

Direct Mapping of Lattice Strain and Structure by Five-Dimensional Scanning X-ray Diffraction Microscopy

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Abstract

Experimental observation of microscopic strain in functional devices has sparked interest in fields ranging from microelectronics to biotechnology, as strain engineering enables tuning of electronic, optical or elastic properties. Moreover, lattice strain can trigger phase transitions giving rise to new physical properties and their coupling phenomena. The study of correlations between structure and function requires an experimental technique to quantify the full deformation state in thin films and microstructures on the length scales relevant for nanotechnology. We highlight the capabilities of four- and five-dimensional Scanning X-ray Diffraction Microscopy to fulfill this role through several showcase experiments, demonstrating spatial resolution below 100 nm, high lattice sensitivity $<10^{-5}$ and full quantification of all nine independent components of the local deformation tensor. Being model-free, non-destructive, universally applicable to crystalline materials and *operando* experiments, this technique has potential to become a gap-bridging technique in the field of strain engineering.

Keywords: x-ray diffraction ~~(XRD)~~₂, nanoscale, elastic properties, microelectronics, energy storage

Introduction

The macroscopic electronic, optical or magnetic properties of solids are inherently linked to details of the atomic crystal structure and can be substantially impacted by its deformation state. In a crystal these physical properties often vary locally due to lattice inhomogeneities, such as lattice defects, grain boundaries, domains or geometrical patterning, which result in three-dimensional (3D) strain variations. This phenomenon is leveraged in many fields, e.g. in micro- and optoelectronics (Tsutsui, Mochizuki, Loubet, Bedell, & Sadana, 2019; Liu, et al., 2021), ferroelectrics (Li, Deng, Liu, & Chen, 2024), catalysis (Miao, Zhao, Zhang, Shi, & Zhang, 2022), bio- and quantum-technology (Burkard, Ladd, Pan, Nichol, & Petta, 2023; Hickey, Leblanc Latour, Harden, & Pelling, 2023). The opportunity to non-destructively map small lattice strains with sub-micron spatial resolution is therefore of fundamental importance for the development of future technologies (Gammer, Richard, & Eberl, 2019).

Stress and strain ~~inhomogeneities~~modulations within a crystal are usually described with continuum mechanics and investigated by diffraction ~~with~~of electrons or photons. X-Ray Diffraction (XRD) is a popular tool to characterize the global strain state of a material, but is limited in spatial resolution (Dolabella, Borzi, Dommann, & Neels, 2022). Nowadays, this capability is expanded towards the nano-cosmos by the continuous development of X-ray focusing optics, enabling X-ray nano-probes that provide a unique glimpse into buried structures, including samples encased within complex environments and operating in realistic conditions. Nano-beam X-ray diffraction can be readily

applied to the vast majority of crystalline samples without relying on sample preparation steps such as those required for Transmission Electron Microscopy (TEM) (Kang, Wang, Kübel, & Mu, 2024), that potentially alter the strain state of the material prior to the measurement.

The elastic response of solids to stress or structural inhomogeneities is often non-trivial. In particular, due to internal elastic interactions within the sample, local sources of stress typically lead to highly anisotropic 3D fields of stress and strain, affecting all components of the strain tensor (Baretin, 2023). However, most available techniques to measure strain deformation in crystalline materials are limited to either a single or a few of its components of the tensor ~~{11}~~ (Naresh-Kumar, et al., 2020), which is why Finite Element Method (FEM) models are typically employed to extrapolate the measured projections to the full strain tensor landscape in 3D- (Zaitsev, et al., 2023). These models rely on the knowledge of mechanical parameters, which in functional materials may deviate significantly from literature values (Bharathan, Narayan, Rozgonyi, & Bulman, 2013). ~~Thus, mechanical FEM models, and thus,~~ should be regularly benchmarked against model-free experimental data on the lattice strain.

In this review, we highlight the capabilities of four- and five-dimensional (4D/5D) Scanning X-ray Diffraction Microscopy (SXDM) (Chahine, et al., 2014), which is universally and non-destructively applicable to any crystal system and in a variety of fields, including quantum computing (Corley-Wiciak, et al., 2023), and sensing (Delegan, et al., 2023), optoelectronics (Zoellner, et al., 2019), semiconductor microstructures (Zatterin, et al., 2025) and nanowires (Hammarberg, et al., 2020), energy storage (Martens, et al., 2023) and more. Initially, like most techniques, SXDM has been restricted in use to single Bragg reflections allowing to extract only projections of the strain tensor (Zoellner, et al., 2015; Richard, et al., 2015). In contrast, this review focuses on latest developments that enable a full strain tensor microscopy based on the combination of at least three SXDM datasets, which we believe to be essential for the understanding of the mechanisms and defects giving rise to strain. Moreover, we showcase *operando* experiments featuring complex electrical setups. Below, we aim to give an overview over the experimental concept and data analysis of SXDM, and showcase the capabilities of the technique in five case studies.

Description of the Scanning X-ray Diffraction Microscopy technique

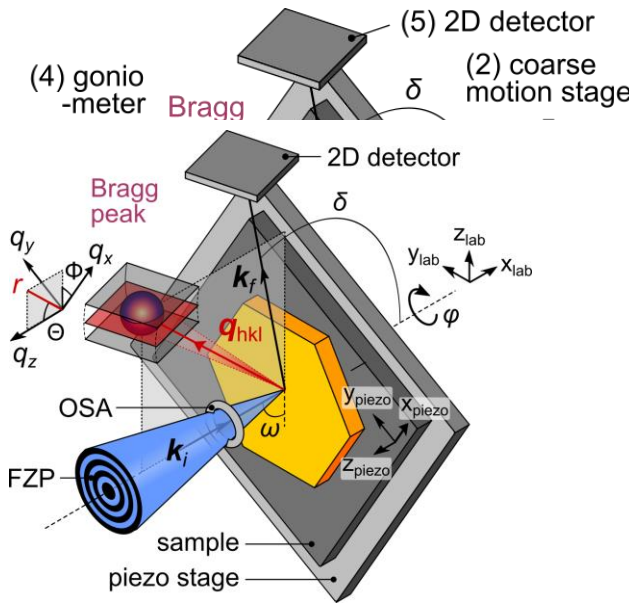


Figure 1 SXDM setup, adapted with permission from [24]. The setup includes a synchrotron source, FZP, OSA, sample on a piezo stage, coarse motion stage (2), goniometer (4), and 2D detector (5). Incident and scattered X-ray wavevectors, k_i and k_f , define the probed region of reciprocal space q . As each detector pixel corresponds to a different k_f , a 2D is spanned. A 3D region is probed by varying the incidence angle η . 2D real-space is mapped by scanning x_{piezo} and y_{piezo} .

equivalent Bragg reflections by rotating the sample about its surface normal. This way, different components of the strain tensor (see below) can be probed, while maintaining the illuminated sample volume. Es ist eine ungültige Quelle angegeben.

Figure 1 summarizes A deformation of the essential components required local unit cell will result in a change of the intensity distribution in 3D reciprocal space $I(q_x, q_y, q_z)$, where q is the momentum transfer. Thus, to obtain a spatial map of lattice strain, this distribution needs to be mapped at each position in real space (x_0, y_0) . A single image of the area detector already represents a 2D cut of the 3D reciprocal space map (RSM). A 3D region is covered by iterating spatial raster scans for performing a series of incidence angles η or different X-ray wavelengths (Richard, et al., 2020). Either approach results in an overall 5D dataset $I(x_0, y_0, q_x, q_y, q_z)$, typically defined in Cartesian coordinates.

