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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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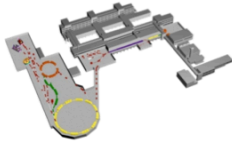
## Motivation

- 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

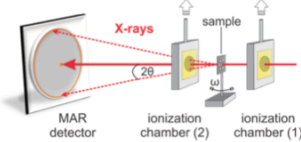
### Swift Heavy Ion Irradiation at GSI

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



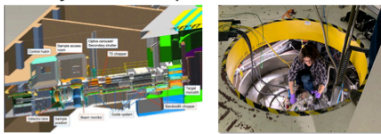
### X-ray Diffraction at APS

- 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



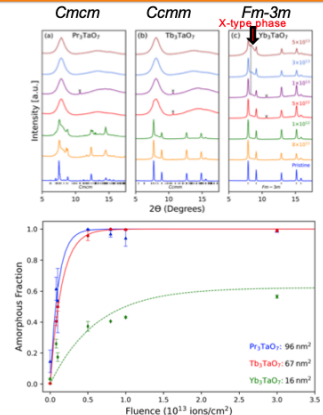
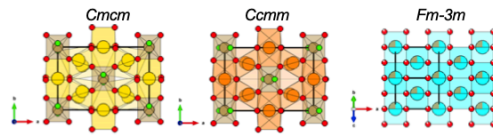
J. Neufeind, M. et al., Nucl. Instruments Methods Phys. Res. Sect. B Beam Interact. with Mater. Atoms, vol. 287, pp. 68-75, 2012.  
 E. C. O'Quinn et al., J. Mater. Sci., vol. 53, no. 19, pp. 13400-13410, 2018.

## 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 ( $Fm-3m$ )

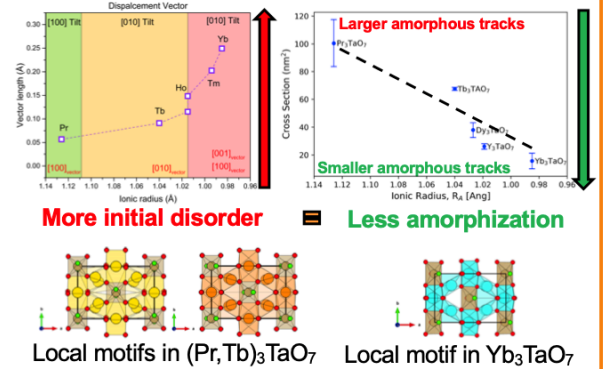
## A-cation Effect on Long-range Structure

- 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  $\text{Pr}_3\text{TaO}_7$ ,  $\text{Tb}_3\text{TaO}_7$
- $\text{Yb}_3\text{TaO}_7$  remain partially crystalline (~40%)
- Formation of X-type phase



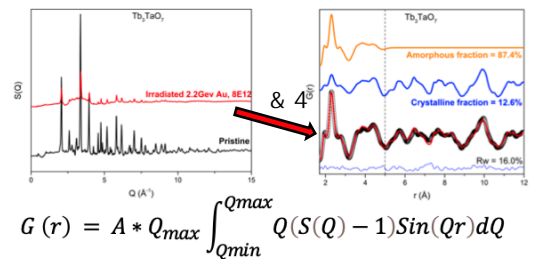
## Radiation Resistance as a Function of Disorder

- 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  $\text{Tb}_3\text{TaO}_7$  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