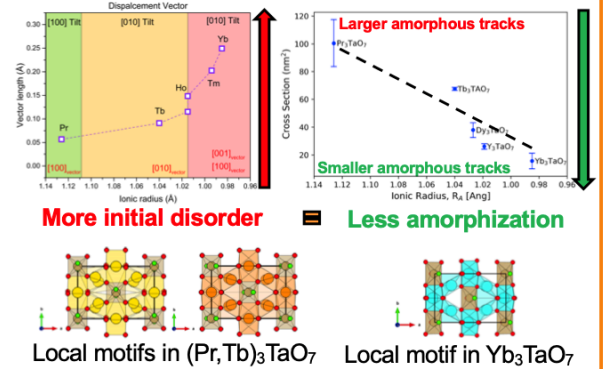
A-cation Effect on Long-range Structure

- A-site is tuned to produce different A_3BO_7 structures
- The radiation responses are dramatically different
- Ion-induced amorphization
- Increase in diffuse scattering beneath Bragg peaks
- Rapid, complete amorphization of Pr_3TaO_7 , Tb_3TaO_7
- Yb_3TaO_7 remain partially crystalline (~40%)
- Formation of X-type phase



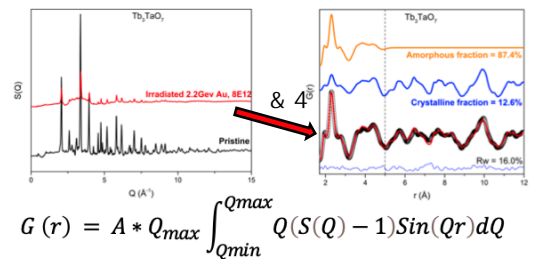
Radiation Resistance as a Function of Disorder

- Radiation resistance in $A_3\text{TaO}_7$ system is correlated with the pre-existing level of local disorder (i.e., local polyhedra distortions away from ideal long-range lattice positions)
- Structures with intrinsically larger level of pre-existing disorder show an improved amorphization resistance



Radiation Resistance of Short-range Structure

- Average, long-range weberite-type structure in Tb_3TaO_7 shows significant amorphization (~80-90% amorphous)
- Local, short-range structure is highly resistant
- No significant local modifications due to large difference in charge states of A^{3+} and B^{5+}
- Cation sites cannot mix



Conclusions

- Radiation response of complex oxides is heterogeneous across different length scales
- Local atomic arrangement must be studied to obtain comprehensive understanding
- In $A_3\text{TaO}_7$ system, materials with pre-existing level of disorder display a higher radiation stability over the long range
- Local weberite-type motif is present even in almost completely amorphous samples