Electromechanical Response of Polycrystalline Barium Titanate Resolved at the Grain Scale
Ferroic materials are critical components in many modern devices. Polycrystalline states of these materials dominate the market due to their cost effectiveness and ease of production. Studying the coupling of ferroic properties across grain boundaries and within clusters of grains is therefore critical for understanding bulk polycrystalline ferroic behavior. Here, three-dimensional X-ray diffraction is used to reconstruct a 3D grain map (grain orientations and neighborhoods) of a polycrystalline barium titanate sample and track the grain-scale non-180° ferroelectric domain switching strains of 139 individual grains in situ under an applied electric field. The map shows that each grain is located in a very unique local environment in terms of intergranular misorientations, leading to local strain heterogeneity in the as-processed state of the sample. While primarily dependent on the crystallographic orientation relative to the field directions, the response of individual grains is also heterogeneous. These unique experimental results are of critical importance both when building the starting conditions and considering the validity of grain-scale modeling efforts, and provide additional considerations in the design of novel ferroic materials.
Grain interaction mechanisms leading to intragranular orientation spread in tensile deformed bulk grains of interstitial-free steel
The spatially resolved intragranular orientation spread in two representative bulk grains of interstitial-free steel deformed to 9% tension has been investigated. A three-dimensional X-ray diffraction microscopy experiment revealed that the two similarly oriented grains are both embedded in local environments representing the bulk texture, yet their deformation-induced rotations are very different. The ALAMEL model is employed to analyse the grain interaction mechanisms. Predictions of this model qualitatively agree with the directionality and magnitude of the experimental orientation spread. However, quantitative agreement requires fine-tuning of the boundary conditions. The majority of the modelled slip is accounted for by four slip systems also predicted to be active by the classical Taylor model in uniaxial tension, and most of the orientation spread along the grain boundaries is caused by relative variations in the activities of these. Although limited to two grains, the findings prove that shear at the grain boundaries as accounted for by the ALAMEL model is a dominant grain interaction mechanism.

**General information**

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Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Physics, Neutrons and X-rays for Materials Physics, European Synchrotron Radiation Facility
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Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.638 SNIP 2.613
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Direct observation of grain rotations during coarsening of a semisolid Al-Cu alloy

Sintering is a key technology for processing ceramic and metallic powders into solid objects of complex geometry, particularly in the burgeoning field of energy storage materials. The modeling of sintering processes, however, has not kept pace with applications. Conventional models, which assume ideal arrangements of constituent powders while ignoring their underlying crystallinity, achieve at best a qualitative description of the rearrangement, densification, and coarsening of powder compacts during thermal processing. Treating a semisolid Al-Cu alloy as a model system for late-stage sintering—during which densification plays a subordinate role to coarsening—we have used 3D X-ray diffraction microscopy to track the changes in sample microstructure induced by annealing. The results establish the occurrence of significant particle rotations, driven in part by the dependence of boundary energy on crystallographic misorientation. Evidently, a comprehensive model for sintering must incorporate crystallographic parameters into the thermodynamic driving forces governing microstructural evolution.

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Ulm, University of Copenhagen, Japan Synchrotron Radiation Research Institute
Authors: Dake, J. M. (Ekstern), Oddershede, J. (Intern), Sørensen, H. O. (Ekstern), Werz, T. (Ekstern), Shatto, J. C. (Ekstern), Uesugi, K. (Ekstern), Schmidt, S. (Intern), Krill III, C. E. (Ekstern)
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Heterogeneous grain-scale response in ferroic polycrystals under electric field

Understanding coupling of ferroic properties over grain boundaries and within clusters of grains in polycrystalline materials is hindered due to a lack of direct experimental methods to probe the behaviour of individual grains in the bulk of a material. Here, a variant of three-dimensional X-ray diffraction (3D-XRD) is used to resolve the non-180° ferroelectric domain switching strain components of 191 grains from the bulk of a polycrystalline electro-ceramic that has undergone an electric-field-induced phase transformation. It is found that while the orientation of a given grain relative to the field direction has a significant influence on the phase and resultant domain texture, there are large deviations from the average behaviour at the grain scale. It is suggested that these deviations arise from local strain and electric field neighbourhoods being highly heterogeneous within the bulk polycrystal. Additionally, the minimisation of electrostatic potentials at the grain boundaries due to interacting ferroelectric domains must also be considered. It is found that the local grain-scale deviations average out over approximately 10–20 grains. These results provide unique insight into the grain-scale interactions of ferroic materials and will be of value for future efforts to comprehensively model these and related materials at that length-scale.
Mapping of strain mechanisms in barium titanate by three-dimensional X-ray diffraction

This thesis presents an in-situ three-dimensional study of the grain-scale response of a prototypical piezoelectric ceramic, barium titanate (BT), to an externally applied electric field. Piezoceramics take advantage of the coupling of electrical and mechanical energies for use in sensors and actuators, found in both common applications such as fuel injectors and specialized applications such as medical imaging equipment. Since piezoceramics are typically used in the polycrystalline state it is important to consider not just the crystal structure but also the role of intergranular effects in the structure-properties relationships. Such effects are difficult to observe using destructive two-dimensional microscopy techniques and averaged over the entire sample in conventional powder diffraction studies. We instead use a combination of
nondestructive three-dimensional X-ray diffraction techniques to study the material at the grain scale. First, we use the intensity ratios of split diffraction peaks to extract grain-scale domain volume fractions for 139 grains. We find that even in the as-processed state there exist unequal volume fractions of each domain type, which we attribute to a heterogeneous local environment at the cubic to tetragonal transition during processing. When a field is applied, we observe a first-order orientation dependence with second order deviations, again attributed to the grain neighbourhood effect. Corelation of this with microstructural parameters such as grain size, neighbour misorientation and position within the sample did not reveal any obvious causes.

Next we develop a novel indexing and refinement method whereby the peak positions of domains are forward projected from crystallographic twinning orientations and the deviation between projected and measured diffraction patterns is minimized to refine domain-scale orientations and lattice parameters. We present the results of refinement for a bulk grain in which the domains are found to be misoriented from perfect crystallographic twins by 0.1-0.3°, suggesting a strained microstructure. The data set was collected by illuminating the entire width of the sample with a box beam, thus it contains a statistically significant number of grains for which domain-scale parameters will be refined in the future.
Time-of-flight 3D Neutron Diffraction for Multigrain Crystallography

This thesis presents a new technique for measuring spatially resolved microstructures in crystalline materials using pulsed neutron beams. The method, called Time-of-Flight Three Dimensional Neutron Diffraction (ToF 3DND), identifies the position, shape, and crystallographic orientation of the individual grains within the sample. The experiments were conducted at the single crystal diffractometer SENJU at the Japanese neutron source J-PARC. The choice of this instrument was motivated by its large coverage of the reciprocal space.

The instrument had to undergo modifications to enable ToF 3DND measurements: a time resolved imaging detector, developed at University of Berkeley, California, was fitted in the interior of SENJU in order to record the extinction spots in the transmitted beam (i.e. areas with missing intensity due to Bragg diffraction of the individual grains).

The arrangement of the two detector systems facilitated two versions of ToF 3DND. The first version, restricted to imaging data, enables reconstruction of the position and shape of the individual grains without the use of crystallography. Afterwords, the orientations of the individual grains are indexed. The algorithms for both steps have been developed in this study. The work also shows that based on the transmission data alone the orientations are not uniquely determined; however, it is possible to find an unique solution by including diffraction signals from the imaging detector. The second version uses an existing method for indexing SENJU data, which then serves as prior information to restrict the extinction spots that belong to the same grain.

The ToF 3DND methods are verified through the study of two different samples: an Iron rod and a shape memory alloy (SMA) CoNiGa bi-crystal. Part of this verification involves comparison with electron backscatter diffraction (EBSD). In the Iron rod, 107 grains were indexed from the SENJU data. As a comparison, 108 grains were reconstructed from the nearfield data alone. This constitutes roughly 10 times as many grains as previously reported using a continuous neutron source.

Thanks to the penetrating properties of the neutron, ToF 3DND complements existing X-ray techniques in those cases where X-rays cannot penetrate the sample. Besides, with ToF 3DND it is also much easier to detect light elements such as those in energy materials.

With a future availability of an energy dispersive x-ray detector with high energy resolution, the methods reported here can be directly transferred to synchrotron and white beam based studies.
3D Neutron Diffraction

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, European Spallation Source ESS AB, Business Region Skåne, University of California at Berkeley, J-PARC, ISIS, Paul Scherrer Institut
Authors: Cereser, A. (Intern), Strobl, M. (Ekstern), Hall, S. (Ekstern), Steuwer, A. (Ekstern), Tremsin, A. (Ekstern), Bergbäck Knudsen, E. (Intern), Willendrup, P. K. (Intern), Kabra, S. (Ekstern), Kelleher, J. (Ekstern), Kockelmann, W. (Ekstern), Peetermans, S. (Ekstern), Shinohara, T. (Ekstern), Schmidt, S. (Intern)
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Dark-field X-ray microscopy for multiscale structural characterization
Many physical and mechanical properties of crystalline materials depend strongly on their internal structure, which is typically organized into grains and domains on several length scales. Here we present dark-field X-ray microscopy; a non-destructive microscopy technique for the three-dimensional mapping of orientations and stresses on lengths scales from 100 nm to 1mm within embedded sampling volumes. The technique, which allows “zooming” in and out in both direct and angular space, is demonstrated by an annealing study of plastically deformed aluminium. Facilitating the direct study of the interactions between crystalline elements is a key step towards the formulation and validation of multiscale models that account for the entire heterogeneity of a material. Furthermore, dark-field X-ray microscopy is well suited to applied topics, where the structural evolution of internal nanoscale elements (for example, positioned at interfaces) is crucial to the performance and lifetime of macro-scale devices and components thereof.

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Materials characterisation tools towards lead-free piezoceramics

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Authors: Oddershede, J. (Intern), Majkut, M. (Intern), Yap, E. (Ekstern), Daniels, J. (Ekstern), Schmidt, S. (Intern)
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On the deformation twinning of Mg AZ31B: A three-dimensional synchrotron X-ray diffraction experiment and crystal plasticity finite element model
Crystals with a hexagonal close-packed (HCP) structure are inherently anisotropic, and have a limited number of independent slip systems, which leads to strong deformation textures and reduced formability in polycrystalline products. Tension along the c-axis of the crystal ideally activates extension twinning as a deformation mode due to the lack of easy-slip systems. In this work, experiments were devised to study extension twinning in a polycrystalline Mg alloy AZ31B with a strong basal rolling texture by tensile deformation parallel to the plate normal. Three-dimensional synchrotron X-ray diffraction (3DXRD) was used to map the center-of-mass positions, volumes, orientations, elastic strains, and stress tensors of over 1400 grains in-situ up to a true strain of 1.4%. More than 700 tensile twins were observed to form in the mapped volume under deformation. The measured center-of-mass positions and grain volumes are used to construct various 3D microstructures and model them with a Crystal Plasticity Finite Element (CPFE) code. It is observed that the average grain-resolved stress did not always select the highest ranked Schmid factor twin variant. In fact, the contribution of lower ranked variants was non-negligible. The CPFE simulation indicates that there is a small variation in the stress within each grain in the elastic regime, which increases drastically upon the onset of plasticity. One of the significant
outcomes of this work is the new statistical information on the interaction between twin and parent grain. It is shown that, on average, there is a small difference between the stress normal to the twin habit plane in the parent and twin, but that this is not the case for the shear acting on the habit plane.
Quantitative grain-scale ferroic domain volume fractions and domain switching strains from three-dimensional X-ray diffraction data

A method for the extension of the three-dimensional X-ray diffraction technique to allow the extraction of domain volume fractions in polycrystalline ferroic materials is presented. This method gives access to quantitative domain volume fractions of hundreds of independent embedded grains within a bulk sample. Such information is critical to furthering our understanding of the grainscale interactions of ferroic domains and their influence on bulk properties. The method also provides a validation tool for mesoscopic ferroic domain modelling efforts. The mathematical formulations presented here are applied to tetragonal coarse-grained Ba$_{0.88}$Ca$_{0.12}$Zr$_{0.06}$Ti$_{0.94}$O$_3$ and rhombohedral fine-grained (0.82)Bi$_{0.5}$Na$_{0.5}$TiO$_3$–(0.18)Bi$_{0.5}$K$_{0.5}$TiO$_3$ electroceramic materials. The fitted volume fraction information is used to calculate grain-scale non-180° ferroelectric domain switching strains. The absolute errors are found to be approximately 0.01 and 0.03% for the tetragonal and rhombohedral cases, which had maximum theoretical domain switching strains of 0.47 and 0.54%, respectively. Limitations and possible extensions of the technique are discussed.