In essence, an SXDM experiment set up at an optimized 3rd or 4th generation synchrotron beamline: needs to combine X-ray focusing with a setup for Bragg diffraction with real space scanning capability over multiple length scales. One concept providing these experimental capabilities is sketched in Figure 1: featuring (1) X-ray focusing optics; (2) stable sample stage, typically a hexapod, translation and rotation stages for coarse motion (e.g. provided by a hexapod); (3) piezo stage for fine scanning motors, e.g. a piezo stage, (4) 3-circle (or more) goniometer and (5) an X-ray area detector to record the diffracted intensity. Often present, an additional energy-resolving X-ray detector allows to map the elemental distribution by their characteristic emission (fluorescence), enabling to correct for sample parasitic drifts occurring during the SXDM measurement as the contrast is independent of geometry, unlike the diffraction signal. —which is independent of the diffraction condition and thus enables to correct for parasitic sample drifts occurring during subsequent SXDM raster scans. In some cases, for instance when using complex sample environment or very sensitive samples, it may be advantageous not to scan and rotate the sample. This can be realized in SXDM by alternatively scanning the focusing optics, which essentially moves the focused beam, and subsequently iterating for a series of X-ray wavelengths to change the diffraction condition and span a 3D region in reciprocal space.

SXDM is a synchrotron-based structural characterization technique pushing that pushes the limit in limits of concurrent fine-resolution in direct real and reciprocal space, and is conceptually similar to Nanobeam Electron Diffraction (NBED) (Ophus, 2023). Usually, SXDM data is acquired by fast scanning (e.g. by piezoelectric actuators) of the sample is scanned, typically with a piezo-driven stage, through a nano-focused X-ray beam, while the Bragg-diffracted X-rays in reflection geometry are collected by a 2D pixelated detector in reflection geometry, as sketched in Figure 1. There are many types of X-ray Various optics for focusing, with X-rays have been developed Es ist eine ungültige Quelle angegeben., where currently the finest X-ray spot size of typically down to ~25-nm is being provided by diffractive lenses, such as Fresnel Zone Plates (FZP) or Multilayer Laue Lenses (MLL) [24]. If experimentally feasible, the it is advantageous to select X-ray energy and the Bragg reflection hkl are selected to achieve near normal incidence of such that the X-ray beam arrives at the sample, avoiding nearly at normal incidence allowing to avoid geometrical broadening of the beam footprint as well as a complex, oblique projection of the interaction volume. If the surface is a high-symmetry crystallographic plane, this also facilitates simple switching between symmetrically

A deformation of the local unit cell will result in a change of the intensity distribution in 3D-reciprocal space $I(q_x, q_y, q_z)$. Thus, to obtain a spatial map of lattice strain, this distribution needs to be probed at a range of locations (x_0, y_0) , which is achieved by scanning the retrieved from such 3D intensity distributions strongly depends on the kind of sample. A single image of the area-detector represents a two-dimensional (2D) cut of 3D reciprocal space, thus in order to obtain the 3D-RSM at each location, spatial raster scans have to be performed for a series of incidence angles ω or different X-ray wavelengths [25]. Either approach results in an overall 5D-dataset $I(x_0, y_0, q_x, q_y, q_z)$, typically described in Cartesian reciprocal space, e.g. defined by Fourier transform the local displacement field $\mathbf{u}(\mathbf{r})$ in the momentum transfer $\mathbf{q}$ in every point of the raster-scan.

Illuminated region, which however, is often not known a-priori. In strain microscopy, a major step of data reduction, is therefore to extract the Bragg peak positions $q_{hkl} = \frac{2\pi n_{hkl}}{d_{hkl}} \langle \mathbf{q} \rangle_{hkl}$ of each distinct layer of interest peak from the RSMs. In this simplification, crystalline phases that are extracted from simultaneously illuminated by the 3D reciprocal space maps, yielding local values of focused beam and have an identical orientation and strain state are indistinguishable and treated as one region. Neglecting refraction effects, the peak positions yield information on the local interplanar spacing d_{hkl} and normal vector $\mathbf{n}_{hkl}$ of the diffracting lattice planes [20] via $\langle \mathbf{q} \rangle_{hkl} = \frac{2\pi n_{hkl}}{d_{hkl}}$ [20].

The extraction of their positions is straightforward if all Bragg peaks in the dataset, e.g. from different layers (depths) in an epitaxial heterostructure, are well separated in comparison to their peak width. In these cases, the peak position can be determined with sub-pixel precision by computing the center of mass of the 3D intensity distribution or of each of the projections on the three Cartesian axes (q_x, q_y, q_z) , which leads to superior strain sensitivity of $< 10^{-5}$ (Chahine, et al., 2014). However, if the lattices of different layers have similar, but not identical, unit cell parameters, their Bragg peaks significantly overlap in 3D reciprocal space and multi-peak fits become necessary. While this type of analysis has been demonstrated, it requires careful fine-tuning and thus represents a primary bottle-neck of the throughput of SXDM data analysis and its potential automation. Nevertheless, the examples below will demonstrate that evaluation of local strain is feasible with precision below 10^{-5} also in these cases. The Python packages *sxdm*, *id01-sxdm*, and *XSOCS* provide functionality for such SXDM data analysis (Judge, Plews, May, Holt, & Cabana, 2021; Zatterin E. , 2024; Vincent, Naudet, Richter, Zatterin, & Zhou, 2024).

As mentioned above, SXDM pushes the physical limits of concurrent resolution in real and reciprocal (angular) space. The finite emittance of the X-ray source translates into a certain volume in phase space occupied by the beam. This volume cannot be reduced by focusing optics, thus leading to a necessary trade-off between beam collimation and size (area). Therefore, reciprocal space maps obtained from a microscopic region by SXDM always exhibit a lower resolution than those obtained from a larger area by illumination with a parallel beam, as in the case of high-resolution XRD. On the other hand, it has been demonstrated that the angular convolution caused by the finite beam divergence inherent in SXDM may be exploited to obtain high-resolution angular scans for the illuminated region by a single detector exposure without the need for sample rotation. **Es ist eine ungültige Quelle angegeben.** This yields useful information (e.g. intensity profiles along crystal truncation rods) in the case of samples with locally well-defined, parallel interfaces, which would reflect collimated X-rays only into one specific direction. It is worth noting that, if the probed volume comprises regions with different lattice parameters, these regions may be separated in reciprocal space allowing to restrict the investigated volume further. This is of particular value for successive epitaxial layers as typically present in electronic devices.

In the following, we showcase the capabilities of SXDM on different material systems. The technique is implemented at several nanoprobe beamlines of synchrotron facilities such as **ID01/ESRF** (Leake, et al., 2019), **NanoMax/Max IV** (Marçal, et al., 2020), **P06/Petra III** (Schroer, et al., 2016), **HXN/APS** (Winarski, et al., 2012), **HXN/NSLS-II** (Xue, Li, Pianetta, & Liu, 2022) and **BL13XU/SPring-8** (Hamachi, et al., 2024), however, full strain tensor microscopy has so far only been performed at **ID01/ESRF** [34].

