



# Threedimensional Xray Diffraction Microscopy

**Turab Lookman, Stephan  
Eidenbenz, Frank Alexander, Cris  
Barnes**



## **Threedimensional Xray Diffraction Microscopy:**

*Three-Dimensional X-Ray Diffraction Microscopy* Henning Friis Poulsen, 2014-01-15      *Three-Dimensional X-Ray Diffraction Microscopy* Henning Friis Poulsen, 2004-08-31 Three dimensional x ray diffraction 3DXRD microscopy is a novel experimental method for structural characterisation of polycrystalline materials The position morphology phase strain and crystallographic orientation of hundreds of grains or sub grain embedded within mm cm thick specimens can be determined simultaneously Furthermore the dynamics of the individual structural elements can be monitored during typical processes such as deformation or annealing The book gives a comprehensive account of the methodology followed by a summary of selected applications The method is presented from a mathematical crystallographic point of view but with sufficient hands on details to enable the reader to plan his or her own experiments The scope of applications includes work in materials science and engineering geophysics geology chemistry and pharmaceutical science      High-resolution Ab Initio Three-dimensional X-ray Diffraction Microscopy, 2006 Coherent x ray diffraction microscopy is a method of imaging nonperiodic isolated objects at resolutions limited in principle by only the wavelength and largest scattering angles recorded We demonstrate x ray diffraction imaging with high resolution in all three dimensions as determined by a quantitative analysis of the reconstructed volume images These images are retrieved from the three dimensional diffraction data using no a priori knowledge about the shape or composition of the object which has never before been demonstrated on a nonperiodic object We also construct two dimensional images of thick objects with greatly increased depth of focus without loss of transverse spatial resolution These methods can be used to image biological and materials science samples at high resolution with x ray undulator radiation and establishes the techniques to be used in atomic resolution ultrafast imaging at x ray free electron laser sources      **A Microstructure Reconstruction Approach for Three Dimensional X-ray Diffraction Microscopy** Changshi Xiao, 2006      **High-resolution Ab-initio Three-dimensional Coherence X-ray Diffraction Microscopy** A. Barty, 2005 Three dimensional diffraction microscopy offers the potential for high resolution aberration free diffraction limited 3D images without the resolution and depth of field limitations of lens based tomographic systems Critical issues in obtaining a high quality image include 1 Data collection signal to noise system stability dynamic range automation 2 Alignment of diffraction patterns with respect to one another 3 Assembly of the diffraction data into a diffraction volume and 4 Efficient algorithms for applying phase retrieval techniques to the diffraction volume 5 Stability of the three dimensional phase retrieval process 6 Techniques for determining the object support and 7 Treatment of missing data both within the beamstop region and elsewhere They have obtained high quality 3D reconstructions from X ray diffraction data alone This is an important step as it does not require a low resolution image to fill in the beamstop region      **International Tables for Crystallography, Volume F** Eddy Arnold, Daniel M. Himmel, Michael G. Rossmann, 2012-03-05 International Tables for Crystallography Volume F is an expert guide to macromolecular crystallography for the structural biologist It was

commissioned by the International Union of Crystallography in recognition of the extraordinary contributions that knowledge of macromolecular structure has made and will make to the analysis of biological systems from enzyme catalysis to the workings of a whole cell The volume covers all stages of a crystallographic analysis from the preparation of recombinant proteins through crystallization diffraction data collection phase determination structure validation and structure analysis Although the volume is written for experienced scientists it is recognized that the reader is more likely to be a biologist interested in structure than a classical crystallographer interested in biology Thus there are chapters on the fundamentals history and current perspectives of macromolecular crystallography as well as on useful programs and databases such as the Protein Data Bank Each chapter is written by one or more internationally recognized experts This second edition features 19 new articles and many articles from the first edition have been revised The new articles cover topics such as standard definitions for quality indicators expression of membrane proteins protein engineering high throughput crystallography radiation damage merohedral twinning low resolution ab initio phasing robotic crystal loading whole cell X ray diffraction imaging and halogen interactions in biological crystal structures There are also new articles on relevant software including software for electron microscopy These enhancements will ensure that Volume F continues to be a key reference for macromolecular crystallographers and structural biologists More information on the series can be found at <http://it.iucr.org>