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of New South Wales, European Synchrotron Radiation Facility, The Advanced Photon Source
Authors: Oddershede, J. (Intern), Majkut, M. (Intern), Caosyd, Q. (Ekstern), Schmidt, S. (Intern), Wright, J. P. (Ekstern), Kenesei, P. (Ekstern), Daniels, J. E. (Ekstern)
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
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ISI indexed (2013): ISI indexed yes
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Three-dimensional X-ray diffraction (3DXRD) microscopy is a fast and non-destructive structural characterization technique aimed at the study of individual crystalline elements (grains or subgrains) within mm-sized polycrystalline specimens. It is based on two principles: the use of highly penetrating hard X-rays from a synchrotron source and the application of “tomographic” reconstruction algorithms for the analysis of the diffraction data. In favorable cases, the position, morphology, phase, and crystallographic orientation can be derived for up to a thousand elements simultaneously. For each grain its average strain tensor may also be derived, from which the type-II stresses can be inferred. Furthermore, the dynamics of the individual elements can be monitored during typical processes such as deformation or annealing. Hence, information on the interaction between elements can be obtained directly. In this chapter we first provide an overview of the various experimental approaches for 3DXRD that have emerged. Following this, a more detailed presentation of work related to the classical 3DXRD setup is given. Some emphasis is also placed on the
mathematical challenges inherent to the reconstruction of grain and orientation maps.

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Main Research Area: Technical/natural sciences
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**A spherical x-ray transform and hypercube sections**
We investigate the problem of sampling a unit great circle on the unit sphere S-3 as a support of orientation distribution functions on which acts the discrete spherical x-ray transform. The circle's partition subsets are gnomonically mapped onto lines that constitute a convex polygon inside the bounding cubes of hypercube. Thus the problem of the great circle tracing is reduced to the problem of the four-dimensional cube sectioning by the plane containing the circle and the intersection figure (the polygon) vertices finding. In this paper, a fast, non-combinatorial approach for the polygon tracing within the general multi-dimensional frame is proposed.

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Institute of Computational Mathematics and Mathematical Geophysics
Authors: Kazantsev, I. G. (Ekstern), Schmidt, S. (Intern)
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Scopus rating (2015): SJR 0.589 SNIP 1.09 CiteScore 0.8
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.663 SNIP 1.205 CiteScore 0.69
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.433 SNIP 1.092 CiteScore 0.74
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.42 SNIP 0.863 CiteScore 0.5
Direct observation of grain boundary migration during recrystallization within the bulk of a moderately deformed aluminium single crystal

A single grain growing in the bulk of a mildly deformed (30% thickness reduction through cold rolling) aluminium single crystal with an \(\{001\}\langle100\rangle\) orientation (Cube orientation), is monitored during recrystallization with synchrotron radiation using topo-tomography. The formation and migration of planar boundary segments (facets) are analyzed using a method that determines the displacements of local boundary segments along parallel lines perpendicular to the facet plane. Facets are observed to form after a certain annealing time. They migrate at a constant rate for extended periods of time and remain planar during their migration. A change in the migration rate for one facet has been observed which is not related to changes in the experimental conditions and is most likely to be driven by the changes in grain orientation and/or the local deformation microstructure. The crystallography of the analyzed facets is not closely related to any crystallographic \(\{111\}\) plane of neither the growing grain nor the disappearing deformed matrix. © 2013 The Japan Institute of Metals and Materials.

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Three-Dimensional X-ray Diffraction (3DXRD) Microscopy is a generic term covering a variety of different techniques for characterising the microstructure within the bulk of polycrystalline materials. One strategy, namely grain centre mapping, enables fast measurements of the average characteristics of each grain (such as their centre-of-mass positions, volumes, phases, orientations and/or elastic strain tensor components), while the exact locations of the grain boundaries are unknown. In the present chapter a detailed description of the setup and software for both grain centre mapping and the closely related boxscan method is given. Both validation experiments and applications for in situ studies of microstructural changes during plastic deformation and crack growth are given. Finally an outlook with special emphasis on coupling the measured results with modelling is given.

**General information**

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Mechanical Engineering, Materials and Surface Engineering, European Synchrotron Research Facility
Authors: Oddershede, J. (Intern), Schmidt, S. (Intern), Lyckegaard, A. (Intern), Lauridsen, E. M. (Intern), Wright, J. P. (Ekstern), Winther, G. (Intern)

**Grain centre mapping - 3DXRD measurements of average grain characteristics.**

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Scopius rating (2014): SJR 0.73 SNIP 1.035 CiteScore 0.91
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopius rating (2013): SJR 0.491 SNIP 0.724 CiteScore 0.69
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopius rating (2012): SJR 0.554 SNIP 0.766 CiteScore 0.7
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopius rating (2011): SJR 0.591 SNIP 0.695 CiteScore 0.78
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopius rating (2010): SJR 0.72 SNIP 0.855
BFI (2009): BFI-level 1
Scopius rating (2009): SJR 0.674 SNIP 0.794
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopius rating (2008): SJR 0.711 SNIP 0.795
Web of Science (2008): Indexed yes
Scopius rating (2007): SJR 0.942 SNIP 1.165
Scopius rating (2006): SJR 0.892 SNIP 0.934
Web of Science (2006): Indexed yes
Scopius rating (2005): SJR 1.031 SNIP 1.104
Scopius rating (2004): SJR 0.927 SNIP 1.168
Scopius rating (2003): SJR 1.145 SNIP 1.116
Scopius rating (2002): SJR 1.191 SNIP 1.184
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GrainSpotter: a fast and robust polycrystalline indexing algorithm

A new approach for indexing multigrain diffraction data is presented. It is based on the use of a monochromatic beam simultaneously illuminating all grains. By operating in sub-volumes of Rodrigues space, a powerful vertex-finding algorithm can be applied, with a running time that is compatible with online analysis. The resulting program, GrainSpotter, is sufficiently fast to enable online analysis during synchrotron sessions. The program applies outlier rejection schemes, leading to more robust and accurate data. By simulations it is shown that several thousand grains can be retrieved. A new method to derive partial symmetries, called pseudo-twins, is introduced. Uniquely, GrainSpotter includes an analysis of pseudo-twins, which is shown to be critical to avoid erroneous grains resulting from the indexing.
Novel applications of the x-ray tracing software package McXtrace

We will present examples of applying the X-ray tracing software package McXtrace to different kinds of X-ray scattering experiments. In particular we will be focusing on time-resolved type experiments. Simulations of full scale experiments are particularly useful for this kind, especially when they are performed at an FEL-facility. Beamtime here is extremely scarce and the delay between experiment and publication is notoriously long. A major cause for the delay is the general complexity of the experiments performed. A complexity which arises from the pulsed state of the source. As an example, consider a pump-and-probe type experiment. In order to get the wanted signal from the sample the X-ray pulse from the FEL source needs to overlap in space and time with the pumping pulse inside the sample. This is made more difficult by several effects: The sample response may be dependent of the polarisation of the pumping and/or probing pulse. There may be significant time-jitter in the pulse arrival times. The composition of the sample may vary depending on local sample geometry and be modified by the probing pulse. Many of the samples considered are in a liquid state and thus have a variable geometry. ...to name some of the issues encountered. Generally more than one or all of these effects are present at once. Simulations can in these cases be used to identify distinct footprints of such distortions and thus give the experimenter a means of deconvoluting them from the signal. We will present a study of this kind along with the newest developments of the McXtrace software package.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, St. Olaf College
Authors: Bergbäck Knudsen, E. (Intern), Nielsen, M. M. (Intern), Haldrup, K. (Intern), Topel, E. (Ekstern), Schmidt, S. (Intern)
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McXtrace: A Monte Carlo software package for simulating X-ray optics, beamlines and experiments

This article presents the Monte Carlo simulation package McXtrace, intended for optimizing X-ray beam instrumentation and performing virtual X-ray experiments for data analysis. The system shares a structure and code base with the popular neutron simulation code McStas and is a good complement to the standard X-ray simulation software SHADOW. McXtrace is open source, licensed under the General Public License, and does not require the user to have access to any proprietary software for its operation. The structure of the software is described in detail, and various examples are given to showcase the versatility of the McXtrace procedure and outline a possible route to using Monte Carlo simulations in data analysis to gain new scientific insights. The studies performed span a range of X-ray experimental techniques: absorption tomography, powder diffraction, single-crystal diffraction and pump-and-probe experiments. Simulation studies are compared with experimental data and theoretical calculations. Furthermore, the simulation capabilities for computing coherent X-ray beam properties and a comparison with basic diffraction theory are presented. © 2013 International Union of Crystallography.
In recent years, increased focus on the potentially harmful effects of x-ray computed tomography (CT) scans, such as radiation-induced cancer, has motivated research on new low-dose imaging techniques. Sparse image reconstruction methods, as studied for instance in the field of compressed sensing (CS), have shown significant empirical potential for this purpose. For example, total variation regularized image reconstruction has been shown in some cases to allow reducing x-ray exposure by a factor of 10 or more, while maintaining or even improving image quality compared to conventional reconstruction methods.

However, the potential in CT has mainly been demonstrated in individual proof-of-concept studies, from which it is hard to distill general conditions for when sparse reconstruction methods perform well. As a result, there is a fundamental lack of understanding of the effectiveness and limitations of sparse reconstruction methods in CT, in particular in a quantitative sense. For example, relations between image properties such as contrast, structure and sparsity, tolerable noise levels,
sufficient sampling levels, the choice of sparse reconstruction formulation and the achievable image quality remain unclear. This is a problem of high practical concern, because the large scale of CT problems makes detailed exploration of the parameter space very time-consuming. Due to the limited quantitative understanding, sparse reconstruction has not yet become the method of choice in practical CT applications.

This thesis takes a systematic approach toward establishing quantitative understanding of conditions for sparse reconstruction to work well in CT. A general framework for analyzing sparse reconstruction methods in CT is introduced and two sets of computational tools are proposed:

1. An optimization algorithm framework enabling easy derivation of algorithms for sparse reconstruction problems, and
2. Tools for characterizing sparse reconstruction in CT, i.e., establishing relations between parameters governing reconstruction quality.

The flexibility of the optimization algorithm framework is demonstrated by constructing convergent optimization algorithms for a range of sparse reconstruction problems of interest to CT. The practical usefulness of the framework is shown through case studies of the effectiveness of specific sparse reconstruction problems in tomographic reconstruction.

The characterization methods proposed in the thesis focus on the role of image sparsity for the level of sampling required for accurate CT reconstruction. While a relation between sparsity and sampling is motivated by CS, no theoretical guarantees of accurate sparse reconstruction are known for CT. In simulation studies, a sparsity-sampling relation is established in CT. This enables quantification of the undersampling allowed by sparse reconstruction methods.

