



HAL
open science

Neutron Total Scattering and X-ray Diffraction Analysis of Radiation Effects in A₃BO₇ Weberite-type Complex Oxides

Igor M Gussev, Eric O'Quinn, Mason King, Christina Trautmann, Jörg Neuefeind, Changyong Park, Gianguido Baldinozzi, Maik Lang

► **To cite this version:**

Igor M Gussev, Eric O'Quinn, Mason King, Christina Trautmann, Jörg Neuefeind, et al.. Neutron Total Scattering and X-ray Diffraction Analysis of Radiation Effects in A₃BO₇ Weberite-type Complex Oxides. 29th international conference on atomic collisions in solids & 11th international symposium on swift heavy ions in matter, Jun 2022, Helsinki, Finland. , 2022. hal-03698305

HAL Id: hal-03698305

<https://cnrs.hal.science/hal-03698305>

Submitted on 17 Jun 2022

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

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

Igor M. Gussev^{1,2}, Eric C. O'Quinn¹, Mason King¹, Christina Trautmann³, Jörg Neufeind⁴, Changyong Park⁵, Gianguido Baldinozzi² and Maik Lang¹

¹ Department of Nuclear Engineering, University of Tennessee, Knoxville, TN, USA
² Laboratoire Structures, Propriétés et Modélisation des Solides CNRS, CentraleSupélec, Université Paris-Saclay, 91190 Gif-sur-Yvette, France
³ GSI Helmholtzzentrum für Schwerionenforschung and Technische Universität Darmstadt, Darmstadt, Germany
⁴ Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, TN, USA
⁵ HPCAT, X-ray Science Division, Argonne National Laboratory, Argonne, IL, USA

igussev@volvs.utk.edu
 igor.gussev@centralesupelec.fr

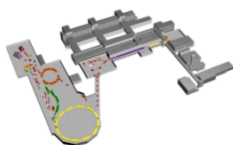
Motivation

- 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

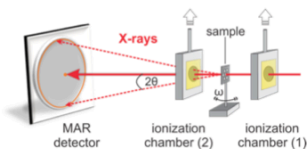
Swift Heavy Ion Irradiation at GSI

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



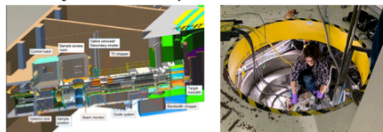
X-ray Diffraction at APS

- 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



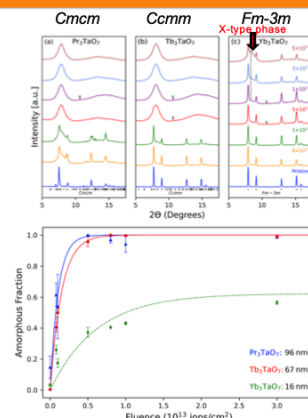
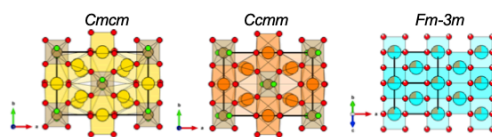
J. Neufeind, M. et al., Nucl. Instruments Methods Phys. Res. Sect. B Beam Interact. with Mater. Atoms, vol. 287, pp. 68-75, 2012.
 E. C. O'Quinn et al., J. Mater. Sci., vol. 53, no. 19, pp. 13400-13410, 2018.

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 ($Fm-3m$)

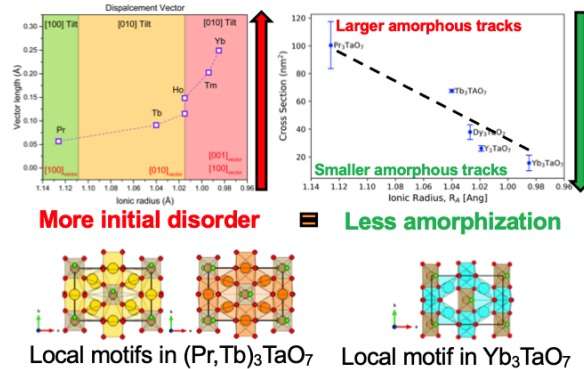
A-cation Effect on Long-range Structure

- 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



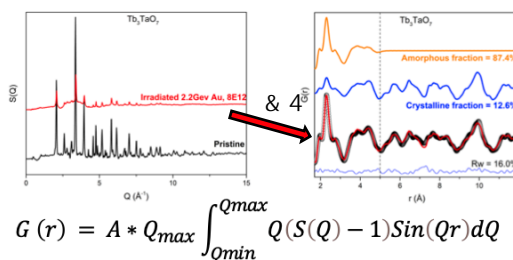
Radiation Resistance as a Function of Disorder

- 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