

ORIGINAL RESEARCH

article

Front. Nucl. Eng.

Sec. Nuclear Materials

Volume 3 - 2024 |

doi: 10.3389/fnuen.2024.1346678

This article is part
of the Research
Topic

Structures and
Properties of
Fluorite-related
Systems for
Nuclear
Applications

[View all articles >](#)

43



Total views

[View article im](#)[View altmetric scor](#)

Charge-Lattice Coupling and the Dynamic Structure of the U-O Distribution in UO_{2+x}

Provisionally accepted

People also
looked at

Ambient
melting
behavior of
stoichiometric
uranium
oxides

Leonid Burakovsky,
Scott D. Ramsey
and Roy S. Baty

Jarrod Lewis^{1,2*}Ross Springell^{1*}Christopher Bell^{1*}Rebeca Nicholls¹Jacek Wasik¹Lottie Harding^{1*}Mahima Gupta^{3*}Janne Pakarinen⁴Gianguido Baldinozzi⁵



Steven Conradson Conradson

¹ School of Physics, Faculty of Science, University of Bristol, Bristol, England, United Kingdom

² Materials Department, University of Oxford, Oxford, England, United Kingdom

³ Meta Corporation, Sunnyvale, United States

⁴ VTT Technical Research Centre of Finland Ltd, Espoo, Uusimaa, Finland

⁵ CentraleSupélec, Université Paris-Saclay, Gif sur Yvette, Île-de-France, France

⁶ Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, United States

⁷ Department of Chemistry, College of Arts and Sciences, Washington State University, Pullman, Washington, United States

! The final, formatted version of the article will be published soon.

Notify me

The different structures and behaviors of UO_{2+x} observed in crystallographic and local structure measurements are examined by Extended X-ray Absorbance Fine Structure (EXAFS) measurements of pristine UO_{2.0}, p + and He²⁺ irradiated UO_{2.0}, and at multiple temperatures bulk U₄O₉ and U₃O₇ and thin film U₄O_{9-δ} on an epitaxial substrate. The disorder caused by irradiation is mostly limited to increased widths of the existing U-O/U pair distributions with any new neighbor shells being minor. As has been previously reported, the disorder caused by oxidative addition to U₄O₉

bulk and thin film U₄O₉. This includes the significant spectral feature near R=1.2 Å for all of the U₄O₉ and U₃O₇ samples that is fit with a U-oxo type moiety with a U-O distance around 1.7 Å. In addition to indicating that these anomalies only occur in the mixed valence materials, this work confirms the continuous rearrangement of the U-O distributions from 10-250 K. Although these variations of the structure are not observed in crystallography, their prominence in the EXAFS indicates that the dynamic structure underlying these effects is an essential factor of these materials.

Keywords: UO_{2+x}, disorder, EXAFS, local structure, Radiation Effects, epitaxial films, Dynamic structure, internal tunneling polarons

Received: 29 Nov 2023; **Accepted:** 18 Jun 2024.

Copyright: © 2024 Lewis, Springell, Bell, Nicholls, Wasik, Harding, Gupta, Pakarinen, Baldinozzi, Andersson, Guo and Conradson. This is an open-access article distributed under the terms of the [Creative Commons Attribution License \(CC BY\)](#). The use, distribution or reproduction in other forums is permitted, provided the original author(s) or licensor are credited and that the original publication in this journal is cited, in accordance with accepted academic practice. No use, distribution or reproduction is permitted which does not comply with these terms.

*** Correspondence:**

Jarrold Lewis, School of Physics, Faculty of Science, University of Bristol, Bristol, BS8 1TL, England, United Kingdom
Ross Springell, School of Physics, Faculty of Science, University of Bristol, Bristol, BS8 1TL, England, United Kingdom
Christopher Bell, School of Physics, Faculty of Science, University of Bristol, Bristol, BS8 1TL, England, United Kingdom

Steven Conradson Conradson, Department of Chemistry,
College of Arts and Sciences, Washington State University,
Pullman, Washington, United States

Disclaimer: All claims expressed in this article are solely those of the authors and do not necessarily represent those of their affiliated organizations, or those of the publisher, the editors and the reviewers. Any product that may be evaluated in this article or claim that may be made by its manufacturer is not guaranteed or endorsed by the publisher.

Similar articles

ORIGINAL RESEARCH

Published on 05 |

Assessing the interfacial corrosion mechanism of Inconel 617 in chloride molten salt corrosion using multi-modal

ORIGINAL RESEARCH

Published on 19 |

The advanced characterization post-irradiation examination and materials informatics for the development of ultra-high-burnup annular

ORIGINAL RESEARCH

Published on 06 |

Oxygen potential, oxygen diffusion, and defect equilibria in UO_{2+x}

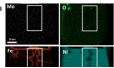
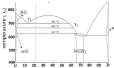
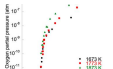
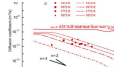
Masashi Watanabe · Masato Kato

ORIGINAL RESEARCH

Published on 27 |

Oxygen diffusion in the fluorite-type oxides CeO₂, ThO₂, UO₂, PuO₂, and (U, Pu)O₂

Masato Kato · Masashi

Frontie...	Articles	Research Topics	Editorial board
<div><div>M. Copeland-Johnson · Daniel J. Murray · Guoping Cao · Lingfeng He</div><div></div><div><div>Frontiers in Nuclear Engineering</div><div>doi 10.3389/fnuen.2024.1346678</div></div><div><div>3,313</div><div>views</div><div>1 citation</div></div></div>	<div><div>Yao · Mukesh Bachhav · Fidelma G. Di Lemma · Fei Xu · Fei Teng · Daniel J. Murray · Michael T. Benson · Luca Capriotti</div><div></div><div><div>Frontiers in Nuclear Engineering</div><div>doi 10.3389/fnuen.2024.1346678</div></div><div><div>1,948</div><div>views</div><div>3 citations</div></div></div>	<div><div></div><div><div>Frontiers in Nuclear Engineering</div><div>doi 10.3389/fnuen.2024.1346678</div></div><div><div>1,774</div><div>views</div><div>4 citations</div></div></div>	<div><div></div><div><div>Frontiers in Nuclear Engineering</div><div>doi 10.3389/fnuen.2024.1346678</div></div><div><div>1,566</div><div>views</div><div>7 citations</div></div></div>

Guidelines

Explore

Outreach

Follow us

f

X

in



[All journals](#)[All articles](#)[Submit your research](#)[Q](#) [Se](#)[Frontie...](#)[Articles](#)[Research Topics](#)[Editorial board](#)

© 2024 Frontiers Media S.A. All rights reserved

[Privacy policy](#) | [Terms and conditions](#)