Both the prototyping framework and the characterization methods add to the understanding of sparse reconstruction methods in CT and serve as initial contributions to a general set of computational characterization tools. Thus, the thesis contributions help advance sparse reconstruction methods toward routine use in.
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  Scopus rating (2013): SNIP 0.342 SJR 0.235 CiteScore 0.28
  ISI indexed (2013): ISI indexed yes
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  BFI (2009): BFI-level 1
  Scopus rating (2009): SNIP 0.389 SJR 0.343
  BFI (2008): BFI-level 1
  Scopus rating (2008): SJR 0.297 SNIP 0.358
  Web of Science (2008): Indexed yes
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  Scopus rating (2006): SJR 0.37 SNIP 0.511
  Web of Science (2006): Indexed yes
  Scopus rating (2005): SJR 0.41 SNIP 0.56
  Web of Science (2005): Indexed yes
  Scopus rating (2004): SJR 0.449 SNIP 0.575
  Web of Science (2004): Indexed yes
  Scopus rating (2003): SNIP 0.548 SJR 0.457
  Web of Science (2003): Indexed yes
  Scopus rating (2002): SNIP 0.514 SJR 0.432
  Web of Science (2002): Indexed yes
  Scopus rating (2001): SNIP 0.524 SJR 0.403
  Web of Science (2001): Indexed yes
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Source: orbit
Source-ID: 315786
Measuring the stress field around an evolving crack in tensile deformed Mg AZ31 using three-dimensional X-ray diffraction

The stress field around a notch in a coarse grained Mg AZ31 sample has been measured under tensile load using the individual grains as probes in an in situ high energy synchrotron diffraction experiment. The experimental set-up, a variant of three-dimensional X-ray diffraction microscopy, allows the position, orientation and full stress tensor of each illuminated grain to be determined and, hence, enables the study of evolving stress fields in coarse grained materials with a spatial resolution equal to the grain size. Grain resolved information like this is vital for understanding what happens when the traditional continuum mechanics approach breaks down and fracture is governed by local heterogeneities (e.g. phase or stress differences) between grains. As a first approximation the results obtained were averaged through the thickness of the sample and compared with an elastic–plastic continuum finite element simulation. It was found that a full three-dimensional simulation was required to account for the measured transition from the overall plane stress case away from the notch to the essentially plane strain case observed near the notch tip. The measured and simulated stress contours were shown to be in good agreement except at the highest applied load, at which stress relaxation at the notch tip was observed in the experimental data. This stress relaxation is attributed to the initiation and propagation of a crack. Finally, it was demonstrated that the measured lattice rotations could be used as a qualitative measure of the shape and extent of the plastic deformation zone.
Multigrain crystallography

We summarize exploratory work on multigrain crystallography. The experimental arrangement comprises a monochromatic beam, a fully illuminated sample with up to several hundred grains in transmission geometry on a rotary table and a 2D detector. Novel algorithms are presented for indexing, integration and filtering with emphasis on handling the complications of spot overlap and the need for on-line analysis. The structure solution and refinement steps are performed by conventional single crystal programs. Simulations are used to verify the algorithms and to probe the overall limitations of the methodology in terms of number of grains, size of unit cell and direct space resolution. First experimental results in the fields of chemistry, structural biology and time-resolved studies in photochemistry are presented. As an outlook, the concept of TotalCrystallography is introduced, defined as the simultaneous characterization of the 3D atomic, and 3D grain-scale structure of polycrystalline specimens with phases of unknown composition and structure.
New 3DXRD results on recrystallization and grain growth

New in-situ 3DXRD results obtained since the last Rex&GG conference are presented and discussed. This includes:

Documentation of the formation of nuclei with new orientations, determination of apparent activation energies for individual bulk grains during recrystallization and evolution in the 3D microstructure during grain growth

General information

State: Published
Organisations: Department of Wind Energy, Materials science and characterization, Department of Energy Conversion and Storage, Department of Physics
Authors: Juul Jensen, D. (Intern), West, S. (Intern), Poulsen, S. O. (Intern), Schmidt, S. (Intern)
Pages: 393-398
Non-destructive identification of micrometer-scale minerals and their position within a bulk sample

Using the conventional techniques of mineralogy, it has been a challenge to determine mineral identity, crystal orientation and spatial position of micrometer-sized crystals that are embedded in a rock, sediment or soil. Traditionally, the individual grains must be extracted and analyzed separately. Crushing or disintegrating a sample annihilates any possibility for gathering information from the texture of the porous media or the mineral assemblage close to the grains in question. A new method using three-dimensional X-ray diffraction (3DXRD) microscopy can be successfully applied to natural materials. We combined X-ray microtomography (XMT) and 3DXRD to investigate a sample of very fine-grained chalk containing fracture minerals. The XMT technique provides three-dimensional images of the particles and pore structure at very high resolution (350 nm voxel dimension) on samples less than 500 μm in diameter. The minor phases present as crystals in fractures were determined nondestructively with 3DXRD microscopy. The chalk fragment investigated is composed predominantly of randomly oriented nanometric crystals of calcite that produce powder rings where no texture can be observed. Superimposed on this pattern, Bragg diffraction peaks from the other crystalline phases were observed. Individual crystals of barite and pyrite only a few micrometers in diameter are present in the fractures. Magnetite, celestine and siderite, other minerals that might have been expected based on the XMT absorption contrast, were not identified. The crystal shape and in-fracture location, derived from the microtomograms, and the mineral identity, derived from 3DXRD, allowed us to propose that the fractures are original in these tiny drill cuttings; they were not induced by drilling and filled with drilling mud particles, thus allowing reliable estimates to be made of rock porosity and permeability.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Informatics and Mathematical Modeling, Department of Energy Conversion and Storage, Electrofunctional materials, Experimental Surface and Nanomaterials Physics, University of Copenhagen
Authors: Sørensen, H. O. (Ekstern), Hakim, S. S. (Ekstern), Pedersen, S. (Ekstern), Christiansen, C. B. (Forskerdatabase), Balogh, Z. I. (Intern), Hem, C. P. (Forskerdatabase), Pasarin, I. S. (Ekstern), Schmidt, S. (Intern), Olsen, U. L. (Intern), Oddershede, J. (Intern), Frandsen, C. (Intern), Feidenhans’L, R. (Ekstern), Stipp, S. L. S. (Forskerdatabase)
Pages: 501-509
Publication date: 2012
Main Research Area: Technical/natural sciences

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BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.504 SNIP 0.716 CiteScore 0.97
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.614 SNIP 0.637 CiteScore 0.96
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.972 SNIP 0.823 CiteScore 1.26
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.015 SNIP 0.846 CiteScore 1.14
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.817 SNIP 1.001 CiteScore 1.26
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.75 SNIP 0.929 CiteScore 1.12
Quantification of mineral behavior in four dimensions: Grain boundary and substructure dynamics in salt

Here we present the first four dimensional (time and three dimensional space resolved) experiment on a strongly deformed geological material. Results show that even complicated microstructures with large continuous and discontinuous changes in crystallographic orientation can be resolved quantitatively. The details that can be resolved are unprecedented and therefore the presented technique promises to become influential in a wide range of geoscientific investigations. Grain and subgrain scale processes are fundamental to mineral deformation and associated Earth Dynamics, and time resolved observation of these processes is vital for establishing an in-depth understanding of the latter. However, until recently, in situ experiments were restricted to observations of two dimensional surfaces. We compared experimental results from two dynamic, in situ annealing experiments on a single halite crystal; a 2D experiment conducted inside the scanning electron microscope and a 3D X-ray diffraction experiment. This allowed us to evaluate the possible effects of the free surface on grain and subgrain processes. The extent to which surface effects cause experimental artifacts in 2D studies has long been questioned. Our study shows that, although the nature of recovery processes are the same, the area swept by subgrain boundaries is up to 5 times larger in the volume than observed on the surface. We suggest this discrepancy is due to enhanced drag force on subgrain boundaries by thermal surface grooving. Our results show that while it is problematic to derive absolute mobilities from 2D experiments, derived relative mobilities between boundaries with different misorientation angles can be used.

General information
State: Published
Organisations: Department of Physics, Stockholm University, Macquarie University, European Synchrotron Radiation Facility
Authors: Borthwick, V. E. (Ekstern), Schmidt, S. (Intern), Piazolo, S. (Ekstern), Gundlach, C. (Ekstern)
Number of pages: 9
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Publication date: 2012
Main Research Area: Technical/natural sciences

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Journal: G3: Geochemistry, Geophysics, Geosystems
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Ratings:
BFI (2017): BFI-level 1
In-situ 3D X-ray diffraction (3DXRD) annealing experiments were conducted at the ID-11 beamline at the European Synchrotron Radiation Facility in Grenoble. This allowed us to nondestructively document and subsequently analyse the development of substructures during heating, without the influence of surface effects. A sample of deformed single crystal halite was heated to between 260-400 °C. Before and after heating a volume of 500 by 500 by 300 μm was mapped using a planar beam, which was translated over the sample volume at intervals of 5-10 μm in the vertical dimension. In the following we present partially reconstructed orientation maps over one layer before and after heating for 240min at 260 °C. Additional small syn-heating "maps" over a constrained sample rotation of 12-30°. The purpose of this was to illuminate a few reflections from 1 or 2 subgrains and follow their evolution during heating. Preliminary results show that significant changes occurred within the sample volume, for which, surface effects can be excluded. Results show a number of processes, including: i) change in subgrain boundary misorientation angle and ii) subgrain subdivision into areas of similar lattice orientation with new subgrain boundary formation. These results demonstrate that 3DXRD coupled with in-situ heating is a successful non-destructive technique for examining real-time postdeformational annealing in strongly deformed crystalline materials with complicated microstructures. © (2012) Trans Tech Publications, Switzerland.
3D grain orientation mapping in the transmission electron microscope

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy, Tsinghua University
Authors: Liu, H. (Ekstern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Godfrey, A. (Ekstern), Liu, Z. (Ekstern), Sharon, J. (Ekstern), Huang, X. (Intern)
Publication date: 2011
Main Research Area: Technical/natural sciences
Materials characterisation and modelling
Source: orbit
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3D grain orientation mapping of polycrystals on scales from 1 mm to 1 nm using 3D-XRD and TEM

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy, Tsinghua University
Authors: Huang, X. (Intern), Poulsen, H. F. (Intern), Schmidt, S. (Intern), Godfrey, A. (Ekstern)
Publication date: 2011
Main Research Area: Technical/natural sciences
Electronic versions:
3d grain.pdf
Source: orbit
Source-ID: 313981
Publication: Research › Conference abstract for conference – Annual report year: 2011

A Monte Carlo approach for simulating the propagation of partially coherent x-ray beams
Advances at SR sources in the generation of nanofocused beams with a high degree of transverse coherence call for effective techniques to simulate the propagation of partially coherent X-ray beams through complex optical systems in order to characterize how coherence properties such as the mutual coherence function (MCF) are propagated to the exit plane. Here we present an approach based on Monte Carlo sampling of the Green function. A Gauss-Shell Stochastic Source with arbitrary spatial coherence is synthesized by means of the Gaussian copula statistical tool. The Green function is obtained by sampling Huygens-Fresnel waves with Monte Carlo methods and is used to propagate each source realization to the detector plane. The sampling is implemented with a modified Monte Carlo ray tracing scheme where the optical path of each generated ray is stored. Such information is then used in the summation of the generated rays at the observation plane to account for coherence properties. This approach is used to simulate simple models of propagation in free space and with reflective and refractive optics. © 2011 COPYRIGHT Society of Photo-Optical Instrumentation Engineers (SPIE). Downloading of the abstract is permitted for personal use only.

General information
State: Published
Organisations: Nano-Microstructures in Materials, Materials Research Division, Risø National Laboratory for Sustainable Energy, Metal Structures in Four Dimensions, European Synchrotron Radiation Facility, University of Copenhagen
Grain-resolved elastic strains in deformed copper measured by three-dimensional X-ray diffraction

This X-ray diffraction study reports the grain-resolved elastic strains in about 1000 randomly oriented grains embedded in a polycrystalline copper sample. Diffraction data were collected in situ in the undeformed state and at a plastic strain of
1.5% while the sample was under tensile load. For each grain the centre-of-mass position was determined with an accuracy of 10 μm, the volume with a relative error of 20%, the orientation to 0.05° and the axial strain to 10−4. The elastic strain along the tensile direction exhibited a grain orientation dependence with grains within 20° of carrying the largest strain. While the width of the strain distribution for all grains did not change upon plastic loading, the grain-resolved data show a significant widening of the distribution evaluated for small subsets of initially elastically similar grains. This widening appears independent of the grain orientation.