Mapping of the Full Strain Tensor – Demonstration in III-nitrides

Semiconductor crystals and epitaxial heterostructures comprised of elements from the groups IV and III-V of the periodic system have been ~~amongst among~~ the first systems targeted by SXDM studies (Zoellner, et al., 2015; Zoellner, et al., 2019; Evans, et al., 2012), motivated by the relevance of lattice strain and its influence on electronic properties in semiconductor technology. III-nitride materials such as $\text{Al}_{1-x}\text{Ga}_x\text{N}$ and $\text{In}_{1-x}\text{Ga}_x\text{N}$ in particular, are of high technological relevance optoelectronics in the blue and ultraviolet spectral ranges (Li, Fu, & Choi, 2020). Since strain engineering allows to optimize the growth and (opto)electronic properties of III-nitride films, many direct and indirect quantitative strain microscopy techniques have been developed for their study ~~{44}~~ (Naresh-Kumar, et al., 2020). SXDM extends these possibilities, allowing to image the 3D strain fields of defects such as dislocations and V-pits in thin nitride layers (Schulz, et al., 2022; Zoellner, et al., 2019) and being model-free, plays an important role to benchmark other techniques.

Since alloying is often used in semiconductor heterostructures to engineer a desired band-structure, local fluctuations of alloy composition, such as in the cases of $\text{In}_{1-x}\text{Ga}_x\text{N}$ and $\text{Si}_{1-x}\text{Ge}_x$, give rise to local variations of lattice parameters that can be probed by diffraction techniques ~~such as SXDM~~—(Zoellner, et al., 2015; Zoellner, et al., 2019). Any inhomogeneities of composition will, in turn, result in stress due to the elastic interaction with their environment. Disentangling the contributions from anisotropic stress and composition, however, strongly depends on assumptions that have to be made, especially if only ~~a single or few~~ projections of the strain tensor are known. For instance, an isotropic change of the crystallographic unit cell parameters may occur either due to hydrostatic strain or ~~due to~~ a change in ~~the composition stoichiometry~~. A common ~~approximation assumption~~ to resolve this issue in the case of thin epitaxial films is, hence, the absence of surface normal stress $\sigma_{zz} = 0$.

A more reliable discussion of these contributions has been enabled by measurements of the full strain tensor. ~~This was first demonstrated for the case of a~~ micro-structured $\text{In}_{1-x}\text{Ga}_x\text{N}$ heterostructure stack ~~and is was the first case where an approach for SXDMs~~ based on combining 5D SXDM datasets obtained for three non-coplanar reflections ~~{46} was demonstrated~~ (Richter, et al., 2022). All six lattice parameters and the orientation of the unit cell become accessible through linear combination of these three scattering vectors, that are determined locally for every point (x_0, y_0) . This is then converted into maps of the full 3×3 tensor of the displacement gradient, which can be decomposed into the tensors of strain ϵ and rotation ω (Richter, et al., 2022).

Quantitative imaging of tensorial strain fields allows better understanding of the sources of lattice inhomogeneities and thus gives deep insights into the effects of growth or strain engineering. Lattice defects, such as dislocations or alloy fluctuations can unambiguously be identified by their characteristic strain fields. For instance, threading edge dislocations only cause variations in the in-plane components of shear strain ϵ_{xy} or rotation ω_{xy} . **Figure 2** shows microscopic maps of ϵ_{xy} for a free-standing $\text{In}_{1-x}\text{Ga}_x\text{N}$ heterostructure investigated in (Richter, et al., 2022), measured by SXDM (top) and calculated based on known strain fields of threading dislocations (bottom). There, a threading edge dislocation density of $2 \times 10^9 \text{ cm}^{-2}$ was found to reproduce the characteristics of the experimental maps in the calculations.

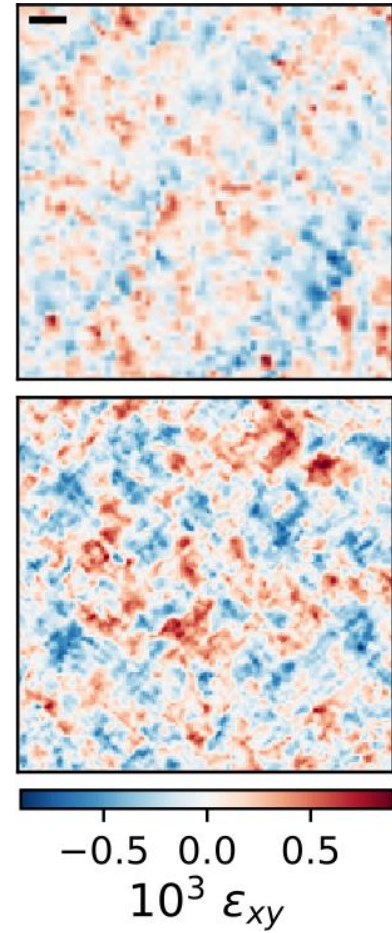


Figure 2: Measured (top) and calculated (bottom) maps of in-plane shear strain due to threading edge dislocations in a free-standing $\text{In}_{1-x}\text{Ga}_x\text{N}$ heterostructure. The scale-bar length is 2 μm .

Approaching the Limit of Spatial Resolution – a Si/Si_{1-x}Ge_x Spin Shuttle

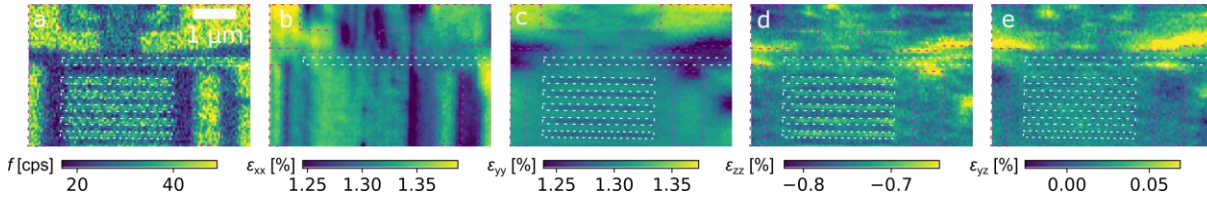


Figure 3 SXDM strain maps in the 10 nm Si QW layer of a Si_{0.67}Ge_{0.33}/Si/Si_{0.67}Ge_{0.33}/Si(001) heterostructure with a test device modeled after the QuBus architecture (a) X-ray fluorescence, (b) ϵ_{xx} , (c) ϵ_{yy} , (d) ϵ_{zz} , (e) ϵ_{yz} , (f) ϵ_{zy} . Adapted with permission from Ref. (Corley-Wiciak C. , et al., 2023)

The spins of electrons or holes confined in electrostatic quantum dots (QDs) are one of the most promising realizations of solid-state quantum bits (qubits) (Burkard, Ladd, Pan, Nichol, & Petta, 2023). Currently, the main challenge towards the development of a functional quantum processor is the fabrication of qubits in large interconnected arrays capable of spin-coherent information exchange (Xue, et al., 2024). However, to-date, massive fluctuations of quantum properties are typically observed between qubits fabricated on the same chip (Volmer, et al., 2024), thus inhibiting their large-scale operation. Modulations of lattice strain within the epitaxial heterostructure and stress induced by metallic gate electrodes represent one contribution to such inhomogeneity (Corley-Wiciak, et al., 2023).