*High-resolution Ab Initio Three-dimensional X-ray Diffraction Microscopy (CXIDB ID 15)*. ,2011 The file contains 125 images corresponding to different tilts of the sample around the y axis at 1 degree intervals Each image is the result of 4 exposures merged together For more details see the citation

**X-ray Tomographic Microscopy and Its Three-dimensional Image Reconstruction with a Limited Number of Views** Heung-Rae Lee,1995

*Materials Discovery and Design* Turab Lookman,Stephan Eidenbenz, Frank Alexander, Cris Barnes,2018-09-22 This book addresses the current status challenges and future directions of data driven materials discovery and design It presents the analysis and learning from data as a key theme in many science and cyber related applications The challenging open questions as well as future directions in the application of data science to materials problems are sketched Computational and experimental facilities today generate vast amounts of data at an unprecedented rate The book gives guidance to discover new knowledge that enables materials innovation to address grand challenges in energy environment and security the clearer link needed between the data from these facilities and the theory and underlying science The role of inference and optimization methods in distilling the data and constraining predictions using insights and results from theory is key to achieving the desired goals of real time analysis and feedback Thus the importance of this book lies in emphasizing that the full value of knowledge driven discovery using data can only be realized by integrating statistical and information sciences with materials science which is increasingly dependent on high throughput and large scale computational and experimental data gathering efforts This is especially the case as we enter a new era of big data in materials science with the planning of future experimental

facilities such as the Linac Coherent Light Source at Stanford LCLS II the European X ray Free Electron Laser EXFEL and MaRIE Matter Radiation in Extremes the signature concept facility from Los Alamos National Laboratory These facilities are expected to generate hundreds of terabytes to several petabytes of in situ spatially and temporally resolved data per sample The questions that then arise include how we can learn from the data to accelerate the processing and analysis of reconstructed microstructure rapidly map spatially resolved properties from high throughput data devise diagnostics for pattern detection and guide experiments towards desired targeted properties The authors are an interdisciplinary group of leading experts who bring the excitement of the nascent and rapidly emerging field of materials informatics to the reader

**Physical Metallurgy** David E. Laughlin, Kazuhiro Hono, 2014-07-24 This fifth edition of the highly regarded family of titles that first published in 1965 is now a three volume set and over 3 000 pages All chapters have been revised and expanded either by the fourth edition authors alone or jointly with new co authors Chapters have been added on the physical metallurgy of light alloys the physical metallurgy of titanium alloys atom probe field ion microscopy computational metallurgy and orientational imaging microscopy The books incorporate the latest experimental research results and theoretical insights Several thousand citations to the research and review literature are included Exhaustively synthesizes the pertinent contemporary developments within physical metallurgy so scientists have authoritative information at their fingertips Replaces existing articles and monographs with a single complete solution Enables metallurgists to predict changes and create novel alloys and processes

**Texture and Anisotropy of Polycrystals II** Claude Esling, Michel Humbert, Robert A. Schwarzer, Francis Wagner, 2005-07-15 ITAP 2 Proceedings of the International Conference on Texture and Anisotropy of Polycrystals ITAP 2

**Textures of Materials - ICOTOM 13** Dong Nyung Lee, 2002-08-20 Proceedings of the 13th Int Conference on Textures of Materials ICOTOM 13 Seoul Korea 26 30 August 2002

**Texture and Anisotropy of Polycrystals** Flavio Deflorian, 1998-02-16 Proceedings of the International Conference on Texture and Anisotropy of Polycrystals ITAP 97 Clausthal Germany September 1997

New Method to Reconstruct Three-dimensional Images Under Limited Number of Angles on Non-crystalline X-ray Diffraction Microscopy □□□, 2009

Aluminium Alloys 2014 - ICAA14 Knut Marthinsen, Bjorn Holmedal, Yan Jun Li, 2014-06-20 Selected peer reviewed papers from the 14th International Conference on Aluminium Alloys ICAA14 June 15 19 2014 Trondheim Norway

Three-dimensional Microscopy, 1995

*Journal of the Optical Society of America*, 2006

*Developments in X-ray Tomography*, 2006

**Applications of X-rays in Mechanical Engineering--2004**, 2004

**Design and Characterization of a Novel Near Field Detector for Three Dimensional X-ray Diffraction** Scott Annett, 2015

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