**General information**
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy, European Synchrotron Research Facility, Max Planck Institute, Technische Universität Berlin
Authors: Oddershede, J. (Intern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Margulies, L. (Intern), Wright, J. (Ekstern), Moscicki, M. (Ekstern), Reimers, W. (Ekstern), Winther, G. (Intern)
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.242 SNIP 1.606 CiteScore 2.61
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.373 SNIP 2.025 CiteScore 2.47
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.183 SNIP 1.79 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.227 SNIP 2.063 CiteScore 2.26
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.132 SNIP 2.21 CiteScore 2.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.231 SNIP 1.767
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.002 SNIP 1.541
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.81 SNIP 1.299
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.623 SNIP 1.16
Scopus rating (2006): SJR 0.625 SNIP 0.948
Scopus rating (2005): SJR 0.693 SNIP 1.218
Scopus rating (2004): SJR 0.67 SNIP 1.017
Scopus rating (2003): SJR 0.468 SNIP 0.899
Web of Science (2003): Indexed yes
Measuring the stress field around an evolving crack in tensile deformed Mg AZ31 using 3DXRD grain centre mapping

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy, Composites and Materials Mechanics
Authors: Oddershede, J. (Intern), Camin, B. (Ekstern), Schmidt, S. (Intern), Mikkelsen, L. P. (Intern), Sørensen, H. O. (Intern), Lienert, U. (Intern), Poulsen, H. F. (Intern), Reimers, W. (Ekstern)
Publication date: 2011
Event: Abstract from MECASENS VI, Hamburg (DE), Sep.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 285479
Publication: Research › Conference abstract for conference – Annual report year: 2011

Simultaneous X-ray diffraction from multiple single crystals of macromolecules

The potential in macromolecular crystallography for using multiple crystals to collect X-ray diffraction data simultaneously from assemblies of up to seven crystals is explored. The basic features of the algorithms used to extract data and their practical implementation are described. The procedure could be useful both in relation to diffraction data obtained from intergrown crystals and to alleviate the problem of rapid diffraction decay arising from the effects of radiation damage.

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Metal Structures in Four Dimensions, Materials Research Division, University of Oxford, European Synchrotron Radiation Facility
Authors: Paithankar, K. S. (Ekstern), Sørensen, H. O. (Intern), Wright, J. P. (Ekstern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Garman, E. F. (Ekstern)
Pages: 608-618
Publication date: 2011
Main Research Area: Technical/natural sciences

Publication information
Journal: Acta Crystallographica. Section D: Biological Crystallography
Three-Dimensional Orientation Mapping in the Transmission Electron Microscope

Over the past decade, efforts have been made to develop nondestructive techniques for three-dimensional (3D) grain-orientation mapping in crystalline materials. 3D x-ray diffraction microscopy and differential-aperture x-ray microscopy can now be used to generate 3D orientation maps with a spatial resolution of 200 nanometers (nm). We describe here a nondestructive technique that enables 3D orientation mapping in the transmission electron microscope of mono- and multiphase nanocrystalline materials with a spatial resolution reaching 1 nm. We demonstrate the technique by an experimental study of a nanocrystalline aluminum sample and use simulations to validate the principles involved.

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy, Tsinghua University, Chinese Academy of Sciences, Johns Hopkins University
Authors: Liu, H. (Intern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Godfrey, A. (Ekstern), Liu, Z. (Ekstern), Sharon, J. (Ekstern), Huang, X. (Intern)
3DXRD measurements of lattice rotations in tensile deformed IF steel

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy, European Synchrotron Research Facility
Authors: Oddershede, J. (Intern), Wright, J. (Ekstern), Margulies, L. (Intern), Huang, X. (Intern), Poulsen, H. F. (Intern), Schmidt, S. (Intern), Winther, G. (Intern)
Pages: 369-374
Publication date: 2010
Conference: 31st Risø International Symposium on Materials Science : Challenges in materials science and possibilities in 3D and 4D characterization techniques, Roskilde, Denmark, 06/09/2010 - 06/09/2010
Main Research Area: Technical/natural sciences

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BFI (2015): BFI-level 1
BFI (2014): BFI-level 1
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BFI (2012): BFI-level 1
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
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BFI (2008): BFI-level 1
Original language: English
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Source: orbit
Source-ID: 266634
Publication: Research - peer-review › Conference article – Annual report year: 2010

4D characterization of metals by 3DXRD

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Materials Research Division, Metal Structures in Four Dimensions, European Synchrotron Radiation Facility
, Olsen, U. L. (Intern), Oddershede, J. (Intern), Reischig, P. (Ekstern), Lyckegaard, A. (Intern), Wright, J. (Ekstern), Vaughan, G. (Ekstern)
Pages: 101-119
A new principle of orientation determination for 3D electron diffraction microscopy

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy, Tsinghua University
Authors: Liu, H. (Intern), Poulsen, H. F. (Intern), Schmidt, S. (Intern), Sørensen, H. O. (Intern), Godfrey, A. (Ekstern), Huang, X. (Intern)
Pages: 311-316
Publication date: 2010
Conference: 31st Risø International Symposium on Materials Science : Challenges in materials science and possibilities in 3D and 4D characterization techniques, Roskilde, Denmark, 06/09/2010 - 06/09/2010
Main Research Area: Technical/natural sciences
Determining grain resolved stresses in polycrystalline materials using three-dimensional X-ray diffraction

An algorithm is presented for characterization of the grain resolved (type II) stress states in a polycrystalline sample based on monochromatic X-ray diffraction data. The algorithm is a robust 12-parameter-per-grain fit of the centre-of-mass grain positions, orientations and stress tensors including error estimation and outlier rejection. The algorithm is validated by simulations and by two experiments on interstitial free steel. In the first experiment, using only a far-field detector and a rotation range of $2 \times 110^\circ$, 96 grains in one layer were monitored during elastic loading and unloading. Very consistent results were obtained, with mean resolutions for each grain of approximately $10 \mu m$ in position, $0.05^\circ$ in orientation, and 8, 20 and $13 \times 10^{-5}$ in the axial, normal and shear components of the strain, respectively. The corresponding mean deviations in stress are 30, 50 and 15 MPa in the axial, normal and shear components, respectively, though some grains may have larger errors. In the second experiment, where a near-field detector was added, ~ 2000 grains were characterized with a positional accuracy of $3 \mu m$.

**General information**

State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy, European Synchrotron Radiation Facility, Technische Universität Berlin
Authors: Oddershede, J. (Intern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Sørensen, H. O. (Intern), Wright, J. (Ekstern), Reimers, W. (Ekstern)
Pages: 539-549
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Main Research Area: Technical/natural sciences

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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.322 SNIP 2.588 CiteScore 3.97
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.585 SNIP 4.371 CiteScore 4.76
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.921 SNIP 6.392 CiteScore 6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.572 SNIP 4.687 CiteScore 4.67
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.015 SNIP 5.863 CiteScore 5.32
ISI indexed (2011): ISI indexed yes
Grain resolved stresses in polycrystalline materials from 3DXRD data

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy
Authors: Oddershede, J. (Intern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Reimers, W. (Ekstern)
Publication date: 2010
Event: Abstract from 8th European Conference on Residual Stresses, Riva del Garda (IT), 26-28 Jun, .
Main Research Area: Technical/natural sciences
Materials characterization and modelling, Materials and energy storage
Source: orbit
Source-ID: 261892
Publication: Research - peer-review › Journal article – Annual report year: 2010

Mapping the stresses of individual grains in a polycrystalline material using 3DXRD

General information
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Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy, Technische Universität Berlin
Authors: Oddershede, J. (Intern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Reimers, W. (Ekstern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Measuring type II stresses using 3DXRD
An algorithm is presented for characterization of the grain resolved (type II) stress states in a polycrystalline sample based on monochromatic X-ray diffraction data. The algorithm is a robust 12-parameter-per-grain fit of the centre-of-mass grain positions, orientations and stress tensors including error estimation and outlier rejection. As examples of use results from two experiments – one on interstitial free (IF) steel and one on copper – will be presented. In the first experiment 96 grains in one layer of IF steel were monitored during elastic loading and unloading. Very consistent results were obtained, with resolutions for each grain of approximately 10 µm in position, 0.05˚ in orientation and 80 µstrain. When averaging over all grains a resolution of 10 µstrain was obtained. In the second experiment it was demonstrated that the strain states of more than 1000 grains in a plastically deformed Cu specimen could be determined to an accuracy of 100 µstrain.

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy
Authors: Oddershede, J. (Intern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Reimers, W. (Ekstern)
Pages: 63-69
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Science Forum
Volume: 652
ISSN (Print): 0255-5476
Ratings:
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.186 SNIP 0.306 CiteScore 0.28
BFI (2015): BFI-level 1
Scopus rating (2015): SNIP 0.337 SJR 0.217 CiteScore 0.29
BFI (2014): BFI-level 1
Scopus rating (2014): SNIP 0.448 SJR 0.269 CiteScore 0.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SNIP 0.342 SJR 0.235 CiteScore 0.28
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SNIP 0.467 SJR 0.279 CiteScore 0.34
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SNIP 0.419 SJR 0.247 CiteScore 0.33
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SNIP 0.406 SJR 0.271
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SNIP 0.389 SJR 0.343
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.297 SNIP 0.358
Web of Science (2008): Indexed yes
Measuring type-II stresses using 3XRD

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy, Technische Universität Berlin
Authors: Oddershede, J. (Intern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Reimers, W. (Ekstern)
Publication date: 2010
Event: Poster session presented at German Conference for Research with Synchrotron Radiation, Neutrons and Ion Beams at Large Facilities, Berlin (DE), 24-26 Feb., .
Main Research Area: Technical/natural sciences
Materials characterization and modelling, Materials and energy storage
Source: orbit
Source-ID: 253771
Publication: Research - peer-review › Conference article – Annual report year: 2010

Monitoring grain boundary migration during recrystallisation using topotomography

General information
State: Published
Pages: 449-456
Publication date: 2010
Conference: 31st Risø International Symposium on Materials Science : Challenges in materials science and possibilities in 3D and 4D characterization techniques, Roskilde, Denmark, 06/09/2010 - 06/09/2010
Main Research Area: Technical/natural sciences

Publication information
Volume: 31
ISSN (Print): 0907-0079
Ratings:
Phase retrieval for superposed signals from multiple binary objects

We introduce the binary superposed phase retrieval problem that aims at reconstructing multiple 0/1-valued functions with nonoverlapping bounded supports from moduli of superpositions of several displaced copies of their individual Fourier transforms. We discuss an application in coherent diffraction imaging of crystalline objects, propose two algorithms, and evaluate their performance by means of simulations. © 2010 Optical Society of America
The extension of ID11 for nanoscale and hierarchical characterization

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Rise National Laboratory for Sustainable Energy, Brookhaven National Laboratory, European Synchrotron Radiation Facility
Pages: 457-476
Publication date: 2010
Conference: 31st Risø International Symposium on Materials Science: Challenges in materials science and possibilities in 3D and 4D characterization techniques, Roskilde, Denmark, 06/09/2010 - 06/09/2010
Main Research Area: Technical/natural sciences

Publication information
Volume: 31
ISSN (Print): 0907-0079
Ratings:
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
BFI (2015): BFI-level 1
BFI (2014): BFI-level 1
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
BFI (2009): BFI-level 1
BFI (2008): BFI-level 1
Original language: English
Materials characterization and modelling, Materials and energy storage
Source: orbit
Source-ID: 266672
Publication: Research - peer-review › Conference article – Annual report year: 2010

A discrete spherical X-ray transform of orientation distribution functions using bounding cubes
We investigate a cubed sphere parameterization of orientation space with the aim of constructing a discrete voxelized version of the spherical x-ray transform. For tracing the propagation of a unit great circle through the partition subsets, the frustums of the cubed sphere, a fast procedure is proposed. The circle's parts in each frustum are gnomically mapped into line segments inside the bounding cubes. The line segments constitute a convex polygon with vertexes indicating frustum exit–entry points. Thus the problem of system matrix calculation is reduced to the tracing of line segments within rectangular voxel arrays partitioning the bounding cubes. Hence algebraic reconstruction techniques can be used in a
comprehensive way for orientation distribution function estimation from diffraction data.