SXDM demonstrated the unique capability of non-destructively and exclusively probing the strain state within the buried epitaxial 10 nm-thin Si/Si_{0.67}Ge_{0.33} Quantum Well (QW) layer, with a spatial resolution matching the typical pitch < 50 nm of the gate electrodes defining the QDs within the QW (Langrock, et al., 2023). These results allowed to predict the electrostatic energy landscape felt by the spin qubit and thus to better understand qubit operation and spin-coherent transport (Corley-Wiciak C. , et al., 2023).

Mapping strain fluctuations between the QDs required to push the spatial resolution limit of the technique. To achieve the ultimate spatial resolution as defined by the focal size of the probe beam, it is critical to ensure a high incidence angle of the beam, preventing geometrical broadening of the X-ray spot on the sample. Moreover, sample drifts during the acquisition of the 5D SXDM dataset and during change of reflection must be accurately tracked. The former was realized by selecting an X-ray energy and a set of symmetry-equivalent Bragg reflections (e.g. {335} reflections for Silicon (001)) that lead to normal incidence and only require a rotation about the surface normal to switch between reflections. The latter can be achieved by recording an orientation-independent signal such as fluorescence, luminescence or beam-induced current, that should not change during subsequent raster scans at varying incidence angle. In this work, this approach was demonstrated by recording X-ray fluorescence from the gate electrodes themselves, enabling to achieve a spatial resolution of ~ 50 nm. We note that nowadays, FZP focusing optics enable focal spots and thus resolution in SXDM down to < 30 nm [24]. **Es ist eine ungültige Quelle angegeben.**

Figure 3 showcases the resulting high-resolution maps of a set of strain tensor components that were reconstructed from SXDM data of the Si QW layer in a QuBus device for spin-coherent electron transport between qubits (Langrock, et al., 2023). It was found that the main source of spatial strain modulations, which are on the order of 5×10^{-4} , are the TiN electrodes fabricated on top of the heterostructure, since they are subjected to considerable internal stress > 1 GPa (Corley-Wiciak C. , et al., 2023). Calculations of the strain-dependent conduction band edge E_c based on the SXDM strain data and the deformation potential predict spatial fluctuations thereof up to ~ 4 meV, which is of a similar magnitude as the QD orbital energy (Zajac, Hazard, Mi, Nielsen, & Petta, 2016).

This work demonstrated how SXDM can provide valuable structural data for the design of functional quantum devices. The potential in a reliable mapping of all components of strain inside QW heterostructures with a resolution matching the size of the qubit has become even more evident since shear-strain-engineering has recently been proposed as a route to enhance valley splitting in semiconductor spin qubits (Zajac, Hazard, Mi, Nielsen, & Petta, 2016). The mapping of ultra-thin layers has become immensely more feasible in generation IV synchrotrons, e.g. after the Extremely Bright Source (EBS) upgrade to the ESRF storage ring (Raimondi, et al., 2023) The intensity is now

sufficient to perform quick mapping, within <12 h, even for ultra-thin layers down to ~4 nm thickness (Wilflingseder, et al., 2024).

Strongly Strained and Bent 3D Microstructures – $\text{Ge}_{1-x}\text{Sn}_x$ Micro-Disks

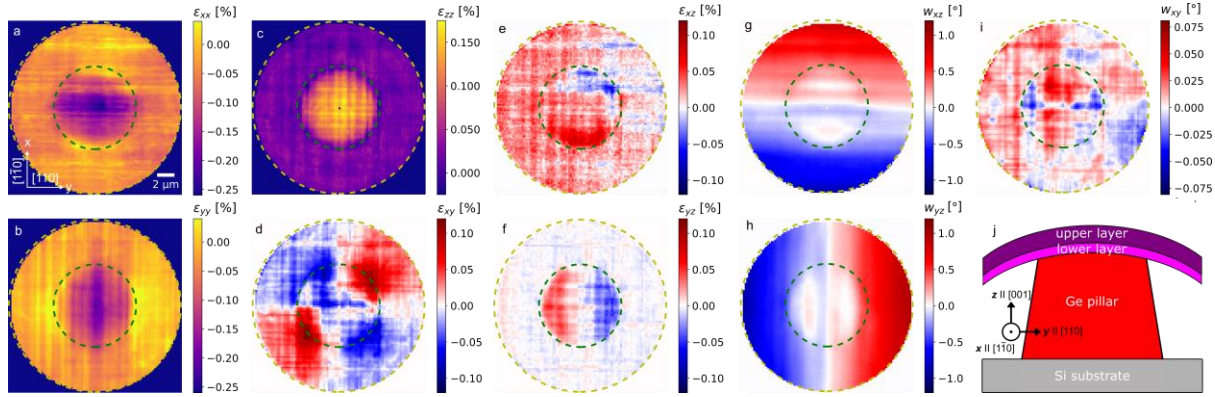


Figure 4 SXDM maps of lattice strain and rotation tensor in a suspended $\text{Ge}_{1-x}\text{Sn}_x$ microdisk. (a) ϵ_{xx} , (b) ϵ_{yy} , (c) ϵ_{zz} , (d) ϵ_{xy} , (e) ϵ_{xz} , (f) ϵ_{yz} , (g) ω_{xz} , (h) ω_{yz} , (i) ω_{xy} , (j) sketch of the microdisk in cross-section view. The inset arrows indicate the direction of the lattice planes within the coordinate system. Reproduced with permission from (Corley-Wiciak C. , et al., 2024).

The realization of CMOS-compatible, on-chip light source holds immense potential for telecommunication and large-scale optoelectronics (Moutanabbir, et al., 2021). One potential material platform for these applications are epitaxial $\text{Ge}_{1-x}\text{Sn}_x/\text{Ge}/\text{Si}$ heterostructures, which in the last decade were the first group IV compound to demonstrate lasing (Wirths, et al., 2015). Bandgap tuning through aggressive strain-engineering has been used to enhance the performance of such devices, e.g. regarding the operating temperature (Stange, et al., 2016). One example of this are $\text{Ge}_{1-x}\text{Sn}_x/\text{Ge}$ microdisks, where the compressive epitaxial strain in the $\text{Ge}_{1-x}\text{Sn}_x$ layer, that counteracts the directness of the bandgap, was released by chemically selective under-etching.

The free-standing regions on the rim of such disks are, on average, nearly unstrained, however they are subject to strong bending. Conversely, the center part of the disk is still in contact with the Ge virtual substrate and is subject to biaxial in-plane strain. Characterizing the strain landscape of the different parts in such strongly deformed, alloyed 3D microstructures is particular challenging for two reasons: (1) Their diffraction signal is spread out widely in reciprocal space, (2) modulations of alloy content and different strain and rotation tensor components are strongly correlated and must be clearly separated. As demonstrated in (Corley-Wiciak C. , et al., 2024), SXDM enabled a quasi-tomographic view on the strain variations due to geometric relaxation in different layers of the disk as well as in from each other and the supporting Ge micro-pillar by discriminating the different regions in reciprocal space—due to their different lattice parameters, driven by their varying stoichiometry and geometric relaxation. This allows for a ‘quasi-tomographic’ view of the disk, as the strain modulations in the individual layers that are located at different depths in the microstructure can be studied separately Es ist eine ungültige Quelle angegeben.

