

PROCEEDINGS OF SPIE

Advances in Computational Methods for X-Ray Optics VI

**Oleg Chubar
Takashi Tanaka**
Editors

**20–21 August 2023
San Diego, California, United States**

Sponsored by
SPIE

Co-sponsored by
RadiaSoft, LLC (United States)

Published by
SPIE

Volume 12697

Proceedings of SPIE 0277-786X, V. 12697

SPIE is an international society advancing an interdisciplinary approach to the science and application of light.

The papers in this volume were part of the technical conference cited on the cover and title page. Papers were selected and subject to review by the editors and conference program committee. Some conference presentations may not be available for publication. Additional papers and presentation recordings may be available online in the SPIE Digital Library at SPIDigitalLibrary.org.

The papers reflect the work and thoughts of the authors and are published herein as submitted. The publisher is not responsible for the validity of the information or for any outcomes resulting from reliance thereon.

Please use the following format to cite material from these proceedings:

Author(s), "Title of Paper," in *Advances in Computational Methods for X-Ray Optics VI*, edited by Oleg Chubar, Takashi Tanaka, Proc. of SPIE 12697, Seven-digit Article CID Number (DD/MM/YYYY); (DOI URL).

ISSN: 0277-786X

ISSN: 1996-756X (electronic)

ISBN: 9781510666085

ISBN: 9781510666092 (electronic)

Published by

SPIE

P.O. Box 10, Bellingham, Washington 98227-0010 USA

Telephone +1 360 676 3290 (Pacific Time)

SPIE.org

Copyright © 2023 Society of Photo-Optical Instrumentation Engineers (SPIE).

Copying of material in this book for internal or personal use, or for the internal or personal use of specific clients, beyond the fair use provisions granted by the U.S. Copyright Law is authorized by SPIE subject to payment of fees. To obtain permission to use and share articles in this volume, visit Copyright Clearance Center at copyright.com. Other copying for republication, resale, advertising or promotion, or any form of systematic or multiple reproduction of any material in this book is prohibited except with permission in writing from the publisher.

Printed in the United States of America by Curran Associates, Inc., under license from SPIE.

Publication of record for individual papers is online in the SPIE Digital Library.

**SPIE. DIGITAL
LIBRARY**

SPIDigitalLibrary.org

Paper Numbering: A unique citation identifier (CID) number is assigned to each article in the Proceedings of SPIE at the time of publication. Utilization of CIDs allows articles to be fully citable as soon as they are published online, and connects the same identifier to all online and print versions of the publication. SPIE uses a seven-digit CID article numbering system structured as follows:

- The first five digits correspond to the SPIE volume number.
- The last two digits indicate publication order within the volume using a Base 36 numbering system employing both numerals and letters. These two-number sets start with 00, 01, 02, 03, 04, 05, 06, 07, 08, 09, 0A, 0B ... 0Z, followed by 10-1Z, 20-2Z, etc. The CID Number appears on each page of the manuscript.

Contents

v *Conference Committee*

COMPUTATION METHODS AND CODES I

- 12697 02 **FOCUS: current status and future perspectives (Invited Paper)** [12697-5]
- 12697 03 **New wavefront split propagator in SRW code and its application in simulation of high-resolution fresnel zone plate** [12697-8]

MIRRORS AND GRATINGS

- 12697 04 **Comparing coherent mode decomposition methods for undulator radiation in modern synchrotron light sources** [12697-9]
- 12697 05 **Exploring the use of x-ray adaptive optics in soft x-ray grating monochromators with wavefront propagation simulations** [12697-20]
- 12697 06 **Machine learning-based alignment for LCLS-II-HE optics** [12697-13]

SIMULATION OF EXPERIMENTS I

- 12697 07 **SimEx-Lite: easy access to start-to-end simulation for experiments at advanced light sources (Invited Paper)** [12697-22]
- 12697 08 **Transverse coherence properties and propagation of x-ray radiation from spontaneous and free-electron laser sources (Invited Paper)** [12697-4]

SIMULATION OF EXPERIMENTS II

- 12697 09 **GPU accelerated simulations of time-dependent coherent x-ray scattering experiments** [12697-27]
- 12697 0A **PyCSFex: an extensible Python three package for calculating x-ray structure factors in complex crystals** [12697-10]
- 12697 0B **Latent Bayesian optimization for the autonomous alignment of synchrotron beamlines** [12697-16]

METHODS FOR BEAMLINE ALIGNMENT AND CONTROL

- 12697 0C **AI-driven real-time optics control system to achieve aberration-free coherent wavefronts at fourth-generation synchrotron radiation and free electron laser beamlines (Invited Paper)**
[12697-12]

POSTER SESSION

- 12697 0D **Recent updates of the Sirepo-Bluesky library for virtual beamline representation** [12697-17]