**General information**
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy
Authors: Kazantsev, I. G. (Intern), Schmidt, S. (Intern), Poulsen, H. F. (Intern)
Pages: 105009
Publication date: 2009
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Inverse Problems
Volume: 25
Issue number: 10
ISSN (Print): 0266-5611
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.502 SNIP 1.386 CiteScore 1.84
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.389 SNIP 1.411 CiteScore 1.82
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.257 SNIP 1.346 CiteScore 1.63
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.19 SNIP 1.566 CiteScore 2.13
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.239 SNIP 1.838 CiteScore 2.15
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.127 SNIP 1.6 CiteScore 1.9
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.365 SNIP 1.587
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.33 SNIP 1.759
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.211 SNIP 1.884
Scopus rating (2007): SJR 1 SNIP 1.984
Scopus rating (2006): SJR 0.893 SNIP 1.763
Scopus rating (2005): SJR 1.129 SNIP 1.954
Scopus rating (2004): SJR 0.795 SNIP 1.615
Scopus rating (2003): SJR 0.723 SNIP 1.389
Scopus rating (2002): SJR 1.114 SNIP 1.457
Scopus rating (2001): SJR 0.987 SNIP 1.502
Scopus rating (2000): SJR 0.896 SNIP 1.52
Scopus rating (1999): SJR 0.815 SNIP 1.347
Original language: English
Materials characterization and modelling, Materials research
DOIs:
An algorithm for determining crystal lattices in unknown polycrystalline compounds

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Rise National Laboratory for Sustainable Energy
Authors: Schmidt, S. (Intern)
Publication date: 2009
Event: Abstract from Total Cryst Workshop, Grenoble (FR), 1-3 Apr., .
Main Research Area: Technical/natural sciences
Materials characterization and modelling, Materials research
Electronic versions:
Schmidt_abstract.pdf
Source: orbit
Source-ID: 254909
Publication: Research › Conference abstract for conference – Annual report year: 2009

Closing the gap between single crystal and powder diffraction

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Rise National Laboratory for Sustainable Energy
Authors: Sørensen, H. O. (Intern), Schmidt, S. (Intern), Wright, J. (Ekstern), Hansen, P. C. (Intern), Poulsen, H. F. (Intern)
Publication date: 2009
Main Research Area: Technical/natural sciences
Materials characterization and modelling, Materials research
Source: orbit
Source-ID: 245305
Publication: Research › Paper – Annual report year: 2009

Direct non-destructive observation of bulk nucleation in 30% deformed aluminum

A 30% deformed aluminum sample was mapped non-destructively using three-dimensional X-ray diffraction (3DXRD) before and after annealing to nucleation of recrystallization. Nuclei appeared in the bulk of the sample. Their positions and volumes were determined, and the crystallographic orientations were compared with the orientations of the deformed grains. It was found that nuclei with new orientations can form and their orientations have been related to the dislocation structure in the deformed grains.

General information
State: Published
Pages: 875-878
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Scripta Materialia
Volume: 61
ISSN (Print): 1359-6462
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Integrated intensities based on grain orientation distribution functions

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy
Authors: Sørensen, H. O. (Intern), Wright, J. (Ekstern), Schmidt, S. (Intern), Hansen, P. C. (Intern), Poulsen, H. F. (Intern)
Publication date: 2009
Main Research Area: Technical/natural sciences
Materials characterization and modelling, Materials research
Source: orbit
Source-ID: 245306
Publication: Research › Paper – Annual report year: 2009

Mapping the elastic strains of individual grains in a polycrystalline material using 3DXRD

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy
Authors: Oddershede, J. (Intern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Sørensen, H. O. (Intern), Reimers, W. (Ekstern)
Publication date: 2009
Main Research Area: Technical/natural sciences
Materials characterization and modelling, Materials research
Source: orbit
Source-ID: 245919
Publication: Research › Conference abstract for conference – Annual report year: 2009

Mapping the elastic strains of individual grains in a polycrystalline material using 3DXRD

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy
Authors: Oddershede, J. (Intern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Sørensen, H. O. (Intern), Reimers, W. (Ekstern)
Publication date: 2009
Event: Abstract from 39th Danish Crystallographer Meeting and 2nd DanScatt Annual Meeting, Lyngby, Denmark.
Main Research Area: Technical/natural sciences
Materials characterization and modelling, Materials research
Source: orbit
Source-ID: 245917
Publication: Research › Conference abstract for conference – Annual report year: 2009

McXtrace - An X-ray Monte Carlo Ray-tracing software package

General information
State: Published
Organisations: Nano-Microstructures in Materials, Materials Research Division, Risø National Laboratory for Sustainable Energy, Metal Structures in Four Dimensions, University of Copenhagen
Authors: Mortensen, K. (Ekstern), Kynde, S. (Ekstern), Knudsen, E. (Ekstern), Willendrup, P. K. (Intern), Schmidt, S. (Intern), Lefmann, K. (Ekstern)
Number of pages: 381
Pages: 328-329
Publication date: 2009

Host publication information
Title of host publication: Programme, Abstracts and Posters
Publisher: SAS-2009 Organising Committee
Measuring residual stresses of individual grains in polycrystalline materials using 3DXRD

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy
Authors: Oddershede, J. (Intern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Reimers, W. (Ekstern)
Publication date: 2009
Main Research Area: Technical/natural sciences
Materials characterization and modelling, Materials research
Source: orbit
Source-ID: 253769
Publication: Research › Conference abstract for conference – Annual report year: 2009

Measuring the elastic strain of individual grains in a polycrystalline material - extending a micro-scale technique to the nano-regime

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy, European Synchrotron Research Facility, Max Planck Institute, Technische Universität Berlin
Authors: Oddershede, J. (Intern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Margulies, L. (Intern), Wright, J. (Ekstern), Moseicki, M. (Ekstern), Reimers, W. (Ekstern)
Pages: 277-283
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Volume: 30
ISSN (Print): 0907-0079
Ratings:
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
BFI (2015): BFI-level 1
BFI (2014): BFI-level 1
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
BFI (2009): BFI-level 1
BFI (2008): BFI-level 1
Original language: English
Materials characterization and modelling, Materials research
Source: orbit
Source-ID: 249784
Publication: Research - peer-review › Conference article – Annual report year: 2009
Measuring the elastic strain of individual grains in polycrystalline materials

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Metal Structures in Four Dimensions, Materials Research Division
Authors: Oddershede, J. (Intern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Sørensen, H. O. (Intern), Reimers, W. (Ekstern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Materials characterization and modelling, Materials research
Electronic versions:
2009_74.pdf
Source: orbit
Source-ID: 245912
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

Measuring the elastic strain of individual grains in polycrystalline materials
3DXRD is not only an excellent tool when it comes to non-destructively determining the positions and orientations of individual grains within the bulk of a polycrystalline material, the experiment can also provide grain resolved elastic strain tensors. To extract this information the program FitAllB, which fits centre-of-mass grain positions, orientations and strain tensors from the experimental far-field 3DXRD data, was developed. The program builds on peaksearch, ImageD11 and GrainSpotter and will eventually be implemented in the Fable GUI. By the use of simulated data the presentation will focus on some of the important aspects you have to take into account in order to determine the strain tensors of the individual grains to the desired accuracy of 10^-4. The first thing is how to handle the peak overlaps that will inevitably occur, especially for textured and/or deformed materials. Secondly a careful calibration of the global parameters relating to the experiment (sample-to-detector distance, tilts of detector and sample and beam centre on detector) must be performed. For this purpose the option of fitting the global parameters simultaneously for any number of indexed grains is included in FitAllB. Finally some examples of applying FitAllB to analyze experimental 3DXRD data will be shown. These will include an experiment performed using both a near- and a far-field detector, thus making it possible to improve the grain positions by fitting these against the near-field data. Again this can be done within FitAllB. In addition to the centre-of-mass grain positions, orientations and strain tensors, FitAllB also calculates the relative volumes of the grains based on the peak intensities, so using a tessellation routine a crude 3D map of the elastic strain in the polycrystal can be obtained.

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Metal Structures in Four Dimensions, Materials Research Division
Authors: Oddershede, J. (Intern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Sørensen, H. O. (Intern), Reimers, W. (Ekstern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Materials characterization and modelling, Materials research
Electronic versions:
2009_74.pdf
2009_74_1.pdf
Source: orbit
Source-ID: 245914
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

Multigrain crystallography - why bother?

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Metal Structures in Four Dimensions, Materials Research Division
New opportunities for 3D materials science of polycrystalline materials at the micrometre lengthscale by combined use of X-ray diffraction and X-ray imaging

Non-destructive, three-dimensional (3D) characterization of the grain structure in mono-phase polycrystalline materials is an open challenge in material science. Recent advances in synchrotron based X-ray imaging and diffraction techniques offer interesting possibilities for mapping 3D grain shapes and crystallographic orientations for certain categories of polycrystalline materials. Direct visualisation of the three-dimensional grain boundary network or of two-phase (duplex) grain structures by means of absorption and/or phase contrast techniques may be possible, but is restricted to specific material systems. A recent extension of this methodology, termed X-ray diffraction contrast tomography (DCT), combines the principles of X-ray diffraction imaging, three-dimensional X-ray diffraction microscopy (3DXRD) and image reconstruction from projections. DCT provides simultaneous access to 3D grain shape, crystallographic orientation and local attenuation coefficient distribution. The technique applies to the larger range of plastically undeformed, polycrystalline mono-phase materials, provided some conditions on grain size and texture are fulfilled. The straightforward combination with high-resolution microtomography opens interesting new possibilities for the observation of microstructure related damage and deformation mechanisms in these materials.
Structured scintillators for X-ray imaging with micrometre resolution

A 3D X-ray detector for imaging of 30–200 keV photons is described. It comprises a stack of semitransparent structured scintillators, where each scintillator is a regular array of waveguides in silicon, and with pores filled with CsI. The
performance of the detector is described theoretically and explored in detail through simulations. The resolution of a single screen is shown to be determined only by the pitch, at least up to 100 keV. In comparison to conventional homogenous screens an improvement in efficiency by a factor 5–15 is obtainable. The cross-talk between screens in the 3D detector is shown to be negligible. The concept of such a 3D detector enables ray tracing and super resolution algorithms to be applied. Realized pore geometries have a lower aspect ratio than used in simulations and the roughness of the pore walls gives a 13% decrease in waveguide efficiency. Compared to currently used regular scintillators with similar resolution an efficiency increase by a factor 4 has been found for the structured scintillator.
Time Evolution in 3D Metal Microstructures—Recrystallization

The three dimensional x-ray diffraction (3DXRD) concept is shortly described and new experimental updates are highlighted. The potentials and limitation of the 3DXRD method are compared to those of other 3D methods. 3DXRD has been used for in-situ studies of recrystallization and new migration rate results are presented. Migration mechanism for boundary segments surrounding a recrystallizing grain are described and discussed.