Figure 4 shows the maps for all components of strain ϵ and rotation ω thus determined for a 900 nm-thick $\text{Ge}_{1-x}\text{Sn}_x$ micro-disk with an average Sn content of $x_{\text{Sn}} \approx 8.9\%$ Ge. The data gives direct evidence of the elastic release of lattice strain on the rim, the resulting bending of the micro-disk and the corresponding dipoles and quadrupoles in the maps of the shear strain components. Additional orthogonal lines in the shape of the quasi-periodic ‘crosshatch pattern’, which is typically observed in the surface morphology of group IV heterostructures (Rovaris, et al., 2019), in all strain components mark the presence of a dense misfit dislocation network at the $\text{Ge}_{1-x}\text{Sn}_x/\text{Ge}$ interface. By comparison of the center of the disk (green dashed circle in **Figure 4**) and the free-standing rim region (yellow circle) and based on

symmetry arguments, ~~the free lower surface was exploited as additional boundary condition, which allowed it was possible~~ to disentangle out-of-plane stress σ_{zz} and local variations in Sn content x_{Sn} (Corley-Wiciak C. , et al., 2024). Experimental strain data such as discussed here may be employed in the development of realistic FEM models of the 3D micro-structure and the calculation of the local band energy levels relevant for optoelectronic applications (Zaitsev, et al., 2023). For this particular micro-disk, spatial fluctuations of the $\text{Ge}_{1-x}\text{Sn}_x$ bandgap on the order of 10 meV are predicted, anticipating a broadening of the laser emission spectrum.

Domains in Ferroic Crystals and Thin Films

~~In addition~~Next to imaging strain fields, a main strength of SXDM is the ability to produce direct space maps filtered for selected features in reciprocal space, which is particularly well suited for the study of crystals that display domains. Different ferroelectric, ferromagnetic or ferroelastic domains can give rise to Bragg peaks of different intensity or position. Most often grown as thin films or as part of complex epitaxial heterostructures, research on these materials has focused on understanding the physics behind their peculiar functionalities with the aim of exploiting them in novel technological devices (Catalan, Seidel, Ramesh, & Scott, 2012). Much of these functionalities depend on the size, type and arrangement of ferroic domains and their boundaries, *domain walls*, so that imaging domain patterns and their response to external stimuli is a crucial aspect of this research effort.

The SXDM imaging mechanism for ferroic domain structures relies on the different symmetry that ~~characterises~~characterizes distinct domain individuals:

Pure *ferroelectric* domains differ only by the direction of the atomic displacements that give rise to the spontaneous electric dipole. In an SXDM map, contrast between oppositely ~~polarised~~polarized domains thus arises from different structure factors, so that the intensity of Bragg peaks is affected (**Fig 5a-c**) (Jo, et al., 2011). Often, ferroelectric domains form dense periodic patterns, comprising individual domains smaller than the X-ray nanoprobe. In such cases, a single nanodiffraction pattern originates from several correlated domains, giving rise to satellite peaks that are representative of the periodicity. SXDM imaging of the satellite peaks then yields the distribution of domain “clusters” that have a uniform periodicity, allowing to determine their local correlation lengths and to contrast these with local strain fields.

Similarly, imaging of *ferromagnetic* domains by SXDM relies on differences in the structure factor under resonant scattering conditions: contrast in SXDM maps is achieved through (i) selecting X-ray energies near an absorption edge of the ion responsible for the magnetic dipole and (ii) ~~analysing~~analyzing the polarization dependence of the diffracted beam (Evans, et al., 2020).

In many ferroelectric systems, notably perovskites, the appearance of the spontaneous dipole is accompanied by a change in crystal family (i.e. in the shape of the unit cell), so that domains are simultaneously ferroelectric and *ferroelastic*. For mechanical compatibility, strain-free boundaries between different ferroelastic domains require the lattice planes to rotate between one domain and its ~~neighbour~~neighbor (i.e. in crossing a domain wall). This leads to a splitting of Bragg peaks in reciprocal space (**Figure 5d-e**), therefore each domain variant can be readily distinguished by the position of the diffraction signal on the detector (**Figure 5f**) (Hruszkewycz, et al., 2011), allowing to image and thus ~~rationalise~~rationalize complex hierarchical domain patterns by SXDM (Yin, et al., 2024). Because an SXDM dataset also contains information on local lattice deformations, the interaction between defects and domain boundaries can additionally be explored (**Figure 5g**) (Zhuo, et al., 2024). ~~Recent works have, furthermore, explored the time domain by means of pump and probe experiments to track the laser excited nanosecond dynamics of domain patterns [57].~~

Compared with other scanning probe and microscopy techniques routinely used to ~~visualise~~visualize ferroic domains, such as TEM/**STEM**, second-harmonic generation microscopy, piezoresponse- or magnetic force microscopy, SXDM has several unique ~~advantages. Firstly, it features. Due to the typical penetration depths of hard X-rays in solids (few to tens of μm),~~ SXDM can image domain patterns in deeply buried layers, such as underneath an electrode

(Lichtensteiger, et al., 2023). ~~For the same reason. Secondly,~~ it allows to study the response of domain patterns to external excitations, such as temperature or a suitable field (Yin, et al., 2024; Marçal, et al., 2020), *in-situ* and in a relatively straightforward manner ~~in devices as-is, without any additional sample preparation being required (Figure 5h,i).~~ ~~Finally,~~ In addition, similarly to 4D-STEM a 5D SXDM dataset will contain not only information on the spatial arrangement of domains and domain walls, but also on their local structure and crystallography. ~~The correlation of such information can yield crucial physical insights.~~ These capabilities offer the possibility of observing lattice dynamics during polarization switching in a ferroelectric capacitor device simply by mounting it onto the scanning stage and applying the necessary bias as SXDM scans are performed **Es ist eine ungültige Quelle angegeben.**