General information
State: Published
Organisations: Materials Research Division. Management, Materials Research Division, Risø National Laboratory for Sustainable Energy, Metal Structures in Four Dimensions
Authors: Juul Jensen, D. (Intern), Schmidt, S. (Intern)
Pages: 1655-1659
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Transactions
Volume: 50
Issue number: 7
ISSN (Print): 1345-9678
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.505 SNIP 0.729 CiteScore 0.86
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.502 SNIP 0.681 CiteScore 0.8
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.73 SNIP 1.035 CiteScore 0.91
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.491 SNIP 0.724 CiteScore 0.69
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.554 SNIP 0.766 CiteScore 0.7
ISI indexed (2012): ISI indexed yes
A high-spatial-resolution three-dimensional detector array for 30-200 keV X-rays based on structured scintillators

A three-dimensional X-ray detector for imaging 30-200 keV photons is described. It comprises a set of semi-transparent structured scintillators, where each scintillator is a regular array of waveguides in silicon, and with pores filled with CsI. The performance of the detector is described theoretically and explored in detail through simulations. Based on available hardware, a spatial resolution of 1 mm is obtainable. The resolution of a single screen is shown to be determined only by the pitch, at least up to 100 keV. In comparison with conventional homogeneous screens, an improvement in efficiency by a factor of 5-15 is obtainable. The cross-talk between screens in the three-dimensional detector is shown to be negligible. The three-dimensional concept enables ray-tracing and super-resolution algorithms to be applied.
Direct observation of 3-D grain growth in Al–0.1% Mn

Grain growth in an Al-0.1% Mn sample has been measured non-destructively using a three-dimensional X-ray diffraction (3DXRD) microscope. The 3-D grain morphology as well as the crystallographic orientation was determined for 483 grains in the illuminated volume prior to annealing. After annealing, a second map revealed that significant grain growth had taken place, with only 27 remaining grains in the same volume. The correlation between grain orientation, growth of grains and neighbouring relationships is explored. (c) 2008 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
Experimental quantification of nucleation

General information
State: Published
Authors: West, S. (Intern), Schmidt, S. (Intern), Juul Jensen, D. (Intern)
Number of pages: 413
Pages: 383-389
Publication date: 2008

Host publication information
Place of publication: Roskilde
Publisher: Danmarks Tekniske Universitet, Risø Nationallaboratoriet for Bæredygtig Energi
ISBN (Print): 978-87-550-3694-9
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 222848
Publication: Research - peer-review › Article in proceedings – Annual report year: 2008

Measuring the elastic strain of individual grains in polycrystalline materials

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy
Authors: Oddershede, J. (Intern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Sørensen, H. O. (Intern), Reimers, W. (Ekstern)
Publication date: 2008
Molecular dynamics simulations of grain boundary migration during recrystallization employing tilt and twist dislocation boundaries to provide the driving pressure

General information
State: Published
Authors: Godiksen, R. B. (Intern), Schmidt, S. (Intern), Juul Jensen, D. (Intern)
Pages: 065002-065021
Publication date: 2008
Main Research Area: Technical/natural sciences
Novel synchrotron based techniques for characterization of energy materials

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Materials Research Division, Metal Structures in Four Dimensions, Nano-Microstructures in Materials, European Synchrotron Radiation Facility
Authors: Poulsen, H. F. (Intern), Nielsen, S. F. (Intern), Olsen, U. L. (Intern), Schmidt, S. (Intern), Wright, J. (Ekstern)
Number of pages: 413
Pages: 101-122
Publication date: 2008

Host publication information
Place of publication: Roskilde
Publisher: Danmarks Tekniske Universitet, Risø Nationallaboratoriet for Bæredygtig Energi
ISBN (Print): 978-87-550-3694-9
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 222830
Publication: Research - peer-review › Article in proceedings – Annual report year: 2008

Three-dimensional geometric simulations of random anisotropic growth during transformation phenomena
In this paper, the effects of anisotropic growth during transformation processes are investigated by geometric simulations of randomly oriented shape preserved ellipsoids in three dimensions and the applicability of idealized models are tested. Surprisingly, the results show that the models can predict the results for random ellipsoids up to aspect ratios of at least four, making the effects of random anisotropic growth less pronounced than what has previously been predicted from two-dimensional simulations or other, more restrictive three-dimensional simulations. (c) 2007 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

General information
State: Published
Pages: 279-282
Publication date: 2008
Main Research Area: Technical/natural sciences

Publication information
Journal: Scripta Materialia
Volume: 58
Issue number: 4
ISSN (Print): 1359-6462
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.71 SJR 1.901 SNIP 1.696
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.3 SNIP 1.876 CiteScore 3.54
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.744 SNIP 2.124 CiteScore 3.55
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.347 SNIP 1.975 CiteScore 3.19
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.309 SNIP 2.022 CiteScore 3.01
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.333 SNIP 2.108 CiteScore 3.21
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.445 SNIP 2.125
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.574 SNIP 2.02
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.634 SNIP 2.128
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.229 SNIP 2.174
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.1 SNIP 1.915
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.831 SNIP 1.915
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.464 SNIP 1.731
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.499 SNIP 1.709
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.509 SNIP 1.345
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.301 SNIP 1.361
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.268 SNIP 1.123
X-ray diffraction contrast tomography: a novel technique for three-dimensional grain mapping of polycrystals. 1. Direct beam case

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy
Authors: Ludwig, W. (Ekstern), Schmidt, S. (Intern), Lauridsen Mejdal, E. (Intern), Poulsen, H. F. (Intern)
Pages: 302-309
Publication date: 2008
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Applied Crystallography
Volume: 41
ISSN (Print): 0021-8898
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.242 SNIP 1.234 CiteScore 2.51
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.322 SNIP 2.588 CiteScore 3.97
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.585 SNIP 4.371 CiteScore 4.76
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.921 SNIP 6.392 CiteScore 6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.572 SNIP 4.687 CiteScore 4.67
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.015 SNIP 5.863 CiteScore 5.32
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.6 SNIP 2.078
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.235 SNIP 2.117
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.126 SNIP 2.101
Atomistisk simulering af rekryrstallisation

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Metal Structures in Four Dimensions, Materials Research Division, Materials Research Division, Management
Authors: Godiksen, R. B. (Intern), Schmidt, S. (Intern), Juul Jensen, D. (Intern)
Pages: 27-37
Publication date: 2007

Host publication information
Title of host publication: Metallurgi, design og innovation
Place of publication: Lyngby
Publisher: DMS
Editors: Brøndsted, P., Kjeldsteen, P., Somers, M.
ISBN (Print): 87-87535-37-8
Main Research Area: Technical/natural sciences
Conference: Middelfart, Denmark, 01/01/2007
Source: orbit
Source-ID: 223110
Publication: Research - peer-review › Journal article – Annual report year: 2008

Development of a high-efficiency high-resolution imaging detector for 30–80 keV X-rays

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy
Authors: Olsen, U. L. (Intern), Badel, X. (Ekstern), Linros, J. (Ekstern), Michiel, M. D. (Ekstern), Martin, T. (Ekstern), Schmidt, S. (Intern), Poulsen, H. F. (Intern)
Pages: 52-55
Publication date: 2007
Conference: International workshop on radiation imaging detectors, Pisa (IT), 01/01/2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Nuclear Instruments and Methods in Physics Research Section A
Volume: 576
Effects of distributions of growth rates on recrystallization kinetics and microstructure

The effects on recrystallization kinetics and microstructure of growth rate distributions rather than a single growth rate for recrystallizing grains were investigated by geometric simulations. The grains were set to grow as spheres with radii \( r = A_1 \alpha \). The results show that distributions in \( A \) and \( \alpha \) may produce significant changes in the microstructure and texture, whereas only distributions in \( \alpha \) may change the overall evolution in kinetics represented by \( V-v(t) \) by completely changing the shape of the kinetics curve. (c) 2007 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
High-resolution three-dimensional mapping of individual grains in polycrystals by topotomography

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy
Authors: Ludwig, W. (Ekstern), Lauridsen Mejdal, E. (Intern), Schmidt, S. (Intern), Poulsen, H. F. (Intern), Baruchel, J. (Ekstern)
Pages: 905-911
Publication date: 2007
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Applied Crystallography
Volume: 40
ISSN (Print): 0021-8898
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.242 SNIP 1.234 CiteScore 2.51
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.322 SNIP 2.588 CiteScore 3.97
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.585 SNIP 4.371 CiteScore 4.76
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.921 SNIP 6.392 CiteScore 6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Mapping partially recrystallised structures by 3DXRD

**General information**

State: Published


Authors: West, S. (Intern), Winther, G. (Intern), Margulies, L. (Intern), Bergbäck Knudsen, E. (Intern), Sørensen, H. O. (Intern), Schmidt, S. (Intern), Juul Jensen, D. (Intern)

Pages: 389-394

Publication date: 2007

Conference: 3rd International Conference on Recrystallization and Grain Growth, Jeju Island, Korea, Republic of, 10/06/2007 - 10/06/2007

Main Research Area: Technical/natural sciences

**Publication information**

Journal: Materials Science Forum

Volume: 558-559

ISSN (Print): 0255-5476

Ratings:
Misorientation aspects of growth during recrystallisation

General information
Simulation of recrystallization using molecular dynamics; Effects of the interatomic potential

General information
State: Published
Authors: Godiksen, R. B. (Intern), Trautt, Z. (Ekstern), Upmanyu, M. (Ekstern), Schmidt, S. (Intern), Juul Jensen, D. (Intern)
Pages: 1081-1086
Publication date: 2007
Conference: 3rd International Conference on Recrystallization and Grain Growth, Jeju Island, Korea, Republic of, 10/06/2007 - 10/06/2007
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Science Forum
Volume: 558-559
ISSN (Print): 0255-5476
Ratings:
  BFI (2017): BFI-level 1
  BFI (2016): BFI-level 1
  Scopus rating (2016): SJR 0.186 SNIP 0.306 CiteScore 0.28
  BFI (2015): BFI-level 1
  Scopus rating (2015): SNIP 0.337 SJR 0.217 CiteScore 0.29
  BFI (2014): BFI-level 1
  Scopus rating (2014): SNIP 0.448 SJR 0.269 CiteScore 0.33
  Web of Science (2014): Indexed yes
  BFI (2013): BFI-level 1
  Scopus rating (2013): SNIP 0.342 SJR 0.235 CiteScore 0.28
  ISI indexed (2013): ISI indexed yes
  Web of Science (2013): Indexed yes
  BFI (2012): BFI-level 1
  Scopus rating (2012): SNIP 0.467 SJR 0.279 CiteScore 0.34
  ISI indexed (2012): ISI indexed yes
  Web of Science (2012): Indexed yes
  BFI (2011): BFI-level 1
  Scopus rating (2011): SNIP 0.419 SJR 0.247 CiteScore 0.33
  ISI indexed (2011): ISI indexed yes
  BFI (2010): BFI-level 1
  Scopus rating (2010): SNIP 0.406 SJR 0.271
  Web of Science (2010): Indexed yes
  BFI (2009): BFI-level 1
  Scopus rating (2009): SNIP 0.389 SJR 0.343
  BFI (2008): BFI-level 1
  Scopus rating (2008): SJR 0.297 SNIP 0.358
  Web of Science (2008): Indexed yes
  Scopus rating (2007): SJR 0.314 SNIP 0.5
Simulations of boundary migration during recrystallization using molecular dynamics

We have applied an atomistic simulation methodology based on molecular dynamics to study grain boundary migration in crystalline materials, driven by the excess energy of dislocation arrangements. This method is used to simulate recrystallization in metals. The simulations reveal that the migration process is not uniform as assumed in many recrystallization models, but that the grain boundaries migrate in an irregular fashion and exhibit a strong dependence on the local presence of dislocations, which can distort the local migration process significantly. (c) 2007 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy, Experimental Surface and Nanomaterials Physics, Department of Physics, Materials Research Division. Management, Center for Individual Nanoparticle Functionality, Center for Nanoteknologi, Colorado School of Mines
Authors: Godiksen, R. B. (Intern), Trautt, Z. (Ekstern), Upmanyu, M. (Ekstern), Schiøtz, J. (Intern), Juul Jensen, D. (Intern), Schmidt, S. (Intern)
Pages: 6383-6391
Publication date: 2007
Main Research Area: Technical/natural sciences

Publication information
Journal: Acta Materialia
Volume: 55
Issue number: 18
ISSN (Print): 1359-6454
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 3.283 SNIP 2.674 CiteScore 5.67
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 3.542 SNIP 2.927 CiteScore 5.22
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 4.045 SNIP 3.348 CiteScore 5.16
Analytical expression for the evolution of interfacial area density between transformed grains during nucleation and growth transformations

This paper shows that interfacial area density between transformed grains during nucleation and growth transformations and the contiguity are useful descriptors of microstructural evolution. These descriptors are evaluated analytically and compared with results from computer simulation. Usage of these descriptors makes microstructural path analysis even more reliable and robust. (c) 2006 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Metal Structures in Four Dimensions, Materials Research Division
Mapping grains and their dynamics in three dimensions

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Nano-Microstructures in Materials, Materials Research Division, Metal Structures in Four Dimensions
Authors: Sørensen, H. (Intern), Jakobsen, B. (Intern), Bergbäck Knudsen, E. (Intern), Lauridsen, E. (Intern), Fæster Nielsen, S. (Intern), Poulsen, H. (Intern), Schmidt, S. (Intern), Winther, G. (Intern), Margulies, L. (Intern)
Pages: 232-237
Publication date: 2006
Conference: E-MRS 2005 Symposium O on Synchrotron Radiation and Materials Science, Strassbourg, France, 31/05/2005 - 31/05/2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Nuclear Instruments & Methods in Physics Research. Section B: Beam Interactions with Materials and Atoms
Volume: 246
ISSN (Print): 0168-583X
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.691 SNIP 0.906 CiteScore 1.22
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.74 SNIP 1.065 CiteScore 1.32
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.616 SNIP 0.905 CiteScore 1.14
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.681 SNIP 1.205 CiteScore 1.47
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.663 SNIP 0.989 CiteScore 1.18
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.685 SNIP 1.071 CiteScore 1.24
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.846 SNIP 0.971
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.672 SNIP 0.925
Non-destructive characterization of recrystallization kinetics using three-dimensional X-ray diffraction microscopy

Three-dimensional X-ray diffraction (3DXRD) is used to characterize the nucleation and early growth of individual bulk nuclei in situ during recrystallization of 92% cold-rolled copper. It is found that some cube nuclei, but not all, have a significantly faster initial growth than the average growth kinetics. These results are discussed and compared to previous 3DXRD results for recrystallization of aluminum alloys, and implications of the results on modeling of recrystallization are considered. Finally, a new 3DXRD technique suitable for non-destructive 3D characterization is outlined and its potential for recrystallization studies is discussed. (c) 2006 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
X-ray microscopy in four dimensions

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Metal Structures in Four Dimensions, Materials Research Division
Algorithms and instrumentation for generating 3D grain maps in polycrystals by 3DXRD

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Knudsen, E. (Ekstern), Poulsen, H. (Intern), Schmidt, S. (Intern), Sørensen, H. (Intern), Lauridsen, E. (Intern), Markussen, T. (Ekstern), Fu, X. (Ekstern)
Publication date: 2005
Event: Abstract from CEPHEUS workshop on advanced method for interpretation of TEM, X-ray and SIMS measurements in nano- and atomic scale, Warsaw (PL), 1-3 Jun.,
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 308630
Publication: Research › Conference abstract for conference – Annual report year: 2005

Image analysis for X-ray studies of the dynamics of individual embedded subgrains during recovery

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Pages: 1476-1479
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Science and Technology
Volume: 21
ISSN (Print): 0267-0836
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.814 SNIP 0.812 CiteScore 1.43
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.632 SNIP 0.764 CiteScore 1.1
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.788 SNIP 1.005 CiteScore 1.1
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.636 SNIP 0.868 CiteScore 0.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.683 SNIP 0.979 CiteScore 0.86
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.674 SNIP 1.059 CiteScore 0.94
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.638 SNIP 0.779
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.876 SNIP 1.08
Mapping grains and their dynamics in 3 dimensions

**General information**
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Publication date: 2005
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 308566
Publication: Research - peer-review › Journal article – Annual report year: 2005


doi:10.1179/174328405X71675

Metals structures in four dimensions

**General information**
State: Published
Organisations: Materials Research Division, Risø National Laboratory for Sustainable Energy
Authors: Schmidt, S. (Intern), Juul Jensen, D. (Intern)
Pages: 181-187
Publication date: 2005
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Archives of Metallurgy and Materials
Volume: 50
ISSN (Print): 1733-3490
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.347 SNIP 0.74 CiteScore 0.85
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.471 SNIP 1.185 CiteScore 1.19
Total crystallography: 3DXRD for molecular compounds

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Sørensen, H. (Intern), Schmidt, S. (Intern), Vaughan, G. (Ekstern), Poulsen, H. (Intern)
Publication date: 2005
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 308344
Publication: Research › Conference abstract for conference – Annual report year: 2005

Towards atomic level simulations of recrystallisation - setting up suitable geometry

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Materials Research Division
Pages: 1373-1375
Publication date: 2005
Main Research Area: Technical/natural sciences
Publication information
3DXRD - Mapping grains and their dynamics in 3 dimensions

**General information**
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Poulsen, H. (Intern), Fu, X. (Ekstern), Knudsen, E. (Ekstern), Lauridsen, E. (Intern), Margulies, L. (Intern), Schmidt, S. (Intern)
Pages: 1363-1372
Publication date: Oct 2004
Conference: 2nd Joint International Conference on Recrystallization and Grain Growth, ReX and GG2, Annecy, France, 30/08/2004 - 30/08/2004
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Materials Science Forum
Volume: 467-470
ISSN (Print): 0255-5476
Ratings:
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.186 SNIP 0.306 CiteScore 0.28
BFI (2015): BFI-level 1
Scopus rating (2015): SNIP 0.337 SJR 0.217 CiteScore 0.29
BFI (2014): BFI-level 1
Scopus rating (2014): SNIP 0.448 SJR 0.269 CiteScore 0.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SNIP 0.342 SJR 0.235 CiteScore 0.28
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SNIP 0.467 SJR 0.279 CiteScore 0.34
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SNIP 0.419 SJR 0.247 CiteScore 0.33
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SNIP 0.406 SJR 0.271
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SNIP 0.389 SJR 0.343
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.297 SNIP 0.358
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.314 SNIP 0.5
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.37 SNIP 0.511
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.41 SNIP 0.56
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.449 SNIP 0.575
Web of Science (2004): Indexed yes
Scopus rating (2003): SNIP 0.548 SJR 0.457
Web of Science (2003): Indexed yes
A method for in-situ measurements of the growth in the bulk of deformed single crystals at the 3DXRD microscope

General information
State: Published
Organisations: Materials Research Division, Risø National Laboratory for Sustainable Energy
Authors: Schmidt, S. (Intern), Juul Jensen, D. (Intern)
Publication date: 2004

Host publication information
Title of host publication: Interfacial engineering for optimized properties 3
Place of publication: Warrendale, PA (US)
Publisher: MRS
Editors: Schuh, C., Kumar, M., Randle, V., Carter, C.
Series: Materials Research Society Symposium Proceedings, v. 819
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 307539
Publication: Research › Article in proceedings – Annual report year: 2004

An algebraic algorithm for generation of three-dimensional grain maps based on diffraction with a wide beam of hard X-rays

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Markussen, T. (Ekstern), Fu, X. (Ekstern), Margulies, L. (Intern), Lauridsen, E. (Intern), Fæster Nielsen, S. (Intern), Schmidt, S. (Intern), Poulsen, H. (Intern)
Pages: 96-102
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Applied Crystallography
Volume: 37
ISSN (Print): 0021-8898
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.242 SNIP 1.234 CiteScore 2.51
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.322 SNIP 2.588 CiteScore 3.97
Web of Science (2015): Indexed yes
Growth aspects of recrystallization

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Materials Research Division
Authors: Juul Jensen, D. (Intern), Lauridsen, E. (Intern), Schmidt, S. (Intern), Vandermeer, R. (Ekstern)
Pages: 69-70
Publication date: 2004
Conference: Symposium on microstructural stability in honor of professor Roger D. Doherty, Charlotte, NC (US), 14-18 Mar, 01/01/2004
In-situ measurements of growth of nuclei within the bulk of deformed aluminum single crystals

General information
State: Published
Organisations: Materials Research Division, Risø National Laboratory for Sustainable Energy
Authors: Schmidt, S. (Intern), Huang, X. (Intern), Juul Jensen, D. (Intern)
Pages: 189-192
Publication date: 2004
Conference: 2nd Joint International Conference on Recrystallization and Grain Growth, ReX and GG2, Annecy, France, 30/08/2004 - 30/08/2004
Main Research Area: Technical/natural sciences
Investigating the effect of grain interaction during plastic deformation of copper

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Lienert, U. (Ekstern), Han, T. (Ekstern), Almer, J. (Ekstern), Dawson, P. (Ekstern), Leffers, T. (Intern), Margulies, L. (Intern), Fæster Nielsen, S. (Intern), Poulsen, H. (Intern), Schmidt, S. (Intern)
Pages: 4461-4467
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Volume: 52
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 3.283 SNIP 2.674 CiteScore 5.67
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 3.542 SNIP 2.927 CiteScore 5.22
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 4.045 SNIP 3.348 CiteScore 5.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 3.29 SNIP 2.709 CiteScore 4.37
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.409 SNIP 2.917 CiteScore 4.28
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.247 SNIP 2.81 CiteScore 4.27
Lattice rotations of individual bulk grains. Part 2: Correlation with initial orientation and model comparison

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Winther, G. (Intern), Margulies, L. (Intern), Schmidt, S. (Intern), Poulsen, H. (Intern)
Pages: 2863-2872
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Volume: 52
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 3.283 SNIP 2.674 CiteScore 5.67
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 3.542 SNIP 2.927 CiteScore 5.22
Web of Science (2015): Indexed yes
Multicrystal approach to crystal structure solution and refinement

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Vaughan, G. (Ekstern), Schmidt, S. (Intern), Poulsen, H. (Intern)
Pages: 813-825
Publication date: 2004
Non-destructive characterisation of grain boundaries in 3D
Simultaneous measurement of the strain tensor of 10 individual grains embedded in an Al tensile sample

First results are presented on the simultaneous observation of the elastic strain tensor as a function of load of 10 individual grains, deeply embedded in the bulk of a polycrystalline Al tensile sample. The experimental technique is based on the use of focused high energy synchrotron radiation in transmission geometry. After each load step diffraction patterns are collected with a large-area X-ray detector system for a series of different angular and lateral sample positions. An automated indexing routine was used to assign sets of diffraction spots to individual grains. The strain tensor components as well as the individual grain position within the sample were then fitted from the diffraction spot positions. A maximum tensile load of 48 MPa was applied. Deviations in strain of up to $600 \times 10^{-6}$ are observed between respective strain components of individual grains.
Watching the growth of bulk grains during recrystallization of deformed metals

We observed the in situ growth of a grain during recrystallization in the bulk of a deformed sample. We used the three-dimensional x-ray diffraction microscope located at the European Synchrotron Radiation Facility in Grenoble, France. The results showed a very heterogeneous growth pattern, contradicting the classical assumption of smooth and spherical growth of new grains during recrystallization. This type of in situ measurement opens up the possibility of obtaining experimental data on scientific topics that before could only be analyzed theoretically on the basis of the statistical characterization of microstructures. For recrystallization, the in situ method includes direct measurements of nucleation and boundary migration through a deformed matrix.