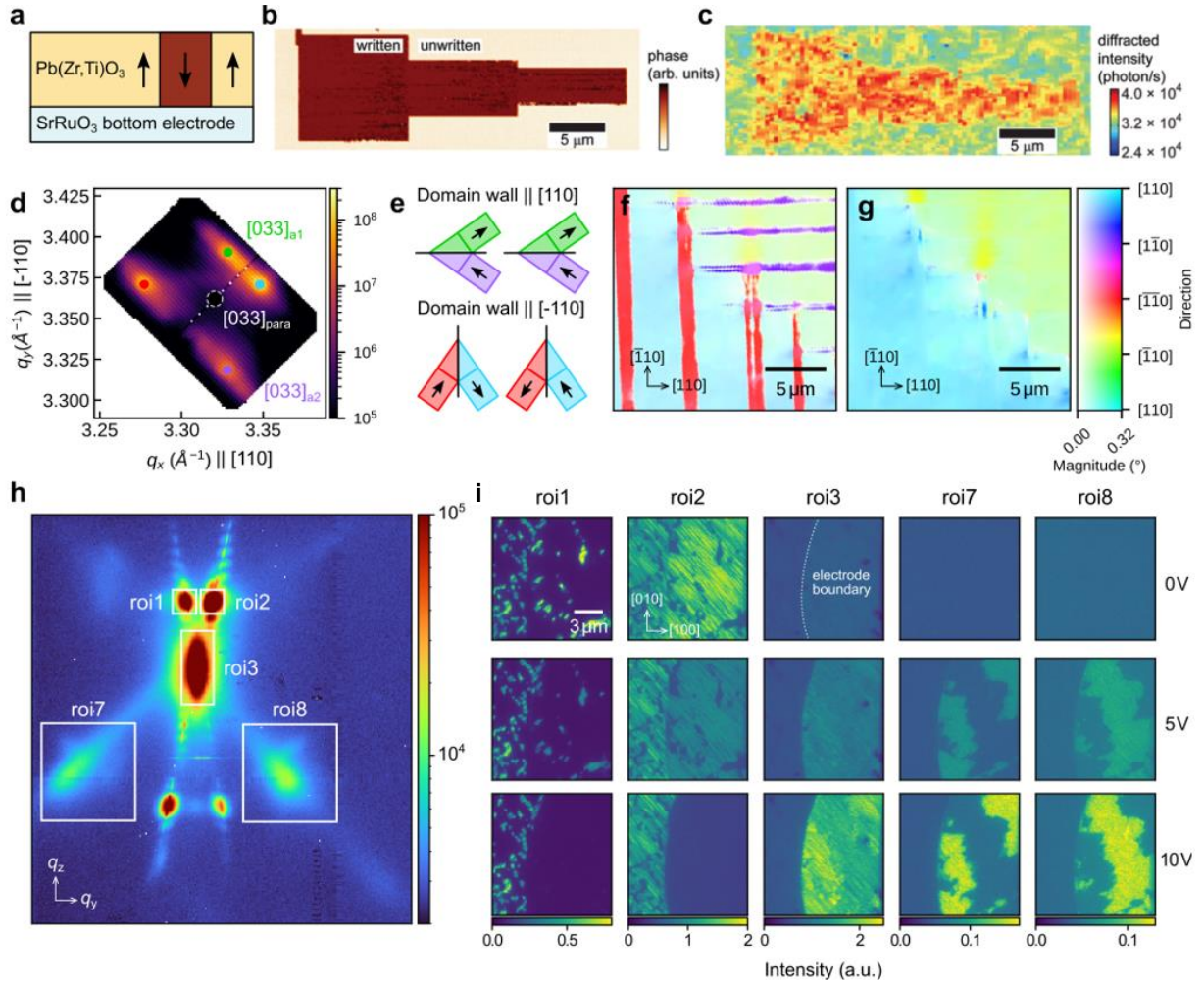


Figure 5. SXDM of ferroelectrics. a) Sketch of a switched ferroelectric domain in a $\text{PbZr}_{0.45}\text{Ti}_{0.55}\text{O}_3$ thin film, where arrows represent the direction of the spontaneous polarisation. b) Piezoresponse microscopy image of the switched domain. c) SXDM image of the switched domain, showing a different diffracted intensity compared to the unswitched matrix for the 002 Bragg reflection. Reproduced from (Jo, et al., 2011). d) Projection along q_z of the large-area 3D-RSM collected around the 033 Bragg condition of a BaTiO_3 crystal with an unfocused beam. The four different peaks which are visible are due to four distinct ferroelectric-ferroelastic domain types, sketched in (e) colour-coded as in (d). f) 5D-SXDM map of the angular tilt of q -vectors normal to 033 lattice planes q_{033} , where colour hue and saturation represent tilt direction and magnitude, respectively. The domains sketched in (e) are visible here. g) The same map as (f), but focusing on local q -vector deviations from the average of two of the four domains, highlighting regions of localized lattice deformations near the domain walls, i.e., dislocations. Reproduced from (Zhuo, et al., 2024). h) Detector frame obtained with an unfocused beam on a $\text{PbTiO}_3/\text{SrTiO}_3 // \text{DyScO}_3$ superlattice, displaying multiple peaks, each due to a different domain or domain bundle variant. i) Evolution of the domain signals seen in (h) as a function of applied voltage; the appearance of some domain variants at the detriment of others is visible underneath the top electrode. Reproduced with

Intra- and Inter-Grain Imaging: Cathode Materials for Li-Ion Batteries

SXDM was proven as a useful tool for analyzing polycrystalline materials as exemplified below on battery materials and their evolution during operation. The deeper understanding and further development of batteries and their

components are a key element for sustainable energy technologies such as electric vehicles, and energy storage (Martens, et al., 2023). By adjusting the scan area and the beam size, it is possible to look into inter-particle variation (**Figure 6a,b**) or intra-particle heterogeneities (**Figure 6c**) of lattice strain in powder samples. Since the fluctuation of the interplanar spacing d is directly related to the Li-ion concentration for most cathode materials, SXDM investigations across an ensemble of particles enable the identification of inter-particle lithiation heterogeneities, as demonstrated on LiNiO₂ (LNO) particles in **Figure 6d,e**. For larger crystals, a more finely resolved SXDM map provides information on strain, defect concentration, lattice rotation and crystallinity within the particle (**Figure 6f**) (Colalongo, et al., 2024). Such an approach assists the quantification of lithiation heterogeneities due to the defective nature of crystals after synthesis, anticipating their impact on the cathode performance and ultimately guiding their technological improvement towards cathode materials with reduced defect densities (Spence, et al., 2022). For example, for a NMC622 (LiNi_{0.6}Mn_{0.2}Co_{0.2}O₂) cathode, SXDM combined with X-ray nanotomography helped to uncover strain gradients and crystal bending present in the particles (Martens, et al., 2023). These types of structural defects can strongly affect the electrochemical stability of the system. *In-situ* SXDM studies of similar NMC622 single crystals under high voltage revealed that the domain boundaries are the fundamental origin for the oxygen redox instability at high voltages and lead to an increase in oxygen release during operation (Liu, et al., 2022).

Relatively few constraints during measurement allows for SXDM to be used in *operando* regime providing unique insights into the local structural evolution of the particle associated with different types of phase transitions (Martens, et al., 2023; Huang, et al., 2024). **Figure 6g-j** showcases a SXDM study of LMNO (LiMn_{1.5}Ni_{0.5}O₄) high voltage spinel cathode where both solid-solution and phase-segregated transitions take place at different points of the charge. In the first half of the charging curve (Martens, et al., 2023), during the solid solution-like phase transition, the average d-spacing value (d_{004}) of the particle is decreasing uniformly as seen in **Figure 6g**, where the color bar spans the full d-spacing range observed during the phase transition. However, by limiting the color bar to the values of d-spacing observed for each individual scan (**Figure 6h**), it becomes possible to visualize very fine local structural changes of the lattice and therefore lithiation inhomogeneities present in the particle at each step of charging. Such gradients are unusually persistent throughout the process and appear to be templated by the lattice defects, guiding the lithiation within single cathode crystals.

During a study on a two-phase transition (**Figure 6i**), where both lithiated and delithiated phases coexist in the particle, one of the crystals measured with SXDM manifested the formation of metastable misoriented domains (Vostrov, et al., 2025). The observed misorientation is due to the accommodation of mechanical stress, arising due to the lattice constant difference between the two phases. Such metastable features affect material stability during continuous charging, as plotted in **Figure 6j**. They were found to be caused by inherent lattice defects due to crystal quality variations of a subset of particles originating after material synthesis and not by the dynamics of lithium ion deintercalation. Such investigations may be coupled with X-ray techniques that probe the statistics of the ensemble and *post-mortem* SXDM studies, allowing to pinpoint the degradation mechanisms and optimize the design of the cathode materials (Martens, et al., 2023; Vostrov, et al., 2025). By a similar approach, a reorientation of the crystal lattice has been observed in Ni-rich layered oxides (NMC), causing lattice distortions and contributing to degradation processes (Huang, et al., 2024).

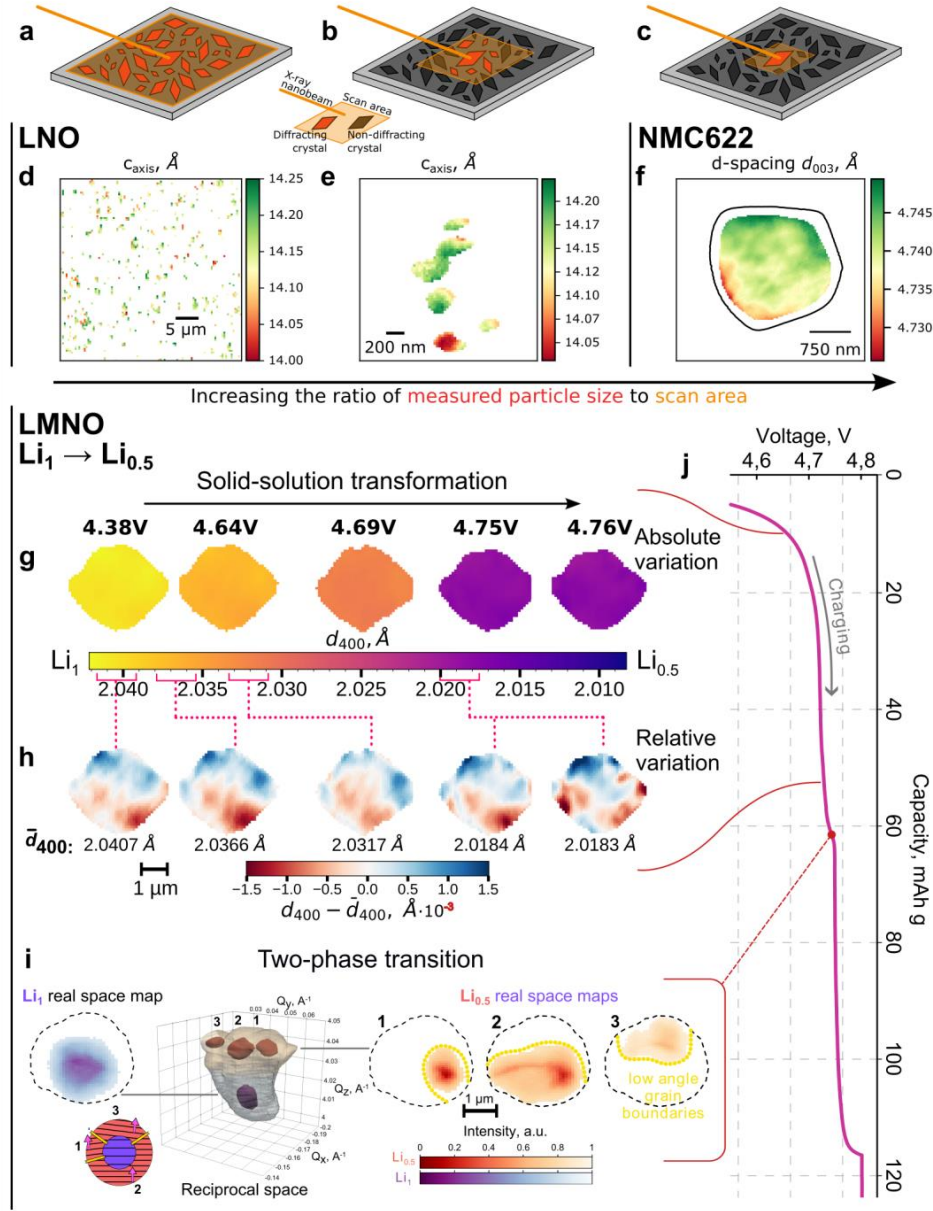


Figure 6. (a-c) A schematic overview of different operation modes of SXDM probing different areas in powder samples. (d-f) 2D maps of structural heterogeneities obtained with each of the operation mode. Reproduced from (Colalongo, et al., 2024). Operando nanodiffraction images of an LMNO micro-crystal at different potentials during the solid-solution region of the $\text{Li}_1 \rightarrow \text{Li}_{0.5}$ phase transition: (g) The color bar uses the complete d_{400} -spacing range observed during $\text{Li}_1 \rightarrow \text{Li}_{0.5}$ transition. (h) The same snapshots are colored showing only variation within the crystal relative to average d -spacing ($\bar{d}_{400}$). Reproduced with permission from (Martens, et al., 2023). (i) Detailed SXDM imaging of the 115 Bragg reflection when Li_1 and $\text{Li}_{0.5}$ phases coexist in the particle during the two-phase region of the transformation. The measured region of reciprocal space contains the intensity integrated over the whole particle in real space. For selected regions of the reciprocal space that correspond to the Li_1 (blue) and $\text{Li}_{0.5}$ (red), the corresponding real-space maps are presented on the right. The red brackets indicate the point in the electrochemical curve (j), where the scans were taken. Reproduced with permission from (Vostrov et al. 2025).

Discussion & Outlook

We have highlighted today's capabilities of 4D and 5D Scanning X-ray Diffraction Microscopy, enabling a complete characterization of nanoscale lattice distortions due to lattice defects, geometric structuring or domain formation with application in a wide range of material systems and functional devices. As a model-free structural characterization method, SXDM especially excels due to its universality, as it can be applied to virtually all crystalline materials and does not require any specific sample preparation. While offering a high penetration depth, the high resolution in reciprocal space allows SXDM to filter out specific regions of interest in the probed volume. This property makes SXDM the tool of choice for imaging of strain in epitaxial layer stacks, particularly relevant in the field of strain engineering, or of complex ~~three-dimensional~~ multidimensional domain patterns.

~~It should be noted that electron probe techniques such as Electron Backscattering Diffraction (EBSD) and NBED bear conceptual similarity to SXDM and naturally allow for strain microscopy with higher (down to atomic scale) spatial resolution (Naresh-Kumar, et al., 2020; Ophus, 2023), but hold the general drawback of a limited, near-surface probing depth or the requirement of a destructive extraction of a thin electron-transparent lamella from the sample.~~ While a comprehensive comparison of experimental techniques for strain mapping is documented in a previous review (Gammer, Richard, & Eberl, 2019), we ~~will~~ briefly outline how ~~compare~~ compare SXDM to other synchrotron-based strain microscopy techniques. Using a polychromatic X-ray beam ~~for~~, X-ray Laue microdiffraction has the ~~benefit~~ advantage that robust information about lattice strain and orientation is obtained in one single exposure. This technique can be applied to both single-crystalline and poly-crystalline materials and ~~nowadays~~ comes with capability for mapping of the full deviatoric strain tensor (Robach, et al., 2013), and 3D spatial resolution (Gürsoy, Sheyfer, Wojcik, Liu, & Tischler, 2023), whereas the resolution in real and reciprocal space are significantly coarser compared to SXDM. Bragg Coherent Diffraction Imaging (BCDI) employs a phase reconstruction algorithm to obtain 3D strain maps with a fine spatial resolution < 10 nm, but is limited to samples smaller than the coherence volume of the beam (typically < 1 µm), making it most suitable for nanoparticles [67]. Dark Field X-ray Microscopy (DFXM), by placing an objective optic between sample and detector (Yildirim, Cook, Detlefs, Simons, & Poulsen, 2020), yields a magnified image of the sample in diffraction contrast by a single exposure. ~~Compared~~ Thus, providing a direct view into real space rather than reciprocal space makes DFXM highly complementary to SXDM. DFXM typically provides a larger field of view at the expense of ~~coarser spatial resolution and~~ a sparse sampling of reciprocal space, which is realized by angular scans of sample and detector. ~~Among these techniques, SXDM stands out by a high-resolution sampling of reciprocal space, resolving inhomogeneities, strain gradients, domain coexistence or layer stacks within the beam footprint.~~

~~It should also be noted that electron probe~~ Among these ~~techniques such as Electron Backscattering Diffraction (EBSD) and NBED bear conceptual similarity to~~ SXDM and allow for strain mapping with fine spatial resolution [69, 23], although these are limited to probing surface near regions of a sample, or require extraction of thin lamella from the bulk sample.

~~In this review, we concentrated on SXDM in~~ stands out by ~~a high-resolution X-ray diffraction geometry giving insights into slight lattice deformations in~~ sampling of real and ~~reciprocal space, which is ideal for highly oriented samples such as epitaxial or textured systems. A low resolution geometry can be~~ resolving slightest inhomogeneities, strain gradients, domain coexistence or layer stacks within the beam footprint. Alternatively, a trade-off between resolution and field of view in reciprocal (angular) space of SXDM is readily ~~realized~~ achieved ~~by~~ reducing ~~changing~~ the distance between sample and the area detector. Short distances correspond to ~~cover large angular ranges. This~~ the Wide-Angle X-ray Scattering (WAXS) geometry, which is particularly beneficial for the study of polycrystalline or semi-crystalline materials (Riekel, Burghammer, & Davies, 2010), and is used in techniques such as scanning 3D XRD (Zhang, et al., 2025), or X-ray strain tensor tomography (Modregger, et al., 2025).

~~Future advances in the fabrication of diffractive X-Ray optics are expected to generate smaller X-ray nano-probes, enabling even finer strain mapping by SXDM [24]. However, greater enhancement of spatial resolution will be realized by leveraging the coherence of latest generation synchrotron sources, which has the potential to unite SXDM~~

and Bragg ptychography. By an iterative phase reconstruction algorithm, this will allow to reconstruct the strain distribution in the crystal with resolution below the beam spot size and provide complete 3D spatial resolution [73]. As of today, although X-ray ptychography in transmission mode is widely used nowadays, the analysis of diffraction-mode ptychography data remains challenging.

Bragg reflections observed using coherent X-rays contain rich information about the 3D distribution of lattice strain expressed in form of strong modulations of the diffracted intensity distribution (speckles) in reciprocal space. However, an inversion of such data is not directly possible and requires prior knowledge of the sample or assumptions that enable recovery of the phase of the recorded X-rays. The latter is done in Bragg Coherent Diffraction Imaging (BCDI) that involves phase retrieval algorithms based on the assumption that the studied sample or lattice dimensions are small (typically $\approx 1 \mu\text{m}$) in all directions. Inversion of BCDI data yields 3D strain maps in high spatial resolution $< 10 \text{ nm}$ (Richard, et al., 2023) and, as for SXDM, the combination of three datasets from different reflections allows to recover the complete strain tensor **Es ist eine ungültige Quelle angegeben.** The limitation to small samples makes BCDI most suitable for the study of nanoparticles, and therefore highly complementary to the use cases of SXDM such as epitaxial thin films. Conversely, SXDM may be applied to samples of any dimension, and is a direct method that does not rely on assumptions.

Coherent Bragg Ptychography is a scanning technique that is experimentally equivalent to SXDM under coherent X-ray illumination. In ptychography, a high data redundancy is achieved by illuminating neighboring regions with significant overlap, thus enabling a robust phase retrieval (Li, et al., 2021), although the data analysis remains a challenge. Indeed, with 4th generation synchrotron sources and improved phase reconstruction algorithms, many of the current limitations of SXDM can potentially be overcome by using highly coherent X-rays and by inverting the resulting Bragg ptychography data. This includes the projection issue, i.e. the lack of surface sensitivity or depth resolution, and the spatial resolution that is limited by the achievable beam spot size of $\approx 25 \text{ nm}$. Although further advances in the fabrication of X-Ray optics are expected and single-digit nanometer focusing of X-rays has been demonstrated **Es ist eine ungültige Quelle angegeben.**, such approaches will be impractical for SXDM due to (a) the short working distances required, (b) vibrations and drift in the setup and (c) the issue of increasing beam convergence described above. In contrast, if phase retrieval and data inversion are successful, Bragg ptychography can provide 3D maps of lattice strain with few-nm resolution, even with moderate focusing and without knowledge of the beam position to this precision.

Another limitation of both SXDM and Bragg ptychography is the time required to perform raster scans, which is currently on the order of minutes for 4D and hours for 5D scans. This prevents capturing fast processes in a time-resolved manner unless they are repeatable and, thus, allow to use stroboscopic techniques. On the other hand, we expect that the SXDM scanning speed will increase through the use of faster positioners and detectors, since already today the recorded signal strength is often not the limiting factor.

We emphasize that, compared to ~~the available alternatives~~ alternative techniques, SXDM ~~is so far the only technique giving access~~ excels when it comes to ~~the entire~~ mapping all components of strain tensor within buried layers at with high lateral resolution ~~<down to~~ 50 nm even for ultra-thin ($< 10 \text{ nm}$) films and at and strain sensitivity of $\sim 10^{-5}$. Furthermore, SXDM data ~~is very robust in its interpretation as no modelling~~ is very robust without the need for structural models or assumptions ~~are made in the analysis~~. The flexibility of SXDM in probing the lattice of samples with any structure and geometry is complemented by the possibility of *in-situ* conditions (Hanke, et al., 2022), utilizing environments such as diamond anvils (Hrubiak, Smith, & Shen, 2019), electrochemical cells (Martens, et al., 2023), as well as cryostats and ovens. Recent works have, furthermore, explored the spatiotemporal evolution of ferroelectric domain patterns under laser excitation by SXDM (Gaal, et al., 2023). Leveraging the time structure of the X-ray bunches in a synchrotron source or an X-ray Free Electron Laser allows for efficient, stroboscopic probing of dynamic processes with temporal resolution in the nanosecond to femtosecond regime, essentially recording movies of lattice strain instead of static maps **Es ist eine ungültige Quelle angegeben.**

In conclusion, SXDM has the potential to become a universal solution to gain insights into lattice inhomogeneities and internal structure in a wide range of ~~problems~~ fields from material science, microelectronics, battery research, and more. In this role, it can leverage the further advantages of synchrotron radiation to obtain elemental sensitivity or time-resolution, especially interesting for *operando* studies on functional devices.

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Declarations

Conflict of interest

On behalf of all authors, the corresponding author states that there is no conflict of interest.

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Availability of data and material

This review article summarizes previously published data, which are available in the cited references. Newly generated data supporting this publication are available upon request.

Authors contributions

All authors contributed to the conceptualization, literature analysis, and writing of the manuscript. All authors reviewed and approved the final version.

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