General information
State: Published
Organisations: Materials Research Division, Risø National Laboratory for Sustainable Energy
Pages: 229-232
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Science
Volume: 305
Issue number: 5681
**3DXRD microscopy (invited talk)**

**General information**
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Number of pages: 7
Publication date: 2003

**Host publication information**
Title of host publication: Final program
Place of publication: Chicago
Publisher: TMS
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 306119
Publication: Research › Conference abstract in proceedings – Annual report year: 2003

**Growth kinetics of individual grains during recrystallization with an intermediate cooling cycle**

**General information**
State: Published
Organisations: Materials Research Division, Risø National Laboratory for Sustainable Energy
Pages: 513-518
Publication date: 2003
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Scripta Materialia
Volume: 48
ISSN (Print): 1359-6462
Ratings:
- BFI (2017): BFI-level 2
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 3.71 SJR 1.901 SNIP 1.696
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 2.3 SNIP 1.876 CiteScore 3.54
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 2.744 SNIP 2.124 CiteScore 3.55
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 2.347 SNIP 1.975 CiteScore 3.19
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 2.309 SNIP 2.022 CiteScore 3.01
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
In situ characterisation of thermomechanical processes

General information
State: Published
Organisations: Materials Research Division, Risø National Laboratory for Sustainable Energy
Pages: 186-192
Publication date: 2003

Host publication information
Title of host publication: Conference proceedings
Place of publication: Sheffield
Publisher: University of Sheffield, Department of Engineering Materials
Editors: Palmiere, E., Mahfouf, M., Pinna, C.
ISBN (Print): 0-9522507-3-X
Main Research Area: Technical/natural sciences
Conference: International Conference on Thermomechanical Processing, Sheffield, United Kingdom, 23/06/2002 - 23/06/2002
Source: orbit
Source-ID: 306014
Publication: Research › Article in proceedings – Annual report year: 2003
Non-destructive mapping of grains in three dimensions

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Materials Research Division
Pages: 1093-1096
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Scripta Materialia
Volume: 49
ISSN (Print): 1359-6462
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.71 SJR 1.901 SNIP 1.696
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.3 SNIP 1.876 CiteScore 3.54
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.744 SNIP 2.124 CiteScore 3.55
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.347 SNIP 1.975 CiteScore 3.19
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.309 SNIP 2.022 CiteScore 3.01
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.333 SNIP 2.108 CiteScore 3.21
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.445 SNIP 2.125
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.574 SNIP 2.02
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.634 SNIP 2.128
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.229 SNIP 2.174
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.1 SNIP 1.915
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.831 SNIP 1.915
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.464 SNIP 1.731
Recrystallization at the 3DXRD microscope

General information
State: Published
Organisations: Materials Research Division, Risø National Laboratory for Sustainable Energy
Authors: Schmidt, S. (Intern), Juul Jensen, D. (Intern)
Pages: 169-174
Publication date: 2003

Host publication information
Title of host publication: Proceedings
Place of publication: Pittsburgh, PA
Publisher: ASM International
Editors: Tiryakioğlu, M., Lalli, L.
ISBN (Print): 0-87170-787-X
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 306170
Publication: Research › Article in proceedings – Annual report year: 2003

Recrystallization kinetics of individual bulk grains in a commercial aluminium alloy

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Materials Research Division
Number of pages: 7
Publication date: 2003

Host publication information
Title of host publication: Abstract booklet
Place of publication: Hamburg
Publisher: DESY
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 306110
Publication: Research › Conference abstract in proceedings – Annual report year: 2003
In-situ characterization of thermomechanical processes

General information
State: Published
Organisations: Materials Research Division, Risø National Laboratory for Sustainable Energy
Publication date: 2002
Event: Abstract from International Conference on Thermomechanical Processing, Sheffield, United Kingdom.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 304525
Publication: Research › Conference abstract in proceedings – Annual report year: 2002

Investigation of recrystallization texture evolution during annealing of hot deformed AA3104 alloy

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Savoie, J. (Ekstern), Yiu, H. (Ekstern), Lauridsen, E. (Intern), Margulies, L. (Intern), Fæster Nielsen, S. (Intern), Schmidt, S. (Intern), Ashton, M. (Ekstern), Sebald, R. (Ekstern)
Pages: 833-838
Publication date: 2002
Main Research Area: Technical/natural sciences
Publication information
Journal: Materials Science Forum
Volume: 408-412
ISSN (Print): 0255-5476
Ratings:
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.186 SNIP 0.306 CiteScore 0.28
BFI (2015): BFI-level 1
Scopus rating (2015): SNIP 0.337 SJR 0.217 CiteScore 0.29
BFI (2014): BFI-level 1
Scopus rating (2014): SNIP 0.448 SJR 0.269 CiteScore 0.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SNIP 0.342 SJR 0.235 CiteScore 0.28
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SNIP 0.467 SJR 0.279 CiteScore 0.34
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SNIP 0.419 SJR 0.247 CiteScore 0.33
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SNIP 0.406 SJR 0.271
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
**Lattice rotations of individual bulk grains during deformation**

**General information**

State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Winther, G. (Intern), Margulies, L. (Intern), Poulsen, H. (Intern), Schmidt, S. (Intern), Larsen, A. (Intern), Lauridsen, E. (Intern), Fæster Nielsen, S. (Intern), Terry, A. (Ekstern)
Pages: 287-292
Publication date: 2002
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Materials Science Forum
Volume: 408-412
ISSN (Print): 0255-5476
Ratings:
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.186 SNIP 0.306 CiteScore 0.28
BFI (2015): BFI-level 1
Scopus rating (2015): SNIP 0.337 SJR 0.217 CiteScore 0.29
BFI (2014): BFI-level 1
Scopus rating (2014): SNIP 0.448 SJR 0.269 CiteScore 0.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SNIP 0.342 SJR 0.235 CiteScore 0.28
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Observation of high-resolution diffraction profiles from single grains within polycrystalline metals

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Lienert, U. (Ekstern), Almer, J. (Ekstern), Margulies, L. (Intern), Fæster Nielsen, S. (Intern), Pantleon, W. (Intern), Poulsen, H. (Intern), Schmidt, S. (Intern)
Publication date: 2002
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 304375
Publication: Research - peer-review › Conference article – Annual report year: 2002

Structural refinement of the individual grains in a polycrystal

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Schmidt, S. (Intern), Vaughan, G. (Ekstern), Poulsen, H. (Intern)
Pages: 57-58
Texture evolution during hot deformation and annealing of AA5182 alloy

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Yiu, H. (Ekstern), Savoie, J. (Ekstern), Lauridsen, E. (Intern), Bosland, A. (Ekstern), Margulies, L. (Intern), Faæster Nielsen, S. (Intern), Schmidt, S. (Intern), Zeng, M. (Ekstern)
Pages: 1501-1506
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Science Forum
Volume: 408-412
ISSN (Print): 0255-5476
Ratings:
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.186 SNIP 0.306 CiteScore 0.28
BFI (2015): BFI-level 1
Scopus rating (2015): SNIP 0.337 SJR 0.217 CiteScore 0.29
BFI (2014): BFI-level 1
Scopus rating (2014): SNIP 0.448 SJR 0.269 CiteScore 0.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SNIP 0.342 SJR 0.235 CiteScore 0.28
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SNIP 0.467 SJR 0.279 CiteScore 0.34
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SNIP 0.419 SJR 0.247 CiteScore 0.33
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SNIP 0.406 SJR 0.271
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SNIP 0.389 SJR 0.343
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.297 SNIP 0.358
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.314 SNIP 0.5
Growth kinetics of individual cube grains as studied by the 3D X-ray diffraction microscope

State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Lauridsen, E. (Intern), Schmidt, S. (Intern), Margulies, L. (Intern), Poulsen, H. (Intern), Juul Jensen, D. (Intern)
Pages: 589-594
Publication date: 2001

Quantification of minor texture components by hard X-rays

State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Pages: 39-54
Publication date: 2001
Three-dimensional maps of grain boundaries and the stress state of individual grains in polycrystals and powders

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Pages: 751-756
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Applied Crystallography
Volume: 34
ISSN (Print): 0021-8898
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.242 SNIP 1.234 CiteScore 2.51
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.322 SNIP 2.588 CiteScore 3.97
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.585 SNIP 4.371 CiteScore 4.76
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.921 SNIP 6.392 CiteScore 6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.572 SNIP 4.687 CiteScore 4.67
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.015 SNIP 5.863 CiteScore 5.32
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.6 SNIP 2.078
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.235 SNIP 2.117
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.126 SNIP 2.101
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.674 SNIP 3.489
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.112 SNIP 7.433
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.817 SNIP 2.339
Scopus rating (2004): SJR 1.618 SNIP 2.239
Web of Science (2004): Indexed yes
Tracking: A method for structural characterization of grains in powders or polycrystals

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy
Authors: Lauridsen, E. (Intern), Schmidt, S. (Intern), Suter, R. (Ekstern), Poulsen, H. (Intern)
Pages: 744-750
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Applied Crystallography
Volume: 34
ISSN (Print): 0021-8898
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.242 SNIP 1.234 CiteScore 2.51
Web of Science (2016): Indexed Yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.322 SNIP 2.588 CiteScore 3.97
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.585 SNIP 4.371 CiteScore 4.76
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.921 SNIP 6.392 CiteScore 6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.572 SNIP 4.687 CiteScore 4.67
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.015 SNIP 5.863 CiteScore 5.32
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.6 SNIP 2.078
Web of Science (2010): Indexed yes
Projects:

3D electron microscopy of nanostructures in energy devices

Department of Energy Conversion and Storage
Period: 01/08/2017 → 31/07/2020
Number of participants: 4
Phd Student:
Colding-Jørgensen, Sofie (Intern)
Supervisor:
Schmidt, Søren (Intern)
Simonsen, Søren Bredmose (Intern)
Main Supervisor:
Kuhn, Luise Theil (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Advanced neutron imaging of energy devices in 2D and 3D

Department of Energy Conversion and Storage
Period: 15/12/2016 → 14/12/2019
Number of participants: 4
Phd Student:
Lacatusu, Monica-Elisabeta (Intern)
Supervisor:
Schmidt, Søren (Intern)
Strobl, Markus (Ekstern)
Main Supervisor:
Kuhn, Luise Theil (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Characterization of Nanomaterials with Experimental Measurements and Atomistic Simulations

Department of Physics
Period: 01/09/2014 → 31/08/2017
Number of participants: 3
Phd Student:
Larsen, Peter Mahler (Intern)
Supervisor:
Schmidt, Søren (Intern)
Main Supervisor:
Schjøtz, Jakob (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Multi-scale mapping of strain mechanisms in lead-free piezoceramics

Department of Physics
Period: 15/03/2013 → 22/06/2016
Number of participants: 6
Phd Student:
Majkut, Marta (Intern)
Supervisor:
Oddershede, Jette (Intern)
Main Supervisor:
Schmidt, Søren (Intern)
Examiner:
Poulsen, Henning Friis (Intern)
Clausen, Bjørn (Intern)
Grant Webber, Kyle (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

3D Neutron Diffraction (3DND) methodology

Department of Physics
Period: 15/02/2013 → 23/09/2016
Number of participants: 8
Phd Student:
Cereser, Alberto (Intern)
Supervisor:
Hall, Stephen A. (Ekstern)
Steuwer, Axel (Ekstern)
Strobl, Markus (Ekstern)
Main Supervisor:
Schmidt, Søren (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet

Relations
Publications:
Time-of-flight 3D Neutron Diffraction for Multigrain Crystallography
Project: PhD

FTP-PIEZO Multi-scale mapping of strain mechanisms in lead-free piezoceramics
Department of Physics
Neutrons and X-rays for Materials Physics
University of New South Wales
Period: 01/01/2013 → 14/03/2016
Number of participants: 3
Project participant:
Oddershede, Jette (Intern)
Schmidt, Søren (Intern)
Phd Student:
Majkut, Marta (Intern)

Relations
Related projects:
Multi-scale mapping of strain mechanisms in lead-free piezoceramics
Activities:
Quantitative grain-scale ferroelectric domain volume fractions and domain switching strains measured by 3DXRD during in situ electrical poling
Strain Mechanisms in Polycrystalline BaTiO3 Measured at the Single Grain Level during In-Situ Electrical Poling
Three-Dimensional X-ray Diffraction (3DXRD) microscopy for studying dynamics in polycrystalline materials
Three-Dimensional X-ray Diffraction (3DXRD) microscopy for studying strain evolution in piezoelectric domain structures and deformation induced twinning
Three-Dimensional X-ray Diffraction (3DXRD) microscopy for in situ studies of polycrystalline materials
Materials characterisation tools towards lead-free piezoceramics
Publications:
Mapping of strain mechanisms in barium titanate by three-dimensional X-ray diffraction
The effect of inter-granular constraints on the response of polycrystalline piezoelectric ceramics at the surface and in the bulk
Maximising electro-mechanical response by minimising grain-scale strain heterogeneity in phase-change actuator ceramics
Heterogeneous grain-scale response in ferroic polycrystals under electric field
Quantitative grain-scale ferroic domain volume fractions and domain switching strains from three-dimensional X-ray diffraction data

Project

Tomography with Prior Information
Department of Informatics and Mathematical Modeling
Period: 01/10/2009 → 17/06/2013
Number of participants: 7
Phd Student:
Jørgensen, Jakob Sauer (Intern)
Supervisor:
Schmidt, Søren (Intern)
Sidky, Emil (Ekstern)
Main Supervisor:
Hansen, Per Christian (Intern)
Examiner:
Larsen, Rasmus Werner (Intern)
Arridge, Simon R. (Ekstern)
Siltanen, Samuli (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD