Electron backscatter diffraction

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This chapter provides an overview of the electron backscatter diffraction (EBSD) modality which, over the past thirty years, has become a core microstructure characterization technique in both the materials and geological fields. EBSD typically produces 2D maps (or 3D volumes in the case of serial sectioning) of the orientations of the constituent crystallites of a sample with respect to an external reference frame. The chapter starts by describing the experimental geometry of the sample and detector inside the chamber of a scanning electron microscope (SEM). This is followed by a review of the kinematical and dynamical theories of electron scattering which, along with the detector geometry, can be used to predict EBSD patterns, including the diffuse background intensity. Since EBSD produces orientations, several commonly used orientation representations and parametrizations are reviewed before explaining how the crystal orientation is extracted from the experimental patterns, using either Hough-transform-based feature extraction, or the whole-pattern-matching approaches known as dictionary indexing and spherical indexing. To obtain accurate results it is crucial that the sample surface be properly prepared and a number of standard techniques for obtaining an optimal sample surface finish are described. Commercial and open-source software solutions for data analysis are described as well as a number of commonly used data formats. The chapter concludes with several examples of applications taken from both the materials and geological literature, and brief ruminations on the future of the EBSD characterization technique.

1. Introduction

1.1. Basic description

Electron backscatter diffraction, most commonly known as EBSD in the community, is a microstructure characterization technique based in the scanning electron microscope (SEM). EBSD patterns are often referred to as EBSPs; the early literature on the technique also included the terms BKD for backscatter Kikuchi diffraction and BEKP for backscatter electron Kikuchi pattern. Orientation mapping of microstructures via automated EBSD is also known under various descriptors, including OIM (orientation imaging microscopy), OM (orientation mapping) and ACOM (automated crystallographic orientation mapping).

The SEM electron beam typically has an energy ranging from 1 to 40 kiloelectronvolts (keV). The beam is focused to a spot size ranging from about 0.4 nm to 5 nm in diameter, resulting in a potential spatial resolution of better than 1 nm. The achievable spatial resolution is generally a function of accelerating voltage and beam current (generally the resolution decreases with increasing current) as well as the sample itself. An SEM produces images from the surface of a specimen by scanning (or rastering) the focused electron beam across the surface. Various signals are emitted by the interaction of the incident electrons with atoms in the sample. The
interaction depth is at most 5 μm and, thus, the SEM is very much a surface-sensitive characterization technique. The signals contain information about the sample, including surface topography, composition and crystallography. As the electron beam is scanned across the sample, the position of the beam is tracked along with the intensity of these detected signals and mapped to a grey scale to produce an image. The most important signals are:

Secondary electrons (SEs) are emitted by atoms excited by the incident electron beam. SE images tend to show contrast dominated by the topography of the sample surface.

Backscattered electrons (BSEs) are those electrons originating in the electron beam that are reflected or backscattered out of the sample after elastic (primarily) scattering interactions with atoms near the sample surface. Heavy elements (high atomic number) backscatter electrons more strongly and thus produce a stronger signal than lighter elements (low atomic number). BSE images will, thus, show image contrast that reflects the chemical composition of the sample. While the BSE signal is strongly sensitive to the atomic number, it is also secondarily affected by the orientation of the atomic planes within the crystal structure with respect to the sample surface plane; this orientation dependence forms the basis for EBSD. Typically, BSEs originate very near the sample surface.

The interaction of the electron beam with the atoms near the sample surface will also produce X-rays. These characteristic X-rays produce a spectrum of energies which can be detected using X-ray energy-dispersive spectroscopy (XEDS or EDS) or wavelength-dispersive X-ray spectroscopy (WDS). When the beam is stationary, these spectroscopic analysis techniques can be used to quantitatively estimate the elemental composition. When the beam is scanning, the X-ray signal can be used to map the distribution of elements in the sample.

Other signals include cathodoluminescence (CL) and electron beam induced current (EBIC); both of these techniques are often used to examine semiconductor materials. Typically samples are mounted flat in the SEM chamber, i.e., normal to the electron beam. If the sample is highly tilted, 70° for example, then the nature of the BSE signal will change so that the signal-to-noise ratio of the crystallographically sensitive portion of the BSE signal is enhanced. In general BSE imaging, the BSE detector simply measures the intensity of the backscattered electrons from the interaction volume. However, the electrons are emitted in all directions from the sample, producing a hemisphere of radiation. The intensity within this cloud of backscattered electrons varies with direction. If a position-sensitive detector is introduced into the SEM to sample the hemisphere, then the directionally varying BSE signal produces a pattern, as can be seen schematically in Fig. 1. Early detection of EBSD patterns was done using film, but modern systems are typically composed of a scintillator, lenses (or a fibre optic) and a low-light camera, such as a charge-coupled device (CCD) or a complementary metal-oxide semiconductor (CMOS) camera. The most commonly used scintillator is a phosphor screen. When electrons impinge on the phosphor, the phosphor fluoresces producing visible light; when many electrons impinge on the phosphor a pattern is formed which can then be captured by the camera. The bands in the EBSD patterns correspond to atomic planes in the crystal structure. If the crystalline phase within the interaction volume is known, then the geometrical arrangement of the bands can be used to determine the orientation of the crystal through a process known as indexing (Section 6). An EBSD pattern can be captured and indexed at each point in a defined raster grid and the orientation (and other descriptive parameters) recorded. Such spatially specific information can then be mapped to a grey or colour scale to form images where the contrast is governed by crystallographic orientation – orientation mapping (Section 9.4). Modern EBSD systems can capture and index patterns at rates exceeding 3000 patterns per second. From such data, orientation maps can be generated so that the crystallographic aspects of the microstructure can be visualized in real time. However, the amount of data generated during automated EBSD scans is large and subsequent analysis of such data can provide statistically reliable information about the crystallographic texture, grain boundaries, strain and other important aspects linking microstructure to material behaviour, often at a sub-micron length scale.

1.2. History

This section intends to provide a broad but not comprehensive review of relevant publications and set the stage for subsequent sections on both the technical aspects of EBSD as well as its applications. Although biased by our personal experiences and familiarity with the field, we have attempted to give a chronological review of the pioneering development work both in terms of the technique itself and also in key applications. Many of the authors cited in these early works have continued to contribute to the EBSD literature and more comprehensive papers reviewing their efforts are available elsewhere. Very good sources for reviewing much of this literature are the two editions of Electron Backscatter Diffraction in Materials Science (Schwartz et al., 2000, 2009).

The first EBSD pattern, then called a ‘P-pattern’, was published in 1928 (Nishikawa & Kikuchi, 1928) and was from
a cleaved face in calcite. Up until the 1970s, a handful of papers were written analysing patterns from different materials. Other names for the patterns included wide-angle and high-angle Kikuchi patterns. These studies typically recorded patterns on photographic plates or electron-sensitive film. For high-angle Kikuchi patterns. These studies typically recorded materials. Other names for the patterns included wide-angle and paper. The effects of the angle of incidence were explored by Alam, Blackman and Pashley, who found the pattern contrast peaked between 20–30° from the incident beam (Alam et al., 1954). The next advancement was the implementation of EBSD into a scanning transmission electron microscope (STEM) (Venables & Harland, 1973), but operated at conditions more typical for an SEM. This implementation was used to measure crystallographic orientations at angular resolutions similar to those routinely measured in today’s automated systems. David Dingley made another significant step forward by developing an online system to analyse the patterns (Dingley et al., 1987). A skilled operator could index patterns at a rate of about one minute per pattern, which was much faster than manual measurements. The online system was achieved by capturing the patterns formed on a scintillator (phosphor screen) using a low-light camera. Dingley presented his work on orientation determination via EBSD at the 1986 International Conference on Textures of Materials, where Brent Adams of Brigham Young University was in attendance. Adams recognized the value of this technique in his research on orientation correlation and, with the help of Dingley, adopted the EBSD technique in his laboratory. After just a few projects using the EBSD system, Adams envisioned the impact a fully automated system could make on microstructural characterization. In 1988, Adams moved to Yale University, where he and Dingley partnered to guide a research team toward realizing the first fully automated EBSD system (Adams et al., 1993) at the end of 1991. This system operated on a four-processor Unix workstation and was capable of collecting and indexing patterns at a rate of one pattern every four seconds. Instead of rastering the beam, this system moved the sample under a stationary electron beam using a piezoelectric stage mounted in the SEM specimen chamber under the control of the EBSD analysis computer. This system was the forerunner of today’s modern systems, which operate at speeds exceeding 3000 points per second while moving the beam under the control of the EBSD computer. As in most research projects, other teams around the world were working in a similar direction. Dorte Juul-Jensen at RISØ National Laboratory in Denmark was also directing a research team focused on EBSD, and the team made several contributions (Juul Jensen & Schmidt, 1991) to successful achievement of a fully automated technique; some of these contributions are highlighted in subsequent sections.

The ability of EBSD to aid in phase identification was recognized early in the development of EBSD (Dingley & Baba-Kishi, 1986). A systematic EBSD procedure was proposed (Michael & Goehner, 1999) a few years after the automation of EBSD. Phase identification has not reached the same widespread application as orientation determination, partly because the same level of robustness and automation compared to orientation determination has not been realized (Section 10.2.2).

Since the early automation of EBSD, the technique has been noted for the colourful orientation maps, where the colour at a given pixel encodes the orientation measured at the corresponding point on the sample. Orientation maps are not unique to EBSD: they have been used for many years albeit constructed manually, grain-by-grain, both in terms of the orientation measurement as well as the colouring of the pixels (Sander, 1950; Wenk et al., 2019). Automated EBSD has made it possible to create orientation maps routinely. The most frequent orientation map shown in the literature is a so-called inverse pole figure (IPF) map (Inokuti et al., 1986). The colours in these maps indicate the crystal direction parallel to a given sample direction (usually the sample normal direction) in the same sense as an inverse pole figure. Various types of maps showing local variations in orientation have become common in EBSD-related publications, particularly in deformation studies; these maps have origins in early EBSD work (Wright, 1993; Lehockey et al., 2000). In addition to orientation maps, maps based on various parameters recorded during the scanning process can also be constructed and correlated with the orientation measurements. The most common of these scalar maps are those showing the quality of the diffraction patterns at each pixel using a grey scale colouring scheme. This was actually the first type of map generated using automated EBSD (Wright, 1992).

A search of EBSD-related publications using any of the scholarly journal indexing services will show that grain-size measurements and deformation are the most common EBSD application areas. While orientation measurements collected using standard EBSD continue to play a significant role in these studies, high-resolution EBSD (HREBSD) is also used (Wilkinson & Dingley, 1991), where high resolution refers to high angular resolution. By using cross-correlation between diffraction patterns from neighbouring points in the microstructure it is possible to measure orientation differences to higher levels of angular resolution than can be achieved using standard indexing (Section 6). In addition to high-resolution misorientation measurements, the technique can be used to estimate a displacement gradient tensor from which the elastic and inelastic strain tensors can be derived (see Section 10.4).

EBSD is a surface-sensitive technique, but it has been adapted in various forms to collect three-dimensional information. The earliest approach was to collect scan data at the edge of the sample. The two surfaces are polished and EBSD collected on the two adjoining surfaces (Randle & Dingley, 1989). More complete three-dimensional EBSD data have been collected through serial sectioning (Groeber et al., 2006; Rowenhorst et al., 2006; Zaefferer et al., 2007; Echlin et al., 2012). G. Rohrer’s team at Carnegie Mellon University has pioneered the collection of three-dimensional data for characterizing the five-dimensional nature of grain boundaries (Saylor et al., 2003) (two dimensions to describe the orientation of the boundary plane, and three for the misorientation across the boundary).
EBSD has been used in situ to characterize the orientation aspects of dynamic materials processes such as deformation, phase transformations, solidification, grain growth, recrystallization etc. Repeatedly measuring scans over the same area on samples while mounted on a deformation stage (Weiland et al., 1996) (tensile, compressive, bending, ...) and/or a heating stage (Seward et al., 2002) provides key information on microstructural evolution which can be linked quantitatively to strain levels and/or temperature.

Samples prepared for transmission electron microscopy (TEM) have been investigated using conventional EBSD systems as well. This can be done in reflection mode (i.e., the standard EBSD geometry) or in transmission mode by tilting the sample away from the detector. The first investigators (Keller & Geiss, 2012) termed this technique transmission EBSD (t-EBSD), as they collected the patterns using their existing EBSD equipment. The term transmission Kikuchi diffraction (TKD) has now become the more accepted term (Trimby, 2012).

Another critical step forward was the development of dynamical pattern simulation algorithms (Winkelmann et al., 2007), which provide simulated patterns that are much more consistent with experimental patterns than those that can be generated using a kinematical model.

2. Experimental geometry

2.1. EBSD setup

While it is not required, the typical geometry for EBSD is to tilt the specimen to approximately 70° from horizontal in the SEM chamber. The detector face is then angled upward by a few degrees (~10°) as shown in Fig. 1. This optimizes the signal intensity on the detector. The actual position of highest intensity on the detector will vary with the atomic density, but the goal is to position the camera such that the point of maximum intensity is just above the midpoint of the detector for a convenient working distance. The working distance can then be changed without significantly altering the performance of the detection system. Some experiments have been made using a non-tilted sample, but this greatly reduces the amount of signal to the detector (Farrer et al., 2003); the untitled geometry does have the advantage of reducing the distortions in the SEM image inherent to the tilted sample (Nolze, 2007).

2.2. Calibration

In order to determine the orientation from a pattern, the so-called pattern centre or projection centre must be located. From the point on the sample where the electron beam impinges (the source point) imagine a vector proceeding in a direction normal to the phosphor screen. The point on the plane of the phosphor screen where this vector hits the screen is the pattern centre. The x, y coordinates of this point as well as the specimen to screen distance are critical parameters, and several approaches have been used to determine these values. One method is to use a single crystal with known orientation, such as a silicon wafer with a [001] normal (Dingley & Baba-Kishi, 1986). Another method is to move the detector in and out of the specimen chamber. As the movement is along the detector normal, the movement of features in the captured patterns will all fall on radial lines through the pattern centre (Hjelen et al., 1993). However, most modern systems are calibrated through an iterative fitting approach (Krieger Lassen, 1999). As HREBSD for strain measurements has become more accepted in the community, the need for more accurate pattern centre determination has been recognized (Britton et al., 2010), and several approaches have been proposed. The shadow-casting approach has been around for many years (Biggin & Dingley, 1977), but improved methodologies have been realized (Mingard et al., 2011; Dingley & Meaden, 2015) that give more accurate pattern centres than can be realized using conventional approaches. As pattern simulation capabilities have become more widespread in recent years, pattern centre determination schemes based on the use of simulated patterns have also recently been explored (Basinger et al., 2011; Alkorta et al., 2017; Friedrich et al., 2018; Tanaka & Wilkinson, 2019; Pang et al., 2020).

Even when the pattern centre can be determined accurately, there are still other potential geometric uncertainties which can effect the absolute orientation accuracy measured by EBSD. These include, but are not limited to, the orientation of the sample (both in terms of the tilt with respect to the horizontal plane but also with any rotations about an axis normal to the tilt axis); rotations between the scintillator plane and the specimen surface; changes to the surface plane during sample preparation; the calibration of the SEM itself in terms of magnification and beam movement; the presumed motion of the sample stage, and other factors.

2.3. Sign and frame conventions

As has been highlighted in several publications (Britton et al., 2016; Rowenhorst et al., 2015) it is important to understand the reference systems used in the measurement of the crystallographic orientations via EBSD. Unfortunately, these definitions vary from system to system. In this example, we will use the definition used in the system from EDAX, but the principles apply to all systems. For details on the definition used for a system, see the documentation supplied by the vendor or contact the vendor. In the schematic shown in Fig. 2, the first axis of the right-handed reference frame for the sample, A1, points downward; the second axis, A2, is to the right (as viewed from the EBSD detector) and the third axis, A3, is parallel to the sample normal. Because some of the first samples investigated by automated EBSD were rolling samples and mounted with the rolling direction parallel to A1, this direction has often been labelled RD; more generally, we call this direction the ‘reference’ direction; the A3 direction is often labelled TD or transverse direction, and A2 as the ND or the normal direction.

It is important to understand how the A1 sample reference system is related to the coordinate system associated with the SEM display. This will be governed by the geometry of the
EBSD system within the SEM and can actually vary through scan rotation. Most modern systems used for EBSD are oriented so that the \( \mathbf{A}_1 \) direction is up in the SEM view and \( \mathbf{A}_2 \) is to the left [(c) in Fig. 2]. If we use a right-handed reference system \((\mathbf{x}, \mathbf{y}, \mathbf{z})\) for the SEM view corresponding to how scanning is performed, then we have \( \mathbf{x} \) equal to \(-\mathbf{A}_2\), \( \mathbf{y} \) equal to \(-\mathbf{A}_1\) and \( \mathbf{z} \) equal to \(-\mathbf{A}_3\). Recognizing that \( \mathbf{z} \) and \( \mathbf{A}_3 \) are antiparallel to each other is particularly important for three-dimensional serial sectioning experiments where the direction the section planes are cut is in the \(-\mathbf{A}_3\) direction.

Furthermore, there is a reference system associated with the bulk material from which a sample was extracted. For example, consider a rolled sheet; a sample from the sheet can be prepared so that the plane polished for microscopy is parallel to the rolling plane or normal to the transverse or longitudinal directions of the rolled sheet. In general, an EBSD user will want to consider the measured orientations with respect to a reference system associated with the processing of the sample. Thus, these directions must be recorded and/or marked on the sample as part of sample preparation and then tracked and recorded when the sample is mounted in the microscope for EBSD investigation. The orientation data collected by the EBSD system may need to be rotated to reflect the geometry desired. While the processing reference frame is generally well known in materials science samples (e.g. Fonda et al., 2014), it may not be as well understood in geological samples; however, the local structure of the rocks can provide indications. There may be planar structural elements, such as the repetitive layering in meta-morphic rocks (foliation), or linear features (lineation) indicating magma flow lines in igneous rocks, paleocurrent in sedimentary rocks or a shearing direction in rock having undergone deformation. Thus, it is good practice to record structural maps of such features with respect to the cardinal directions when extracting samples from a rock formation and consider these structural maps in preparing samples for EBSD investigation.

If there is any question regarding sample, image and diffraction pattern orientation on a particular EBSD system, one approach for checking the system is to use a coin, as shown schematically in Fig. 2. For more details in checking a system, see Britton et al. (2016). Keeping track of all these coordinate systems is important; fortunately, most mistakes can be corrected through 90° rotations of the orientation data about the principal axes of the sample.

Another variation on coordinate systems that can occur is the convention used to convert crystal axes to Cartesian axes in non-cubic crystals. Consider, for example, a hexagonal or trigonal crystal. There are, generally, two conventions for assigning a right-handed Cartesian coordinate system \((\mathbf{x}, \mathbf{y}, \mathbf{z})\) to the hexagonal crystal. In both cases \( \mathbf{A}_1 \) is aligned with the \( c \) axis of the crystal but in case (1) the \( \mathbf{a}_1 \) axis is assigned to \([2\bar{1}10]\) and the \( \mathbf{a}_2 \) axis to \([0110]\), and in case (2) \( \mathbf{a}_1 \) is assigned to \([0110]\) and \( \mathbf{a}_2 \) to \([2\bar{1}10]\). There is a 30° degree rotation that must be accounted for when comparing data acquired using these two definitions. Similarly, care must be taken for other crystal systems. For example, monoclinic crystals have their unique axis aligned with the \( b \) axis. These factors must all be considered both in comparing EBSD orientation measurements from different systems or with other orientation measurement techniques as well as in using crystal definitions from different crystallographic databases (for instance, non-standard space-group settings).

3. Physics of pattern formation

3.1. Geometric description

Kikuchi patterns are formed when inelastically scattered electrons inside a sample are scattered again in an elastic (Bragg) scattering process (Kikuchi, 1928). After an inelastic scattering event, an electron is free to travel in any direction through the crystal lattice; the distribution of directions is
determined by the angular part of the differential scattering cross section for the particular inelastic event (plasmon, phonon, inner-core excitation etc.), but is typically a continuous distribution with a maximum in or near the forward scattering direction. Within this continuous distribution, a subset of electrons will travel in a direction that precisely corresponds to the Bragg angle, $\theta_{hk0}$, for a particular lattice plane ($hk0$), i.e., the electron travels on the incident Kossel cone for that plane; thus, this electron will have a finite probability of Bragg scattering and travelling on the outgoing Kossel cone, with a directional change of twice the Bragg angle, $2\theta_{hk0}$. Each set of lattice planes has two associated Kossel cones, one on each side of the plane. The cone surfaces subtend an angle $\theta_{hk0}$ with respect to the plane, or $\pi/2 - \theta_{hk0}$ with respect to the plane normal. Since Bragg angles for high-energy electrons are of the order of tens of milliradians, the Kossel cone surfaces remain close to the corresponding lattice planes, as illustrated in Fig. 3(a), in which the lines represent the intersections of all low-order Kossel cones for an Ni single crystal with a surrounding unit sphere, the Kikuchi sphere, at 20 keV beam energy. The darkness of the lines is proportional to the electron structure factor squared for each reflection.

EBSPs are obtained by inserting a planar rectangular detector tangent to the sphere and determining the gnomonic projection of the relevant Kossel cones onto the detector plane. Each pair of Kossel cones forms a pair of curved lines (hyperbolae) in the gnomonic projection; the area between the two lines is known as the Kikuchi band, and the point of contact between the detector plane and the Kikuchi sphere is known as the pattern centre. The intensity inside a Kikuchi band is generally higher than the background, although contrast inversions can be observed when the path length travelled by BSEs inside the sample becomes larger than the extinction distance for dynamical scattering from a given set of lattice planes (see Section 3.2.2).

3.2. Elastic electron scattering

Elastic scattering of high-energy electrons in a crystalline material is described by the scalar relativistic Klein–Gordon equation (Fujiwara, 1961; Ferwerda et al., 1986):

$$\Delta \Psi + 4\pi^2 K_0^2 \Psi = -\frac{8\pi^2 m_e}{\hbar^2} [V(\mathbf{r}) + iW(\mathbf{r})] \Psi;$$  

(1)

$\Psi$ is the electron wavefunction, $K_0 = 1/\lambda$ the relativistic wavenumber, $m$ the relativistically corrected electron mass, and the other constants have their usual meanings. The electrostatic lattice potential $V(\mathbf{r})$ is augmented by an imaginary component $W(\mathbf{r}) > 0$ describing absorption, i.e., a phenomenological approach to include all inelastic scattering processes. Both potential functions have the periodicity of the crystal lattice and can be expanded in Fourier series:

$$U(\mathbf{r}) = \frac{2m_e}{\hbar^2} \sum_{\mathbf{g} \neq \mathbf{0}} V_{\mathbf{g}} \exp(2\pi i \mathbf{g} \cdot \mathbf{r});$$

$$U'(\mathbf{r}) = \frac{2m_e}{\hbar^2} \sum_{\mathbf{g}} W_{\mathbf{g}} \exp(2\pi i \mathbf{g} \cdot \mathbf{r}).$$

In the definition of $U(\mathbf{r})$, the mean inner potential term $V_0$ is omitted from the series and instead included in the wavenumber; writing $k_0 \equiv (2m_0(\Psi^* + \gamma V_0))^{1/2}/\hbar$ with $\Psi$ the relativistic accelerating potential and $\gamma$ the relativistic correction factor, we obtain the starting equation for elastic electron scattering:

$$\Delta \Psi + 4\pi^2 k_0^2 \Psi = -4\pi^2 [U + iU'] \Psi.$$  

(2)

To solve the equation, an assumption is made about the functional form of the solution; the two leading solution approaches are as follows.

(i) Write the solution as a superposition of plane waves travelling in all directions allowed by Bragg’s law, $\mathbf{k}' = \mathbf{k}_0 + \mathbf{g}$:

$$\Psi(\mathbf{r}) = \sum_{\mathbf{g}} \psi_{\mathbf{g}} \exp(2\pi i (\mathbf{k}_0 + \mathbf{g}) \cdot \mathbf{r}).$$  

(3)

Substitution in equation (2) along with the use of the high-energy approximation (van Dyck, 1976) leads to the Darwin–Howie–Whelan (DHW) system of coupled first-order differential equations (Howie & Whelan, 1961). Writing the scattered amplitudes $\psi_{\mathbf{g}}$ as a column vector $S$, the DHW equations can be written compactly as

$$\frac{d\mathbf{S}}{d\varepsilon} = i\mathcal{A}\mathbf{S};$$  

(4)

the structure matrix $\mathcal{A}$ is defined below.

Figure 3

Representations on a unit-radius sphere surrounding an Ni single crystal with 20 keV beam energy of (a) the intersections of the Kossel cones of all low-order lattice planes; (b) Kikuchi bands with intensities proportional to $|F_{hk0}|^2$; (c) the intensity distribution under kinematical scattering conditions; and (d) the intensity distribution using a full dynamical scattering computation. Note that both (b) and (c) are typically referred to as kinematical representations.
(ii) Alternatively, write the solution as a function that has the periodicity of the crystal lattice:

\[ \Psi(r) = C(r) \exp(2\pi i k \cdot r) = \sum_g C_g \exp(2\pi i (k + g) \cdot r); \]

the function \( C(r) \) is known as a Bloch wave (Bethe, 1928; Bloch, 1929), and after application of the high-energy approximation leads to an eigenvalue problem (Metherell, 1975; Humphreys, 1979) of the form

\[ \mathbf{A} \mathbf{C}^{(0)} = 2\pi i k \mathbf{N} \mathbf{C}^{(0)}, \]

where \( \mathbf{C}^{(0)} \) is a vector with Bloch-wave coefficients, \( k_n \) the normal component of the incident wavevector and \( \mathbf{N} = \gamma^{(0)} + i \theta^{(0)} \) the complex eigenvalues.

The structure matrix \( \mathbf{A} \) which appears in both solution approaches is defined as follows:

\[ \mathbf{A}_{gg'} = \begin{cases} 2\pi i q_{g-g'} + (\pi/q_0) & g = g' \, \text{and} \, g \\ \pi/q_{g-g'} & g 

\neq g' \end{cases}; \]

The factor \( q_{g-g} \) is the excitation error for the planes \( g \) and describes the deviation from the Bragg condition, \( \mathbf{N} \) is the structure matrix, enters the relations via \( \mathbf{A} \).


\[ 1 \sum |U_g|/|k_0 + g| + i |U_g| \exp(i \beta_g) = 1 \exp(i \beta_{g'})/\xi_g, \]

where \( \beta_g \) is the phase difference between the Fourier coefficients \( U_g \) and \( U_{g'} \); \( \xi_g \) is known as the extinction distance and \( \xi_g \) is the anomalous absorption length. The normal absorption length, \( \xi_{g'} \) which is part of the diagonal elements of the structure matrix, enters the relations via

\[ 1 \sum \xi_{g'} = 0. \]

3.2.1. Kinematical diffraction model. In the kinematical diffraction theory, the assumption is made that an electron can undergo only one elastic scattering event; thus, the electron either remains in the incident beam or it scatters in the direction \( \mathbf{k}' = \mathbf{k}_0 + g_{hkl} \). In the case of backscattered electrons, \( \mathbf{k}_0 \) lies along the exit trajectory of the electron, and the wavelength corresponds to the electron energy, decreased by energy losses due to prior inelastic scattering events. While these losses are taken into account in some of the dynamical models discussed in the next section, they are generally ignored for the kinematical approach; in fact, the kinematical approach replaces the imaginary part \( W(r) \) of the lattice potential by a constant \( W_0 \). In addition, all the interaction factors \( q_{g-g}^{-1} \) vanish, except for those for which \( g' = 0 \), \( \mathbf{N} \), i.e., only scattering from the incident beam into one of the scattered beams is considered; once in a diffracted beam, the electron cannot be scattered into any other beam.

There are two basic approaches to the kinematical diffraction problem; in the first approach, the probability of scattering into a diffracted beam is taken to be proportional to the modulus squared of the structure factor, \( F_{hkl} \), computed using standard electron scattering factors. This assumption effectively means that there is no coupling between the various diffracted beams, so that the diffraction pattern is a simple linear superposition of Kikuchi bands with constant intensity proportional to \( |F_{hkl}|^2 \). At zone-axis locations, where multiple Kikuchi bands intersect, the intensities of the individual bands are simply added together, leading to the Kikuchi sphere shown in Fig. 3(b) for Ni at 20 keV incident beam energy. The kinematical intensity distribution on the Kikuchi sphere has at least the point-group symmetry of the underlying crystal structure; owing to Friedel’s law, however, the kinematical Kikuchi sphere will be centrosymmetric, even when the point group is not. Thus, the kinematical Kikuchi sphere belongs to one of the eleven Laue classes. This is not true for the dynamical Kikuchi sphere, as discussed in the next section.

In the second approach, the dynamical diffraction model of the next section is employed, but with a structure matrix that has only the diagonal and the first column different from zero, i.e.,

\[ \mathbf{A}_{kin} = \pi/q_0 \delta_N + \pi \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ q_{r_1}^{-1} & 2x_{r_1} & 0 & \cdots & 0 \\ q_{r_2}^{-1} & 0 & 2x_{r_2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ q_{r_{N-1}}^{-1} & 0 & 0 & \cdots & 2x_{r_{N-1}} \end{pmatrix}, \]

where \( \delta_N \) is the \( N \times N \) identity matrix. The resulting intensity distribution for 20 keV electrons and nickel is shown in Fig. 3(c). Note that in this form, the kinematical Kikuchi sphere does have the symmetry of the complete point group, i.e., Friedel’s law does not apply in this case.

3.2.2. Dynamical diffraction model. The goal of a dynamical diffraction model for EBSD is to determine the BSE yield as a function of the exit direction relative to the crystal reference frame. A complete quantum-mechanical solution of this problem requires consideration of the crystal state as well as the backscattered electron state; this results in the need to solve the Yoshioka equations (Yoshioka, 1957) and include a variety of inelastic scattering mechanisms, which represents a significant challenge. Progress can be made, however, by using the phenomenological approach and considering all inelastic processes to be covered by means of the absorption potential \( W(r) \) introduced in Section 3.2. The detailed theory of the depth and energy distribution of BSEs inside a crystal lattice is a topic of ongoing research.

Since BSEs can arise from any depth inside the material, the total yield will be described by an integral over the depth. For simplicity, consider an elemental crystal with atomic number \( Z \). The probability of a backscatter event happening for a given atom at position \( r \), is proportional to the square of the atomic number, \( Z^2 \), multiplied by the probability that the beam electron will be found at that location \( r \), in the first place; this probability is given by the modulus squared of the electron wavefunction evaluated at \( r \). Since atoms of type \( Z \) can be found at nominally the same position in each unit cell, but at different distances (depths) from the sample surface, the
probability of backscattering in a direction \( \mathbf{k} \) can be written as follows:

\[
P(\mathbf{k}) \simeq \frac{1}{z_0} Z^2 \exp(-M) \sum_{i=1}^{N} \int_{z_0}^{z} \mathrm{d}z' |\Psi_{n}(r; z')|^2.
\]

(11)

where the third factor is the Debye–Waller exponential, and the sum runs over all equivalent atom positions in the unit cell. The integration upper bound \( z_0 \) is often chosen to be a fraction of the Bethe parameter (Reimer, 1985), but can also be determined from Monte Carlo simulations of the electron backscattering process (Callahan & De Graef, 2013). The wavefunction \( \Psi_{n} \) is usually determined using the Bloch-wave formalism; the general solution is given by

\[
\Psi(r) = \sum_{l} a^{(l)} \sum_{n} C_{n}^{(l)} \exp(2\pi i \mathbf{k}_{n} \cdot \mathbf{r}) \cdot \mathbf{r},
\]

(12)

where \( a^{(l)} \) are the Bloch-wave excitation amplitudes and \( \mathbf{n} \) is the sample normal; for normal incidence we have \( \mathbf{n} \cdot \mathbf{r} = z \).

Substituting the wavefunction into equation (11) and allowing for multiple sites in the asymmetric unit results in

\[
P(\mathbf{k}, E) \simeq \sum_{\mathbf{g}} \sum_{\mathbf{k}} S_{\mathbf{gh}} \lambda_{\mathbf{gh}}(E),
\]

(13)

with

\[
S_{\mathbf{gh}} = \sum_{n} \sum_{\mathbf{r}_n} I^{(n)}_{\mathbf{h} - \mathbf{g}}(\mathbf{h} - \mathbf{g}) \cdot \mathbf{r}_n;
\]

(14a)

\[
I_{\mathbf{gh}} = \sum_{j} \sum_{k} C_{j}^{(n)} \alpha_{\mathbf{h} \mathbf{g}}^{(n)} \lambda_{\mathbf{kh}}(E) \alpha_{\mathbf{h} \mathbf{g}}^{(k)} C_{k}^{(g)}.
\]

(14b)

The first sum in equation (14a) runs over all sites in the asymmetric unit, and the symbol \( S_{n} \) in the second summation represents the number of equivalent sites for site \( n \). The matrix \( S_{\mathbf{gh}} \) is reminiscent of a structure factor, but is weighted by the Rutherford scattering cross section \( Z_{\mathbf{h} \mathbf{g}}^{(n)} \) for each atom. The matrix \( I_{\mathbf{gh}} \) contains all the scattering information [obtained by solving the eigenvalue problem in equation (6) for the correct boundary conditions], including the depth integration in the form of the matrix \( \lambda_{\mathbf{kh}}(E) \) defined by

\[
\lambda_{\mathbf{kh}}(E) = \frac{1}{z_0(E)} \int_{z_0(E)}^{z_0} \lambda(E, z) \exp(-2\pi i(\alpha_{\mathbf{h} \mathbf{k}} + i\beta_{\mathbf{h} \mathbf{k}})z) \mathrm{d}z,
\]

(15)

where \( \alpha_{\mathbf{h} \mathbf{k}} = q^{(l)} + q^{(k)} \) and \( \beta_{\mathbf{h} \mathbf{k}} = \gamma^{(l)} - \gamma^{(k)} \). The function \( \lambda(E, z) \) in the integral is set equal to 1 in some models (e.g., Winkelmann et al., 2007) or can be determined from Monte Carlo simulations, as in Callahan & De Graef (2013).

When \( \lambda(E, z) = 1 \), we have \( P(\mathbf{k}, E) = P(\mathbf{k}) \), i.e., there is no integration over the electron energy; when using Monte Carlo results, a second integration over the electron energy is needed, which can be discretized as a summation over energy bins. The most basic Monte Carlo model employs Bethe’s continuous slowing down approximation (CSDA), in which an electron has a constant energy loss rate as it travels between Rutherford scattering events; the crystal lattice is completely ignored and replaced by a simple mean-free-path model (Joy, 1995). While this approach is known to be incorrect with respect to the elastic peak, it does produce a realistic BSE distribution.

Improvements to the CSDA approach involve explicit accounting for discrete energy losses by incorporating plasmon and phonon scattering cross sections as well as core losses and other atomic excitations; this is an area of active research.

Since the matrix \( S_{\mathbf{gh}} \) depends explicitly on the atom type, one can separate the contributions from individual sites in the asymmetric unit. As an example, Figs. (a–c) show equal-area Lambert projections of the Kikuchi sphere for the three general sites in the CaTiO$_3$ perovskite structure with space group Pnma: Ti at 1\( f(1/2, 1/2, 1/2) \), Ca at 1\( a_0 \) (0, 0, 0) and O at 3\( d \) (1/2, 1/2, 0). An electron energy of 20 keV was used and the projections show the distribution of BSEs with energies in the range 18–20 keV. Note that some of the Kikuchi bands show contrast inversions; these are caused by the fact that the extinction distance for scattered beams arising from some atomic sites can be significantly larger than for beams that are dominated by other sites. The projection in Fig. 4(d) is the (incoherent) sum of the three separate patterns; note that each projection is proportional to \( Z_{\mathbf{h} \mathbf{g}}^{(n)} \), so that the Ca, Ti and O intensities account for 37.2, 45.0 and 17.8%, respectively, of the total intensity.

The total number, \( N \), of scattered beams taken into account in a simulation depends strongly on the size of the unit cell (a larger cell has a more densely populated reciprocal lattice, hence more diffracted beams, than a smaller unit cell), as well as the average atomic number of the crystal structure, since heavier atoms have a larger Rutherford scattering cross...
section which, in turn, means that more beams (i.e., beams corresponding to longer reciprocal-lattice vectors) are needed to obtain convergence of the simulation. Since the Debye–Waller (DW) factor is essentially an exponential damping factor, it is important to take into account the correct DW factors, or at the very least a close estimate; DW factors that are too small will unnecessarily increase the number of beams that needs to be taken into account to achieve convergence. Finally, to reduce $N$ as much as possible (since the computation time of all algorithms increases as $N^3$), it is common to employ first-order perturbation theory to handle the weakest Fourier coefficients of the lattice potential; this leads to the introduction of the so-called Bethe potentials (Bethe, 1928), which render the algorithm more difficult to implement but can provide a significant speed up over the brute-force inclusion of all beams. An analysis of $N$ as a function of accelerating voltage, atomic number, structure complexity, beam tilt and temperature can be found in Wang & De Graef (2016).

All available computational models in the end produce an EBSD master pattern, i.e., the distribution of the BSE yield on the Kikuchi sphere, as illustrated in Fig. 3(d) for nickel at 20 keV. Individual EBSD patterns can be extracted from such a master pattern by means of an interpolation process that depends on accurate knowledge of the detector geometry and the pattern-centre coordinates.

4. Detectors

4.1. Scintillator-based detectors

Initially, EBSD patterns were recorded using photographic plates or film. In modern systems, a scintillator, usually a phosphor screen, is placed in the path of the diffracted electrons and the image from the scintillator is acquired using a digital camera. When the electrons impinge on the phosphor, the phosphor luminesces, creating an image that can be captured by a low-light camera. YAG (yttrium aluminium garnet) single crystals have also been used as scintillators (Michael & Goehner, 1993). The scintillator can be coupled to the camera using lenses or a fibre optic. Early cameras were SIT (silicon-intensified-target) video cameras and the video signal was converted to a digital signal using a video capture card in the computer. The next generation of cameras were CCD (charge-coupled-device) cameras and these evolved from cameras producing a video signal to fully digital systems. In 2017, CMOS (or complementary metal-oxide-semiconductor) cameras were introduced; modern CMOS cameras are particularly well suited for very high speed data-acquisition applications.

4.2. Direct electron detectors

While scintillator-based detectors meet the need for many EBSD applications, higher sensitivity, particularly at lower voltages, is desired. To this end, various research groups have experimented with direct electron detection (beyond the photographic plates and films) (Wilkinson et al., 2013; Vespucci et al., 2015). In a conventional scintillator-based detector when the diffracted electrons strike the phosphor screen, the energy is converted into light (photons) which are focused through a lens onto an imaging sensor (CCD or CMOS) where the photons are converted back to electrons. In a direct electron detector, the diffracted electrons are essentially counted directly, removing the intermediate electron-to-light-to-electron steps. Such systems have single electron sensitivity and zero readout noise, which makes them promising for low-voltage applications. They also have some potential for differentiating the energy of the diffracted electrons. Another advantage is that the need for a lens or fibre optic is eliminated; this is particularly useful in the technique of high-resolution EBSD used for strain measurements as the lenses introduce distortions which must be accounted for to achieve the desired accuracy.

5. Orientations, symmetry and fundamental zones

The principal output of an EBSD experiment is the orientation of the crystal lattice at each scan point; this orientation is measured with respect to a reference frame that is attached to the sample. Traditionally, the choice of sample reference frame has been different in the materials and geology communities: in the materials community, the sample axes are usually taken to be along orthogonal directions associated with the sample processing or growth history, whereas in the geological community the axes are typically related to foliation and lineation orientations.

Each orientation is expressed mathematically as the ‘passive’ rotation that brings the sample reference frame into coincidence with the crystal reference frame (in contrast to an ‘active’ rotation, which rotates an object with respect to a single reference frame). Once the orientations are known, the orientation field can be analysed to detect orientation gradients that, in turn, can be used to extract the local strain state or the local density of geometrically necessary dislocations. While the orientations are usually expressed as Euler angle triplets $(\varphi_1, \Phi, \varphi_2)$ (the so-called Bunge convention corresponding to consecutive $zxz$ rotations), for computations involving orientations one resorts to other representations that offer more numerical convenience. The most important representations will be introduced in Section 5.1. Usually, the presence of rotational crystal symmetry allows for a reduction of the measured orientations to a subset of all possible orientations; this involves the concept of the fundamental zone (FZ), which will be introduced in Section 5.2 for orientations and in Section 5.3 for misorientations.

5.1. Orientation representations relevant to EBSD

Crystallite orientations are represented by passive rotations from the sample reference frame $e_i^S$ to the crystallite reference frame $e_i^C$ (all reference frames are Cartesian and right-handed). Each rotation is characterized by a positive rotation angle $\omega$ and an invariant line, described by a unit rotation axis vector $\mathbf{n}$. Consistency between the eight rotation representa-
tions described in the following sections requires that the rotation angle and axis be defined such that a positive rotation angle \( \omega \) corresponds to a counterclockwise rotation when looking from the endpoint of \( \mathbf{n} \) towards the origin. In the definitions below, the symbol \( P \) takes on the value of either +1 or −1; for either choice, a fully internally consistent set of conversion routines between the representations can be obtained (Rowenhorst et al., 2015).

5.1.1. Axis–angle pair. The axis–angle pair combines \( \omega \) and \( \mathbf{n} \) into a single symbol \((-P \mathbf{n}, \omega)\), sometimes written as \( \omega\hat{\mathbf{n}} \). Since some rotation axes may fall along crystal symmetry axes, the notation \( \omega\hat{\mathbf{n}} \) is also used frequently (i.e., without normalizing the rotation axis indices). As an example, a rotation by 120° around the [111] axis of a crystal is described by the axis–angle pair \((2\pi/3)\hat{[111]}\) for the choice \( P = -1 \), and \((2\pi/3)\hat{[111]}\) for \( P = +1 \). The axis–angle pair representation is useful to describe particular rotations, but has limited computational value; in particular, there is no direct way to compute the result of consecutive rotations expressed as axis–angle pairs.

5.1.2. Euler angles. Euler has shown that any 3D rotation can be decomposed into three consecutive rotations around the reference axes; the order of rotations is denoted by a triplet of coordinate axes, e.g. \( xyz \) or \( yzx \), with rotations applied from left to right. While there are many combinations of three axes, the so-called Bunge convention, with rotation order \( xzx \), has become the standard in texture research; the corresponding angles are represented by the triplet \((\varphi_1, \Phi, \varphi_2)\) with angular ranges \([0, 2\pi]\), \([0, \pi]\) and \([0, 2\pi]\), respectively.

Euler space is traditionally represented using a left-handed orthogonal reference frame with \( \varphi_1 \) along \( x \), \( \varphi_2 \) along \( y \) and \( \Phi \) along \( z \). It should be noted that for every Euler angle triplet \((\varphi_1, \Phi, \varphi_2)\) there is an equivalent triplet \((\varphi_1 + \pi, 2\pi - \Phi, \varphi_2 + \pi)\); the second angle in this equivalent triplet lies in the range \([\pi, 2\pi]\), and the two points are related to each other by a diagonal glide plane \( n \) at angle \( \Phi = \pi \) with glide vector \((\pi, 0, \pi)\). Thus, the symmetry of Euler space can be described in terms of the monoclinic space group \( P \) (No. 7, \( P1n1 \), unique axis \( b \), cell choice 2) (Pospiech et al., 1974).

The metric tensor for Euler space is given by (we use the notation \( G_{ij} \) to avoid confusion with rotation matrices typically represented by \( g_{ij} \) in the literature):

\[
G_{ij} = \frac{1}{4c} \begin{bmatrix}
1 & 0 & \cos \Phi \\
0 & 1 & 0 \\
\cos \Phi & 0 & 1
\end{bmatrix},
\]

(16)

which results in a differential volume element

\[
dV = \frac{1}{8c^{3/2}} \sin \Phi \, d\varphi_1 \, d\Phi \, d\varphi_2.
\]

(17)

The constant \( c \) can be selected to obtain a unit total volume (for \( c = \pi^{3/2} \)) or the standard volume of \( 8\pi^2 \) (for \( c = 1/4 \)). It should be noted that the volume element is degenerate when \( \sin \Phi = 0 \) (i.e. \( \Phi = 0 \) or 2\( \pi \)). As a consequence, rotations of the form \((\varphi_1, 0, \varphi_2)\) and \((\varphi_1, \pi, \varphi_2)\) are degenerate; in particular, the identity rotation is given by \((\varphi_1, 0, -\varphi_1)\), i.e., by the straight lines \( \varphi_2 = 2n\pi - \varphi_1 \) (with \( n \in \mathbb{Z} \)) in the plane \( \Phi = 0 \).

Note that the Euler angle representation does not depend on the choice of the constant \( P \).

5.1.3. Rotation matrix representation. 3D rotations can be represented by orthogonal \( 3 \times 3 \) matrices with unit (positive) determinant; the set of all such matrices forms a group denoted by \( SO(3) \), the group of special orthogonal \( 3 \times 3 \) matrices. The axis–angle pair \( \omega\hat{\mathbf{n}} \) can be converted to a rotation matrix using the relation

\[
g_{ij} = \delta_{ij} \cos \omega + (1 - \cos \omega)n_in_j - \sin \omega \epsilon_{ijk}n_k,
\]

(18)

where \( n_i \) are the components of \( \mathbf{n} \), \( \delta_{ij} \) is the identity matrix and \( \epsilon_{ijk} \) is the permutation symbol. The Euler angle triplet \((\varphi_1, \Phi, \varphi_2)\) can be converted to a rotation matrix as follows:

\[
g_{ij} = \frac{g_{ij}(\varphi_2)g_{ij}(\Phi)g_{ij}(\varphi_1)}{4} = \begin{bmatrix}
1 & -c_2s_1 & s_1s_2 + c_1c_2s_2 \\
-c_2s_1 & c_1 & -s_1s_2 + c_1c_2s_2 \\
s_1 & c_1s_2 & c
\end{bmatrix},
\]

with \( c_i = \cos \varphi_i \), \( s_i = \sin \varphi_i \), \( c = \cos \Phi \) and \( s = \sin \Phi \). For passive rotations, concatenation of rotations occurs from left to right, i.e., rotation \( g^1 \) followed by rotation \( g^2 \) is represented by the matrix product \( g^2g^1 \); for active rotations, the matrix product order should be inverted.

The rotation matrix \( g_{ij} \) converts the sample reference frame into the crystallite frame by

\[
e^{\mathbf{C}} = g_{ij}e^j_i.
\]

(19)

For a vector \( \mathbf{t} \) with components \( t^i_j \) in the sample reference frame, the components in the crystallite reference frame are given by \( t^i_j = g_{ij}t^j_i \). It is common in texture analysis to represent sample directions in the crystal reference frame, which leads to inverse pole figures (IPFs); the reverse, a crystal direction represented in the sample reference frame, requires the inverse \( g_{ij}^{-1} \) of the rotation matrix and leads to pole figures (PFs).

5.1.4. Quaternion representation. Quaternions are four-component complex numbers with one real and three imaginary parts. They were introduced into mathematics by Hamilton in 1844 (Hamilton, 1844), and are defined by

\[
q = q_0 + q_1i + q_2j + q_3k = [q_0, \mathbf{q}],
\]

(20)

with \( q_i \in \mathbb{R} \), \( \mathbf{q} \) the vector part of the quaternion and

\[
i^2 = j^2 = k^2 = -1, \quad ij = -ji = k, \quad jk = -kj = i, \quad ki = -ik = j.
\]

The quaternion norm is defined as \( |q| = (q_0^2 + q_1^2 + q_2^2 + q_3^2)^{1/2} \). Just as regular unit complex numbers describe 2D rotations, unit quaternions correspond to 3D rotations. The axis–angle pair \((-P\mathbf{n}, \omega)\) can be converted into a unit quaternion by the relation

\[
q = \left[\cos \frac{\omega}{2}, -P \sin \frac{\omega}{2}(n_i i + n_j j + n_k k)\right].
\]

(21)

Owing to the half-angle argument of the trigonometric functions, unit quaternions provide a double cover of the rotation group, i.e., \( q \) and \(-q \) (i.e., a rotation by \( \omega + 2\pi \)) are equivalent.
rotations. It is customary to consider only half of the unit quaternion sphere \( S^3 \) by restricting the range of \( \omega \) to \([0, \pi]\) so that \( q_0 \geq 0 \); the quaternion 'Northern' hemisphere is denoted by \( S^3_+ \) with hyper-area \( \pi^2 \).

Quaternion multiplication is non-commutative (as is the composition of rotations), and is written compactly in vector form as

\[
pq = [p_0, \ p][q_0, \ q] = [p_0q_0 - p \cdot q, \ p_0q + q_0p + P(p \times q)].
\]

(22)

Note that the conventional quaternion product is recovered for \( P = +1 \); for \( P = -1 \), the product must be redefined to maintain consistency with all other rotation representations.

A 3D vector \( r \) can be rotated by means of a (passive) quaternion \( q \) by pre-multiplication with \( q \) and post-multiplication by the conjugate \( q^* \equiv [q_0, -q] \). The vector \( r \) is first converted to a quaternion with zero scalar part and then the following relation is applied:

\[
r' = \text{vec}[q_0, \ r]q^* = (q_0^2 - ||q||^2)r + 2(q \cdot r)q + 2Pq_0(q \times r).
\]

(23)

The symbol ‘vec’ indicates the vector part of the quaternion in the argument.

It was stated in Section 5.1.2 that Euler space can be described by the space group \( P_{\text{c}} \), corresponding to the presence of a diagonal glide plane at \( \Phi = \pi \). When the conversion relation between Euler angles and the quaternion representation is considered, the double-cover property of the quaternion representation implies that the true range of the Euler angles should be \([0, 4\pi]\) for each of the angles. As a consequence (Callahan et al., 2017), the true space-group symmetry of Euler space corresponds to the monoclinic magnetic space group \( P_{\text{c}}c \) (7.6.37) in the Opechowski and Guccione nomenclature. The relevant symmetry elements are \( a \) a glide, \( b \) a time-reversing diagonal glide \( n' \), and \( c \) two time-reversing translations \( t_{000} \) and \( t_{000} \). The time-reversal operation maps onto the equivalence of the quaternions \( q \) and \( -q \).

5.1.5. Neo-Eulerian representations. The axis–angle pair representation \( \omega \theta (q = -\hat{P}u) \) can be converted into a class of representations, the ‘neo-Eulerian’ representations, of the form \( -\hat{P}u f(\omega) \), where \( f(\omega) \) is an arbitrary monotonic function of \( \omega \) satisfying \( f(0) = 0 \). The metric tensor for this class of representations is given by (Kumar & Dawson, 1998)

\[
G_\theta = \frac{1 - \cos \omega}{2c^2(\omega)} \delta_{ij} - n_in_j + \frac{1}{4c^2(\omega)}n_in_j,
\]

(24)

where a prime indicates a derivative with respect to \( \omega \). Note that this metric tensor does not depend on \( P \) due to the quadratic appearance of the components \( n_i \). Three frequently used representations are described below: the Rodrigues–Frank vector, the homochoric vector and the 3D stereographic vector. The vector part \( q \) of the quaternion representation in Section 5.1.4 can also be regarded as a neo-Eulerian representation with \( f(\omega) = \sin(\omega/2) \). The neo-Eulerian representations share the convenient property that all rotations around a given axis lie along a straight line in all representations.

Rodrigues–Frank representation. Setting \( f(\omega) = \tan(\omega/2) \) results in the Rodrigues–Frank vector \( \rho = -\hat{P}u \tan(\omega/2) \). For rotations by an angle of \( \omega = \pi \), the Rodrigues–Frank (RF) vector has infinite length; thus, RF space maps onto \( \mathbb{R}^3 \) with the identity rotation at the origin and metric tensor

\[
G_\theta = \frac{1}{c} \left( \frac{\cos^2 \omega}{2} - \delta_{ij} - \frac{1}{4} \sin^2 \omega n_i n_j \right). 
\]

(25)

Despite the infinite range of RF space, this representation is frequently used for two main reasons:

(i) concatenation of two or more rotations can be expressed by a compact rule; and

(ii) fundamental zones (defined in Section 5.2) have planar bounds, and, for all but the cyclic rotational point groups, a finite volume.

Concatenation of two passive rotations \( \rho \) and \( \sigma \) (\( \rho \) first, followed by \( \sigma \)) can be performed by means of the \( \circ \) multiplication of the two RF vectors:

\[
\rho \circ \sigma \equiv \rho + \sigma + \rho \times \sigma. 
\]

(26)

Note that the RF vector can also be defined in terms of the rotation quaternion by

\[
\rho = \frac{q}{q_0}.
\]

(27)

Homochoric representation. In cartography, the Lambert projection represents an equal-area projection from the 2-sphere, \( S^2 \), to the disc, \( \mathbb{B}^2 \). Since unit rotation quaternions live on the 3-sphere, \( S^3 \), and an equivalent Lambert equal hyper-area (volume) projection can be constructed to map the quaternions into a ball, \( \mathbb{B}^3 \). This projection is known as the ‘homochoric’ projection, and is achieved by defining the homochoric vector \( h \) as

\[
h = -\hat{P}u f(\omega) \text{ with } f(\omega) = \left[ \frac{3}{4} (\omega - \sin \omega) \right]^{1/3}. 
\]

(28)

This results in a 3D equal-volume representation of the quaternion unit sphere; all rotations by \( \omega = \pi \) lie on the outer surface of the ball \( \mathbb{B}^3 \), which has volume \( \pi^2 \). There is no known analytical inverse transformation from a homochoric vector to a quaternion or RF vector. The metric tensor of homochoric space is given by

\[
G_\theta = \frac{1}{9} \left( \frac{\cos \omega - 1}{c(\omega - \sin \omega)^2} \delta_{ij} + \frac{9(\omega - \sin \omega)^2}{2(1 - \cos \omega)^3} - 1 \right)n_in_j.
\]

(29)

3D stereographic representation. Similar to the 2D stereographic projection, which is an equal-angle projection from \( S^2 \) onto \( \mathbb{B}^2 \), the 3D stereographic projection maps \( S^3_+ \) onto the unit ball \( \mathbb{B}^3 \) through an equal-angle projection, resulting in the 3D stereographic vector \( s \) defined by

\[
s = \frac{q}{1 + q_0} = \frac{q_0\rho}{1 + q_0} = -\hat{P}u \tan \frac{\omega}{4}. 
\]

(30)
The stereographic projection maps the infinite RF space $\mathbb{R}^3$ onto the unit ball; rotations by $\omega = \pi$ lie on the surface of the ball, and the identity rotation lies at its centre. The equal-angle nature of the projection means that angles between rotation axes are faithfully represented. In addition, circular trajectories on $S^3$ are represented by circles inside the unit ball $B^3$. Note that $s$ is sometimes defined by twice the value above, to ensure that the first term in the Taylor expansion with respect to $\omega$ is identical to that of the Rodrigues, homochoric and quaternion expansions. The metric tensor for the 3D stereographic representation is a diagonal tensor of the form

$$G_{ij} = \frac{1}{4c} \cos^{\frac{\omega}{2}} \delta_{ij},$$

(31)

5.1.6. Cubochoric representation. The cubochoric representation was introduced (Rosca et al., 2014) to facilitate uniform sampling of orientation space by performing an equal-volume mapping from the homochoric ball to a cube of volume $\pi^2$. The equal-volume nature of the mapping means that angles between rotation axes are not preserved, so that this representation does not belong to the class of neo-Eulerian representations. Closed-form expressions for the forward and reverse mapping from the cubochoric vector $c$ to the homochoric vector $h$ can be found in Rosca et al. (2014). Applications of this representation are discussed in Section 5.4.

5.1.7. Summary of rotation representations. Table 1 lists the rotation representations covered in this section along with the mathematical spaces to which they belong and the volume of that space. An open-source numerical library, implementing conversions between all the representations in this section, is available from GitHub (De Graef, 2019); the library provides conversion routines in Fortran90, C, MATLAB, Python and the Interactive Data Language (IDL; L3Harris Geospatial, 2020).

Table 1

<table>
<thead>
<tr>
<th>Representation</th>
<th>Symbol</th>
<th>Space</th>
<th>Volume</th>
</tr>
</thead>
<tbody>
<tr>
<td>Axis–angle</td>
<td>$\omega$((-P\hat{u}))</td>
<td>$\mathbb{R}^3$</td>
<td>$\infty$</td>
</tr>
<tr>
<td>Euler angles</td>
<td>$(\psi_1, \Phi, \psi_2)$</td>
<td>$[0, 2\pi] \times [0, \pi] \times [0, 2\pi]$</td>
<td>$8\pi^2$</td>
</tr>
<tr>
<td>Rotation matrix</td>
<td>$g_{ij}$</td>
<td>$SO(3)$</td>
<td>$-$</td>
</tr>
<tr>
<td>Quaternion</td>
<td>$q = [q_0, q]$</td>
<td>$S^3$</td>
<td>$\pi^2$ for $S^3$</td>
</tr>
<tr>
<td>Rodrigues–Frank</td>
<td>$\rho$</td>
<td>$\mathbb{R}^3$</td>
<td>$\infty$</td>
</tr>
<tr>
<td>Homochoric</td>
<td>$h$</td>
<td>$B^3 ([3\pi/4)^{1/3}]$</td>
<td>$\pi^2$</td>
</tr>
<tr>
<td>3D stereographic</td>
<td>$s$</td>
<td>$B^3 [1]$</td>
<td>$4\pi/3$</td>
</tr>
<tr>
<td>Cubochoric</td>
<td>$c$</td>
<td>$C [\pi/2]$</td>
<td>$\pi^2$</td>
</tr>
</tbody>
</table>

Figure 5

(a)–(c) Rodrigues fundamental zones (RFZs) for the non-cyclic crystallographic rotational point groups; note that the trigonal point group 312 has an RFZ that is rotated by $30^\circ$ around the $z$ axis with respect to the one shown in (b). (d) RFZ for the icosahedral rotational group 532; a fivefold axis is oriented along $z$ and a twofold axis along the $y$ direction. The length of the coordinate axis segments between the origin and the end-point sphere is unity in each of the drawings.
be defined separately in each of the eight representations from the previous section. In the Rodrigues–Frank representation, however, the FZ takes on a particularly simple form, namely the region enclosed between pairs of parallel planes normal to each of the rotational symmetry axes. It is customary to transform this Rodrigues FZ (RFZ) into the other rotation representation spaces. In Euler space, one can also define FZs, some of which (for cubic symmetry) have curved boundaries.

5.2.1. Fundamental zones in Rodrigues space. The RFZ for a given rotational symmetry group can be determined by generating all equivalent rotations for a given rotation and selecting the representative with the smallest rotation angle. Starting from the quaternion representation, the smallest rotation angle \( \omega \) corresponds to the largest scalar quaternion part \( q_0 = \cos(\omega/2) \). All symmetry-equivalent quaternions have components that can be expressed as linear combinations of the original components \( q_i \); in particular, the scalar component \( q_0^* \) of an equivalent quaternion can be written as

\[
q_0^* = c_0 q_0 + c_1 q_1 + c_2 q_2 + c_3 q_3
\]

with \( c_i \in \mathbb{R} \) (He & Jonas, 2008). For one of the symmetry operators, this scalar part will be maximal, i.e.,

\[
\pm (c_0 q_0^* + c_1 q_1 + c_2 q_2 + c_3 q_3) \leq q_0^*.
\]

### Table 2
General vertex coordinate and volume for the Rodrigues fundamental zones for all rotational point-group symmetries.

The complete set of vertices is generated by application of the rotational group elements to \( \rho \). The letter following some of the RFZ shape entries refers to the labels in Figs. 5 and 11.

<table>
<thead>
<tr>
<th>Point group ( G )</th>
<th>No. of vertices</th>
<th>Edge length ( a )</th>
<th>Volume ( V/a^3 )</th>
<th>Volume ( V )</th>
<th>RFZ shape</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>( \infty )</td>
<td>( \mathbb{R}^3 )</td>
</tr>
<tr>
<td>2</td>
<td>( (\rho_x, \rho_y, \pm \tan(\pi/4)) )</td>
<td>—</td>
<td>—</td>
<td>( \infty )</td>
<td>infinite slab</td>
</tr>
<tr>
<td>3</td>
<td>( (\rho_x, \rho_y, \pm \tan(\pi/6)) )</td>
<td>—</td>
<td>—</td>
<td>( \infty )</td>
<td>infinite slab</td>
</tr>
<tr>
<td>4</td>
<td>( (\rho_x, \rho_y, \pm \tan(\pi/8)) )</td>
<td>—</td>
<td>—</td>
<td>( \infty )</td>
<td>infinite slab</td>
</tr>
<tr>
<td>6</td>
<td>( (\rho_x, \rho_y, \pm \tan(\pi/12)) )</td>
<td>8</td>
<td>2</td>
<td>1</td>
<td>8.00000 infinite slab</td>
</tr>
<tr>
<td>32</td>
<td>( (1, \pm \tan(\pi/6), \tan(\pi/6)) )</td>
<td>12</td>
<td>( 2/(3)^{1/2} )</td>
<td>( 3(3)^{1/2}/2 )</td>
<td>4.00000 hexagonal prism (h)</td>
</tr>
<tr>
<td>422</td>
<td>( (1, \pm \tan(\pi/8), \tan(\pi/8)) )</td>
<td>16</td>
<td>( 2 \tan(\pi/8) )</td>
<td>( 2\cot(\pi/8) )</td>
<td>2.74517 octagonal prism (g)</td>
</tr>
<tr>
<td>622</td>
<td>( (1, \pm \tan(\pi/12), \tan(\pi/12)) )</td>
<td>24</td>
<td>( 4 - 2(3)^{1/2} )</td>
<td>( 3(2 + 3^{1/2}) )</td>
<td>1.72312 dodecagonal prism (f)</td>
</tr>
<tr>
<td>23</td>
<td>( (1, 0, 0) )</td>
<td>6</td>
<td>( 2^{1/2} )</td>
<td>( 2^{1/2}/3 )</td>
<td>1.33333 octahedron (d)</td>
</tr>
<tr>
<td>432</td>
<td>( (2^{1/2} - 1, 2^{1/2} - 1, 3 - 2(2)^{1/2}) )</td>
<td>24</td>
<td>( 6 - 4(2)^{1/2} )</td>
<td>( (21 + 14(2)^{1/2})/3 )</td>
<td>0.54949 truncated cube (c)</td>
</tr>
<tr>
<td>532</td>
<td>( ((10 - 22(5)^{1/2})^{1/2}, 0, (41 - 18(5)^{1/2})^{1/2}) )</td>
<td>12</td>
<td>( 2(41 - 18(5)^{1/2})^{1/2} )</td>
<td>( (15 + 7(5)^{1/2})/4 )</td>
<td>0.30931 dodecahedron</td>
</tr>
</tbody>
</table>

Figure 6: 3D representations of the Rodrigues fundamental zones for the ten non-trivial rotational point groups in the stereographic, Rodrigues, homochoric and cubochoric spaces. All renderings are shown at the same scale, except for the Rodrigues representation for the cyclic point groups.
taking into account the double-cover nature of the quaternion representation. Dividing both sides of the inequality by $q_0$ we obtain a similar relation in Rodrigues–Frank space:

$$\pm(c_0 + c_1\rho_1 + c_2\rho_2 + c_3\rho_3) \leq 1.$$  

This equation represents a region of space between a pair of planes, one plane on each side of the origin. The positions of the planes depend on the order of the rotational symmetry axis; it can be shown (e.g. Morawiec, 1995) that the planes are located at $\pm \tan(\pi/2n)$ from the origin and normal to the rotation axis of order $n$. In particular, for a twofold rotation axis, the planes are at unit distance from the origin.

Application of the above inequalities to the rotational point groups and finding all unique intersections between three or more planes using a vertex enumeration scheme (He & Jonas, 2008) results in the vertices listed in Table 2; the crystallographically relevant RFZs are illustrated in Fig. 5. The letter labels in parentheses following the point-group symbols will be used for the description of misorientation fundamental zones in Section 5.3.

5.2.2. Graphical representations for RFZs in other spaces. The RFZs can be mapped onto any of the other rotational spaces. Fig. 6 shows the Rodrigues FZs mapped onto the stereographic, homochoric and cubochoric spaces. Note that the Rodrigues representations for the cyclic groups consist of an infinite volume between parallel planes at distance $\pm \tan(\pi/2n)$ from the origin; they are represented by 2D cross sections normal to the $\rho_y$ axis, and the arrows have unit length.

5.2.3. Fundamental zones in Euler space. Historically, the texture community has used $zxz$ Euler angles as the main rotation/orientation representation, and the concept of fundamental zones in Euler space is well established. The crystallographic rotational symmetry elements can be represented by lines or points in Euler space. All rotations with axis normal to the $a\ b$ plane are represented by continuous lines in the $\Phi = 0$ plane in Fig. 7(a); similar to the identity operation, those rotations are degenerate in Euler space due to the vanishing of the volume element [equation (17)]. Rotations with axis in the $a\ b$ plane are represented by dashed lines in the $\Phi = \pi$ plane [Fig. 7(a)]; once again, all these rotations have degenerate Euler representations. Finally, rotations with inclined rotation axes fall on a regular grid of points in the $\Phi = \pi/2$ plane, as shown in Fig. 7(b). The subscripts on the labels indicate the direction of the rotation axis, with $x$ and $y$ representing the coordinate directions, and $a = [111]$, $b = [\bar{1}\bar{1}\bar{1}]$, $c = [11\bar{1}]$ and $d = [\bar{1}\bar{1}\bar{1}]$. The 11 rotational crystallographic point groups are shown in Euler-space representation in Fig. 8; note that, with the exception of the cubic point groups, all rotations in the other nine point groups are degenerate in this representation.

The presence of crystallographic rotational symmetry operations introduces a natural subdivision of Euler space into unique disjoint regions that can be considered as Euler fundamental zones (EFZs). A cubic rotational symmetry operation generates an equivalent point $\theta'$ for any given point $\theta = (\varphi_1, \Phi, \varphi_2)$ in Euler space. The fourfold rotation operator $4_z$ generates a translation by $\pi/2$ along the $\varphi_2$ axis, whereas $4_x$ generates a set of twofold screw axes parallel to the $\varphi_1$ axis (Hansen et al., 1978). These operations subdivide Euler space into eight equivalent rectangular prisms of extent $[0 \leq \varphi_1 \leq 2\pi, 0 \leq \Phi \leq \pi/2, 0 \leq \varphi_2 \leq \pi/2]$. The threefold rotational operator gives rise to a non-planar subdivision and introduces a quasi threefold screw axis parallel to the $\varphi_1$ axis and located at $\varphi_2 = \pi/4, \Phi = \arccos(1/3^{1/3})$. Fig. 9(a) shows the locations of the twofold screw axes and the translational cells (dashed lines), whereas the curved surfaces caused by the threefold symmetry are illustrated in Fig. 9(b); note that it is common to
orient Euler space so that the \( \Phi \) axis points downwards in planar projections. The surfaces delineating the area shaded in grey are described by the relation

\[
0 < \varphi_1 < 2\pi; \quad \Phi_1 < \Phi < \frac{\pi}{2}; \quad 0 < \varphi_2 < \frac{\pi}{2}.
\]

where

\[
\Phi_1 = \arccos \left( \frac{\cos \varphi_2}{(1 + \cos^2 \varphi_2)^{1/2}} \right), \quad \sin \varphi_2 = \left( \frac{1 + \sin^2 \varphi_2}{(1 + \cos^2 \varphi_2)^{1/2}} \right)^{1/2}.
\]

The resulting volume is shown in rendered form in Fig. 9(c).

It should be noted that these Euler FZs typically do not contain the identity rotation, which lies in the degenerate \( \Phi = 0 \) plane. This failure to contain the identity inside the EFZ can be avoided by instead mapping the Rodrigues FZs directly into Euler space, as shown in Fig. 10 for the ten non-trivial rotational point groups (the reference frame is shown in the lower left corner). The mapping relations from a Rodrigues vector \( \mathbf{r} = (x, y, z) \) to the Bunge Euler triplet are given by

\[
\varphi_1 = \arctan \left( \frac{-y + xz}{-x - yz} \right); \quad (34a)
\]

\[
\Phi = \arctan \left( \frac{2((x^2 + y^2)(1 + z^2))^{1/2}}{1 - x^2 - y^2 + z^2} \right); \quad (34b)
\]

\[
\varphi_2 = \arctan \left( \frac{-2z}{1 - z^2} \right) - \varphi_1. \quad (34c)
\]

For the cyclic groups, the RFZs become diagonal rectangular prisms with thickness depending on the order of the rotation axis. For all other rotational point groups, the RFZs map onto closed (finite) volumes with curved top surfaces, also aligned along the diagonal \((\varphi_1, 0, 2\pi - \varphi_1)\). The cusps in the top surfaces correspond to the vertical edges (i.e., parallel to the \( z \) axis) of the RFZs in Rodrigues space (shown in Fig. 5), whereas the points along the \( z \) axis inside the RFZ are mapped onto degenerate diagonal lines in the \( \Phi = 0 \) plane in Euler space.

5.2.4. Sample symmetry. In addition to the crystallographic symmetry of the crystal structure, the processing conditions of a sample, or its thermomechanical history in the case of geological samples, may impose additional symmetry. For instance, during a (hot or cold) rolling process, the thickness of a block of material is reduced and an elongated slab is produced. The texture of this slab will reveal the symmetry of

\[
\begin{align*}
\varphi_1 = \arctan \left( \frac{-y + xz}{-x - yz} \right); \\
\Phi = \arctan \left( \frac{2((x^2 + y^2)(1 + z^2))^{1/2}}{1 - x^2 - y^2 + z^2} \right); \\
\varphi_2 = \arctan \left( \frac{-2z}{1 - z^2} \right) - \varphi_1.
\end{align*}
\]

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\varphi_2 = \arctan \left( \frac{-2z}{1 - z^2} \right) - \varphi_1.
\end{align*}
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the processing conditions in addition to the crystallographic symmetry; for rolling, the orthorhombic point group $mmm$ describes this sample symmetry, with the twofold axes normal to the slab surfaces, and an orientation distribution function derived from texture measurements can be expected to exhibit this symmetry. Representing the Cartesian basis vectors of the crystal and sample by $\{K_c\}$ and $\{K_s\}$, respectively, and taking the point groups to be represented by $G_c$ and $G_s$, we have the relations

$$\{K'_c\} = g_c \{K_c\} \quad \text{and} \quad \{K'_s\} = g_s \{K_s\},$$

where $g_c \in G_c$ and $g_s \in G_s$ and the primed symbols represent equivalent orientations of the reference frames. We also have the relation

$$\{K'_c\} = g \{K'_c\},$$

with $g$ representing a rotation taking the sample reference frame into the crystal reference frame. Combining both relations, we have

$$\{K_c\} = g_c^{-1} g_s \{K_s\} = g' \{K_s\},$$

with $g' = g_c^{-1} g g_s$; thus, there is a symmetry operation $g'$ that contains both crystal and sample symmetry and transforms the sample reference frame to the crystal reference frame. The combination of the two point groups $G_c$ and $G_s$ results in an effective or induced space-group symmetry for Euler space; the 729 pairs of non-cubic point groups combine to generate 21 space-group symmetries for Euler space (for details, see Pospiech et al., 1974), namely space-group numbers 6, 7, 10, 13, 28, 29, 30, 32–34, 40, 41, 49, 50, 52–54, 56, 60, 66 and 68; note that the highest rotational symmetry order in these groups is 2.

The additional sample symmetry reduces the size of the Euler FZ that needs to be considered. For non-cubic point groups, the relevant range of the Euler angles is reduced to $\varphi_1 \in [0, 2\pi/f], \Phi \in [0, \pi]$ and $\varphi_2 \in [0, 2\pi/i]$, where $i$ is the highest rotational order along the $z$ axis for the crystal point group $G_c$ and $j$ the same for the sample point group $G_s$. For cubic crystal symmetry, the Euler FZs with curved boundaries described in Section 5.2.3 must be used, and their size along the $\varphi_1$ axis is correspondingly shortened.

### 5.3. Fundamental zones for misorientations

Consider two different crystal structures, $\alpha$ and $\beta$, each with a rotational point group $G^i$ with $i \in \{\alpha, \beta\}$; the groups can be identical to or different from each other, and their order is represented by $N^i$. The elements of $G^i$ are represented by $S^i_j$ ($j \in [1, \ldots, N^i]$) and the elements of $G^\alpha$ by $T^\beta_k$ ($k \in [1, \ldots, N^\alpha]$). Consider two crystallites, one belonging to each phase, with orientations $A$ and $B$ represented by the matrices $s^\alpha_A$ and $s^\beta_B$ (or quaternions $q^\alpha_A$ and $q^\beta_B$). For a given orientation matrix, $g$, of phase $\alpha$, the equivalent orientations are given by the set

$$\{g | g_j = S^\alpha_j g, j \in [1, \ldots, N^\alpha]\}.$$  

In quaternion form, the symmetry elements are written as $q_S^\alpha$ and $q_T^\alpha$, respectively.

The misorientation between $A$ and $B$ is defined as the rotation that takes $A$ to $B$ or $B$ to $A$. Since orientations

---

**Figure 10**
Graphical representation of the Rodrigues FZ of the ten non-trivial rotational crystallographic point groups mapped into Euler space. Note that all zones line up along the diagonal line corresponding to the identity rotation. In the bottom two rows, the segment that has a slightly lighter shade of grey corresponds to the repeat unit of the FZ.
represent the (passive) transformation from the sample reference frame to the crystal frame, the misorientation matrix, $g_{AB}$, is obtained by undoing the first orientation, $(g_A^0)^{-1}$, and then applying the second one:

$$g_{AB} = (g_A^0)^{-1}g_B$$ and $g_{BA} = (g_B^0)^{-1}g_A \rightarrow g_{AB} = g_{BA}^{-1}$, \hspace{1cm} (39)

note that the sequence of matrix multiplications reflects the passive nature of the rotations. In quaternion form we have

$$q_{AB} = (q_A^0)^*q_B^0$$ and $q_{BA} = (q_B^0)^*q_A^0 \rightarrow q_{AB} = q_{BA}^*$. \hspace{1cm} (40)

The misorientation angle $\omega_{AB}$ is then given by

$$\omega_{AB} = 2 \arccos(q_{AB,0}) \equiv \text{ang}[q_{AB}]$$ \hspace{1cm} (41)

where the subscript 0 refers to the scalar part of the quaternion and the operator $\text{ang}$ returns the rotation angle; in matrix form, the misorientation angle is given in terms of the trace, $\text{Tr}$, of the misorientation matrix as

$$\omega_{AB} = \arccos \left( \frac{\text{Tr}[g_{AB}] - 1}{2} \right) \equiv \text{ang}[g_{AB}]$$. \hspace{1cm} (42)

In the presence of crystallographic symmetry, each misorientation matrix/quaternion has $N - 1$ equivalent orientations, where $N$ is the order of the rotational point group. The disorientation is then defined as the smallest misorientation angle for the set of equivalent misorientations:

$$\omega_{AB} = \min_{j,k} \{ \text{ang}[(S_j g_A^0)^{-1}(T_k g_B^g)] \}$$ \hspace{1cm} (43)

or

$$\omega_{AB} = \min_{j,k} \{ \text{ang}[(q_S q_A^0)^*q_{T_k} g_B^g] \}. \hspace{1cm} (44)

These sets contain $N_g \times N_p$ elements; thus, for an $\alpha$ phase with rotational point group 432 and a $\beta$ phase with point group 622, there are $24 \times 12 = 288$ equivalent misorientations, and the disorientation is defined as the smallest misorientation angle in this set. The maximum possible number of misorientations is $24^2 = 576$.

For the special case where the $\alpha$ and $\beta$ phases are identical, the relations above can be simplified and the number of equivalent misorientations is reduced. We have

$$\omega_{AB} = \min_{j,k} \{ \text{ang}[(S_j g_A^0)^{-1}S_k g_B^g] \}$$ \hspace{1cm} (45)

$$= \min_{j,k} \{ \text{ang}[(g_A^0)^{-1}S_j g_B^g] \}$$ \hspace{1cm} (46)

$$= \min_{j} \{ \text{ang}[(g_A^0)^{-1}S_j g_B^g] \}. \hspace{1cm} (47)$$
where \( S_1 = S^{-1}_1 S_k \) belongs to the point group \( G' \) due to the closure property; hence, there are only \( N_a \) misorientations to be considered.

For the general case of two different crystal symmetries, the combined operators \( S_1^{-1} T_k \) must be considered in the same way as before (Section 5.2.1) to determine the fundamental zone of misorientations for the pair of point groups \( G, G'' \). Table 3 lists the shape of the misorientation fundamental zones for all point-group combinations (He & Jonas, 2008). Shapes labelled \( c, d, f, g, h \) and \( i \) were defined in Fig. 5; shapes \( a, b \) and \( e \) are shown in Fig. 11. All shapes indicated by \( x \) correspond to an infinite volume and are thus not representable in a finite drawing. The coordinates for the vertices of the shapes in Fig. 11 are listed in Table 4; note that shapes \( a \) and \( b \) can occur in two mirror-related variants, depending on the point-group pair.

### 5.4. Orientation sampling and statistics

The most straightforward random sampling approach for orientations is the Marsaglia algorithm (Marsaglia, 1972), which operates in the quaternion representation. Select two numbers \( x_1 \) and \( y_1 \) uniformly in the interval \([-1, 1] \) until \( s_1 = x_1^2 + y_1^2 < 1 \); repeat this step for two additional numbers \( (x_2, y_2) \), with \( s_2 = x_2^2 + y_2^2 < 1 \). One can then show that the unit quaternion

\[
q = \left[ x_1, y_1, x_2 \left( \frac{1 - s_1}{s_2} \right)^{1/2}, y_2 \left( \frac{1 - s_1}{s_2} \right)^{1/2} \right]
\]  

is uniformly distributed on the unit 3-sphere \( S^3 \).

To obtain a sample of orientations on a uniform grid in orientation space, three approaches are available in the literature. In the robotic motion community, a multi-resolution sampling scheme has been developed that is based on the Hopf fibration (Górski et al., 2005; Yershova et al., 2010), i.e., a parametrization \((\theta, \phi, \psi) \) of \( SO(3) \) in terms of an angle \( \psi \in [0, 2\pi] \) (i.e., the unit circle \( S^1 \)) and \((\theta \in [0, \pi], \phi \in [0, 2\pi]) \), i.e., spherical angles on \( S^2 \). This is then transformed into a quaternion by the following relation:

\[
q = \left( \begin{array}{c} \cos \frac{\theta}{2} \cos \frac{\psi}{2} \\ \cos \frac{\theta}{2} \sin \frac{\psi}{2} \\ \sin \frac{\theta}{2} \cos (\phi + \frac{\psi}{2}) \\ \sin \frac{\theta}{2} \sin (\phi + \frac{\psi}{2}) \end{array} \right).
\]  

A second approach (Górski et al., 2005) produces a uniform incremental grid on \( SO(3) \), by means of a HEALPix grid on \( S^2 \) and a regular grid on \( S^1 \). While both of these approaches produce uniform grids, they are not easily combined with crystallographic symmetry and fundamental zones. The cubochoric orientation representation, described in Section 5.1.6, allows for a straightforward uniform sampling of a cube of volume \( \pi^2 \) and results in a uniform (in the equal-volume sense) sampling of \( S^3 \). Sampling in the presence of rotational symmetry only requires the introduction of a binary test: for each sampling point in the cube, the orientation is transformed to the Rodrigues representation and tested against the RFZ boundaries; if the point falls inside the RFZ, it is kept, otherwise the orientation is discarded from the sample.

When working with sets of orientations on \( S^3 \), techniques from the field of ‘directional statistics’ become relevant (Mardia & Jupp, 2009). The equivalent of a normal distribution on the \( n \)-sphere in \( \mathbb{R}^n \) is the von Mises–Fisher distribution:

\[
f_{\text{vMF}}(x; \mu, \kappa) \equiv \left( \frac{\kappa}{\Gamma(p/2)} \right)^{p/2 - 1} \frac{1}{2 I_{p/2-1}(\kappa)} \exp(\kappa \mu \cdot x),
\]  

with \( \kappa \) the concentration and \( \mu \) the mean direction, \( \Gamma \) Euler’s gamma function, and \( I_p \) a modified Bessel function of the first kind and order \( p \). For \( \kappa \to 0 \) this becomes a uniform distribution, and for \( \kappa > 0 \) the function clusters around the mean direction \( \mu \). For quaternions we have \( p = 4 \) and

\[
f_{\text{vMF}}(q; \mu, \kappa) = \frac{\kappa}{2 I_2(\kappa)} \exp(\kappa \mu \cdot q).
\]

Incorporating the equivalence of \( q \) and \( -q \), one obtains the axial Watson distribution which, for quaternions, reduces to

![Figure 11](image-url)
6. Indexing

Strictly speaking, ‘indexing’ an EBSD pattern refers to the assignment of Miller indices to the bands in the pattern. However, the EBSD community commonly uses the term ‘indexing’ to describe the complete procedure for determining the crystallographic orientation of the crystal lattice from a pattern. The crystal structures of the various phases present in the sample are assumed to be known. Various indexing approaches have been developed since the beginning of EBSD work; since they build upon each other, this will be presented somewhat chronologically, albeit with some skipping of intermediate steps for brevity.

6.1. Algorithm types

Since the inception of EBSD as a tool in materials and geological laboratories, there have been four main approaches to indexing patterns. The first two are manual approaches but they do represent important steps in the evolution towards automated indexing.

(1) The user must manually identify zone axes in the pattern; once the crystallographic indices of the zone axes are identified and their location determined in terms of pattern coordinates, then the crystallographic orientation can be determined. This approach requires a knowledgeable operator capable of correctly recognizing the crystallographic direction associated with a zone axis (Dingley, 1984). This approach is briefly introduced in Section 6.2.1.

(2) The user must manually draw the bands in the pattern (Schmidt & Olesen, 1989). By comparing the angles between these bands to the interplanar angles of prominent reflecting planes (known as ‘reflectors’ in EBSD) in the material, it is then possible to identify a list of possible orientations. The user would then select the correct orientation from the list. This was a significant step forward as the user would not need to be nearly as skilled as needed to employ method (1). The basic steps of this approach are covered in Section 6.2.2.

(3) Full automation of the procedure by detecting Kikuchi bands using feature-recognition techniques (Adams et al., 1993) and then using the detected bands and knowledge of the interplanar angles to hone in on a unique orientation. This technique has been coupled with automation of beam movement leading to a fully automated system for rapidly measuring orientations. This is the core of commercial EBSD systems and has led to their becoming relatively commonplace in materials and geology characterization facilities. The algorithms involved are covered in Section 6.3. There are several commercial EBSD vendors offering automated indexing systems. The commercial EBSD system sold by EDAX is based on an indexing algorithm developed by Adams’ research team at Yale University; as this work is well documented in the scientific literature, we present this approach. The other commercial vendors’ indexing algorithms are, to the knowledge of the authors, unpublished, but it is assumed that they use a derivative of the approach presented here. While other approaches to automated indexing have been developed (Morawiec, 1995; Britton, Tong et al., 2018), the approach covered here is the most common.

(4) Taking advantage of dynamical simulations of diffraction patterns to create a dictionary of patterns (Chen et al., 2015). Experimental patterns can then be compared against the patterns in the dictionary to determine the orientation. Dictionary indexing and the related spherical indexing approaches are described in Section 6.5.1.

6.2. Operator-assisted indexing

6.2.1. Zone axis indexing. As outlined in some of the early papers on indexing, one approach, implemented in David Dingley’s early online indexing software (Dingley, 1984), is to identify two zone axes. This methodology is relatively straightforward in an EBSD pattern from a high-symmetry material such as a face-centred cubic (f.c.c.) crystal where, with a little practice, the major zone axes are relatively easy to recognize (see Fig. 12). Given the location of two zone axes, the orientation can be determined using the following approach (see schematic in Fig. 13). Define two vectors from the origin (the point where the incident electron beam hits the sample) to the two zone axes in pattern coordinates:

$$f_W(\pm q; \mu, \kappa) = \frac{\exp(-\kappa/2)}{I_0(\kappa/2) - I_1(\kappa/2)} \exp(\kappa(\mu \cdot q)^2).$$

Both the von Mises–Fisher and Watson distributions are rotationally symmetric around the mean direction. For more general distributions on the n-sphere, with anisotropic peak shapes, one must resort to the use of the Bingham distribution, which poses significant numerical challenges (Niezgoda et al., 2016).

Figure 12

Typical zones axes used in manual indexing of patterns from face-centred cubic crystals.
Generally, this consists of the tilt sample reference frame. To do this, the geometrical relationship between the two zones is a mirror plane. However, if the (130) and (121) zone axes are identified, then there would be two possible solutions, only one of which is correct. An operator must choose between these two possibilities to select the correct orientation.

6.2.2. Band indexing. Instead of a user being required to identify two zone axes, the user could be required to identify two bands in a pattern. To determine the orientation, two vectors representing two plane normals need to be defined in pattern coordinates (refer to the schematic in Fig. 14).

\[
\mathbf{n}_A^P = \frac{\mathbf{OA}_1 \times \mathbf{OA}_2}{\| \mathbf{OA}_1 \times \mathbf{OA}_2 \|} \quad \text{and} \quad \mathbf{n}_B^P = \frac{\mathbf{OB}_1 \times \mathbf{OB}_2}{\| \mathbf{OB}_1 \times \mathbf{OB}_2 \|}. \tag{59}
\]

From these two normalized vectors an orthogonal frame can be constructed as follows:

\[
\mathbf{e}_i^A = \mathbf{n}_A^P \times \mathbf{n}_B^P \quad \text{and} \quad \mathbf{e}_i^B = \mathbf{e}_i^A \times \mathbf{e}_i^P. \tag{60}
\]

Similarly, an orthogonal frame can be constructed in the crystal frame given the indices associated with the bands used in the calculation of the plane normals \( \mathbf{n}_A^C \) and \( \mathbf{n}_B^C \) shown previously. This is done as follows:

\[
\mathbf{e}_i^C = \frac{(hkl)_A^C}{\| (hkl)_A^C \|} \quad \text{and} \quad \mathbf{e}_i^C = \frac{(hkl)_B^C}{\| (hkl)_B^C \|}. \tag{61}
\]

As for the zone axes, the orientation (representing the rotation required to bring the pattern coordinate frame into coincidence with the crystal lattice reference frame) can be calculated from these vectors. The crystallographic orientation, \( \mathbf{g}^S \), is calculated by taking into account the sample and detector geometries.

6.3. Hough indexing

To automate the indexing, the bands in the pattern must be detected and then the reflectors \((hkl)\) associated with each band identified. We focus on the latter step first.

6.3.1. Identifying reflectors. As mentioned in Section 6.2.2, the interplanar angles provide a means of identifying the reflectors associated with specific bands. As an introductory case, consider the face-centred cubic (f.c.c.) crystal system. In f.c.c. crystals the reflecting planes \([200],[311],[111]\) and \([220]\) produce the most prominent bands in EBSD patterns. We can construct an interplanar angle \((\alpha)\) look-up table from these

\[
\mathbf{g}^S = \mathbf{g}^P \mathbf{g}^{PS}, \tag{58}
\]

where \( \mathbf{g}^S \) represents the crystallographic orientation, i.e., the rotation that brings the sample reference frame into coincidence with the crystal reference frame.

It should be noted that the indexing solution obtained is not necessarily unique when only the families of indices \((uvw)\) are associated with a zone axis pair as opposed to the exact \([uvw]\) pair. Consider the pattern shown in Fig. 12 for an f.c.c. crystal. If the (110) and (010) zone axes are identified, then there would only be one possible solution because the band joining the two zones is a mirror plane. However, if the (130) and (121) zone axes are identified, then there would be two possible solutions, only one of which is correct. An operator must choose between these two possibilities to select the correct orientation.

Figure 13
Schematic of indexing using a pair of zone axes in an EBSD pattern.

\[
\mathbf{v}_A^p = \frac{\mathbf{OA}}{\| \mathbf{OA} \|} \quad \text{and} \quad \mathbf{v}_B^p = \frac{\mathbf{OB}}{\| \mathbf{OB} \|}. \tag{53}
\]

[The notation \( \| \mathbf{v} \| \) denotes the magnitude of a vector \( \mathbf{v}, \text{i.e.,} \| \mathbf{v} \| = (\mathbf{v} \cdot \mathbf{v})^{1/2} = (v_1 v_1 + v_2 v_2 + v_3 v_3)^{1/2} \) and \( \hat{\mathbf{v}} \) denotes a normalized vector, i.e. \( \| \mathbf{v} \| = 1 \).] From these two normalized vectors an orthogonal frame can be constructed as follows:

\[
\hat{\mathbf{e}}_3^A = \hat{\mathbf{v}}_3^A \quad \text{and} \quad \hat{\mathbf{e}}_3^B = \hat{\mathbf{v}}_3^B \times \hat{\mathbf{v}}_2^B. \tag{54}
\]

Similarly, an orthogonal frame can be constructed in the crystal frame given the indices \([uvw]\) associated with the zone axes used in the calculation of \( \mathbf{v}_A^p \) and \( \mathbf{v}_B^p \) shown previously. This is done as follows:

\[
\hat{\mathbf{e}}_3^C = \frac{[uvw]_A}{\| [uvw]_A \|} \quad \text{and} \quad \hat{\mathbf{e}}_3^C = \frac{[uvw]_B}{\| [uvw]_B \|}. \tag{55}
\]

The orientation (representing the rotation required to bring the pattern coordinate frame into coincidence with the crystal lattice reference frame) can be calculated from these vectors as follows:

\[
g_i^P = \hat{\mathbf{e}}_3^C \times \hat{\mathbf{e}}_3^P. \tag{56}
\]

One more step is needed to bring this orientation into the sample reference frame. To do this, the geometrical relationship between the detector and the sample must be considered. Generally, this consists of the tilt \( \chi \) of the sample (typically \( \theta \approx 70^\circ \)) as well as the tilt of camera (sometimes referred to as the elevation angle) as shown schematically in Fig. 1. The rotation matrix can be written:

\[
g_{PS} = \begin{pmatrix}
0 & -c_x s_y + s_x c_y & s_x s_y + c_x c_y \\
1 & 0 & 0 \\
0 & c_y s_x + s_y c_x & -s_y s_x + c_y c_x
\end{pmatrix}, \tag{57}
\]

where \( s_x = \sin \alpha, c_x = \cos \alpha \) and

\[
g^S = g^P g_{PS}. \tag{58}
\]
reflector angles as shown in Table 5; while the exact \((hkl)\) pairs are shown in the table, the subsequent text focuses only on the families \([hkl]\).

If two bands are identified either manually by an operator or automatically by a band-detection routine, then a measured interplanar angle \(\alpha_M\) can be calculated from the dot product of the two vectors formulated in (59) and compared against the look-up table to find a match. For example, if \(\alpha_M = 45^\circ\) then the two bands are very likely to be produced by the \((200)\) and \((220)\) reflectors. However, band 1 may be \((200)\) and band 2 may be \((220)\) or vice versa. Since the band widths are a function of the interplanar \(d\)-spacing, in principle it is possible to positively identify which reflector is associated with which band. In practice, the difference in band widths may be just a few pixels or even sub-pixels and thus, if the measured band widths are used in the identification procedure, it is usually as a secondary criterion. Another uncertainty exists in the precision of the measurement of the positions of the bands. Typically, this is of the order of a few degrees, and, thus, a tolerance is needed for the comparison. If a typical tolerance value of \(3^\circ\) is used, then an additional pair of reflectors would be those for \(\alpha = 50.5^\circ\), \((311)\) and \((311)\). Thus, several orientations could be calculated for the two bands. If the measured interplanar angle were within the tolerance of \(90^\circ\), then an inspection of the table shows that there would be at least five different reflector pairs possible.

The uncertainty can be greatly reduced if three bands are considered instead of just two. Consider, for example, a band triplet with measured interplanar angles of 55, 59 and 72\(^\circ\). If a tolerance angle of \(5^\circ\) is used then the possible reflector pairs for each measured interplanar angle are listed in Table 6. The number of possible orientations from this table would be \(4 \times 4 \times 2 = 32\). But the following logic chain reduces the possibilities: consider the third pair of candidate bands in the list for \(\alpha_M = 55^\circ\); if band 1 is of \([111]\) type, then band 2 must be of \([311]\) type. Now consider the candidate pairs for the second interplanar angle \(\alpha_M = 59^\circ\) with the condition that the first reflector in the pair is of \([311]\) type. This eliminates two of the candidate pairs leaving only \([311]\) & \([111]\) and \([311]\) & \([311]\). So band 3 is either \([111]\) or \([311]\). We now consider the third interplanar angle with the condition that one member of the pair is either \([111]\) or \([311]\) and the other member must be \([111]\) (band 1 from the first condition). The only pair that matches both the interplanar angle criterion and the reflector matching criterion is the \([111]\) & \([111]\) pair. For this triplet example, there are three possible solutions as shown in the diagram in Fig. 15.

Of course, there are many more bands in a pattern and thus many more triplets can be formed. The number of triplets \(n_T\) than can be formed from a set of \(n_B\) bands is given as

\[
n_T = \frac{n_B!}{(n_B - 3)!n_B^3}.
\]

Each triplet will produce a few possible orientations, but it is assumed that the correct orientation for the pattern will be that which appears most frequently among the sets of orientations for all the triplets. The most probable orientation can then be determined using a voting scheme. An example of the voting scheme is shown in the diagram in Fig. 16 for a pattern from an f.c.c. material where five bands are detected (only five are used to keep the example simple). From this diagram, it is clear that orientation 1 is the most probable orientation, receiving all 10 of 10 possible votes. We denote the number of votes received for the top solution as \(V_1\) and use \(V_2\) for the solution receiving the second most votes.

It should be noted at this juncture that band doublets, triplets, quadruplets and so on can all be used. Increasing the number of bands in the set will reduce the number of possible orientations at the beginning of the procedure. However, some cursory experiments by the authors have shown that using more than three bands introduces more sensitivity to rogue bands sometimes found by the band-detection schemes, particularly for poor-quality patterns. This leads to less robustness in the automated indexing routine. Once again, since the measurement of the position of the bands in the pattern is not exact, the orientations in the voting table are not all exactly the same, but similar within a tolerance angle typically of just a few degrees. To hone in on the correct orientation a quaternion average of all the similar orientations is used (Kunze et al., 1993). Recall that for each orientation

### Table 5

<table>
<thead>
<tr>
<th>Interplanar angle (\theta )</th>
<th>((hk)f_1)</th>
<th>((hk)f_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.2</td>
<td>200</td>
<td>311</td>
</tr>
<tr>
<td>29.5</td>
<td>111</td>
<td>311</td>
</tr>
<tr>
<td>31.5</td>
<td>220</td>
<td>311</td>
</tr>
<tr>
<td>35.1</td>
<td>311</td>
<td>311</td>
</tr>
<tr>
<td>35.3</td>
<td>111</td>
<td>220</td>
</tr>
<tr>
<td>45.0</td>
<td>200</td>
<td>220</td>
</tr>
<tr>
<td>50.5</td>
<td>311</td>
<td>311</td>
</tr>
<tr>
<td>54.7</td>
<td>111</td>
<td>200</td>
</tr>
<tr>
<td>58.5</td>
<td>111</td>
<td>311</td>
</tr>
<tr>
<td>60.0</td>
<td>220</td>
<td>202</td>
</tr>
<tr>
<td>63.0</td>
<td>311</td>
<td>131</td>
</tr>
<tr>
<td>64.8</td>
<td>220</td>
<td>311</td>
</tr>
<tr>
<td>70.5</td>
<td>111</td>
<td>111</td>
</tr>
<tr>
<td>72.5</td>
<td>200</td>
<td>131</td>
</tr>
<tr>
<td>80.0</td>
<td>111</td>
<td>311</td>
</tr>
<tr>
<td>84.8</td>
<td>311</td>
<td>131</td>
</tr>
<tr>
<td>90.0</td>
<td>111</td>
<td>220</td>
</tr>
<tr>
<td>90.0</td>
<td>200</td>
<td>020</td>
</tr>
<tr>
<td>90.0</td>
<td>200</td>
<td>022</td>
</tr>
<tr>
<td>90.0</td>
<td>220</td>
<td>113</td>
</tr>
<tr>
<td>90.0</td>
<td>220</td>
<td>220</td>
</tr>
</tbody>
</table>

### Table 6

Candidate reflector pairs for a triplet of bands with measured interplanar angles of 55, 59 and 72\(^\circ\) in a face-centred-cubic crystal.

This table was constructed using the look-up table in Table 5 with a 5\(^\circ\) tolerance.

<table>
<thead>
<tr>
<th>(\alpha_M = 55^\circ)</th>
<th>(\alpha_M = 59^\circ)</th>
<th>(\alpha_M = 72^\circ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>([311]) &amp; ([311])</td>
<td>([111]) &amp; ([200])</td>
<td>([111]) &amp; ([111])</td>
</tr>
<tr>
<td>([111]) &amp; ([200])</td>
<td>([111]) &amp; ([311])</td>
<td>([200]) &amp; ([311])</td>
</tr>
<tr>
<td>([111]) &amp; ([311])</td>
<td>([220]) &amp; ([220])</td>
<td>([311]) &amp; ([311])</td>
</tr>
</tbody>
</table>

there are several symmetry-equivalent variants. The variants considered must be close to each other in orientation space. For the quaternion averaging scheme we use the symmetric variants with maximum values for quaternion components $q_0$, $q_2$ and $q_3$. The average orientation can then be calculated using these symmetric variants according to

$$
\tilde{q}_i = F \sum_{n=1}^{N} q_i(n),
$$

where $q(n)$ is quaternion representation of the $n$th triplet and $F$ is a normalization factor such that $\|\tilde{q}\| = 1$.

6.3.2. Detecting bands. Full automation of the system requires that the bands be found by feature detection. While various approaches have been proposed (Juul Jensen & Schmidt, 1990; Wright & Adams, 1992), the one most commonly used in modern systems is based on the Hough transform. It should be noted that the Hough transform is related to the Radon transform (van Ginkel et al., 2004). The Hough transform is inherently a discrete algorithm for detecting lines in grey scale images (but can be extended to other shapes as well). The Radon transform is a mathematical integral transform on a continuous parameter space. The Hough transform is well suited to the band-detection problem in EBSD pattern given its robustness and computational speed.

Krieger Lassen et al. first proposed using the Hough transform to extract the bands (Krieger Lassen et al., 1992). The equation governing the Hough transform is

$$\rho = x \cos \theta + y \sin \theta. \quad (63)$$

$(x, y)$ are the coordinates of a pixel in the image with intensity $I(x, y)$ and $\rho, \theta$ are the magnitude and angle, respectively, of a vector normal to a line from the origin to a line passing through the pixel, as shown in Fig. 17.

The Hough transform is represented by an accumulator array calculated using the following pseudo-code:

```plaintext
for each pixel in the image (x, y)
    for each $\theta_i$ in (in $\Delta \theta$ steps)
        calculate $\rho_i^k = x_i \cos \theta_i + y \sin \theta_i$
        round $\rho_i^k$ to the closest value $\rho_k$ in $H(\rho_k, \theta_i)$
        add $I(x, y)$ to $H(\rho_k, \theta_i)$
    end
end
```

A pixel in the image space becomes a sinusoidal curve in Hough space. For a set of pixels in a line, the sinusoidal curves for each pixel intersect at a point in Hough space. Since the accumulator array sums the intensities, this point becomes a high-intensity peak in the Hough transform. Thus, the problem of finding a line of high-intensity pixels in an image is reduced to finding a peak of high intensity in the Hough transform. The most prominent bands in the EBSD patterns approximate a line of high intensity at the centreline of the band edged by lines of low intensity. Thus, the centrelines of the bands appear as peaks in the Hough transform with valleys above and below the peaks, as can be seen in Fig. 18, which
shows a sample EBSD pattern and the corresponding Hough transform.

As the bands in the diffraction pattern are not of uniform size or a single line of bright pixels, the peaks in the actual Hough transform are not as simple as shown in Fig. 17. However, they all tend to have a characteristic shape. Krieger Lassen (1994) noted that this characteristic shape mimics a butterfly. The Hough transform can be convolved with a ‘butterfly mask’ to enhance the peaks corresponding to real bands in the diffraction pattern. The convolved Hough transform corresponding to Fig. 18 is shown in Fig. 19. Comparing these two transforms shows that the butterfly-mask convolution also removes some of the artefacts in the raw Hough transform. These artefacts, which arise from the digital nature of the images and the transform in capturing continuous lines, are generally negligible except in the case of very poor patterns where the peaks in the Hough transform are weak and the artefacts become more prominent. Other methodologies can be used to mitigate these artefacts (Tao & Eades, 2005).

The need to use a butterfly mask is a weakness of the Hough-transform approach for locating bands; the butterfly mask assumes that each band in the pattern has the same width and intensity profile as well as a symmetric intensity profile. This is less of an issue when the patterns are compressed. Thus, for Hough-transform-based indexing, patterns between 60 × 60 to 120 × 120 pixels are typically used. Another potential solution has been proposed by Krieger Lassen (1998), and the commercial vendors have also made adaptations to the Hough-transform workflow to reduce these effects.

One additional weakness of the Hough-transform approach is that it is sensitive to the overall intensity gradient typical of raw EBSD patterns. Thus, it is helpful to remove this gradient through some form of image pre-processing. One simple and common approach is to generate a background pattern for a sample by decreasing the magnification until the field of view in the SEM contains many grains (more than 50); collecting a pattern while the beam scans the field of view essentially creates an average background pattern that is then subtracted or divided from the patterns when the beam is stationary within individual grains. This results in a flattened overall pattern intensity. Any additional image processing, such as
smoothing or sharpening, prior to applying the Hough transform tends to provide only a marginal improvement in the Hough results.

The edges of the Kikuchi bands are not actually straight lines, but rather segments of hyperbolae; this is due to the projection of the diffraction cones onto the flat detector surface. This is generally not a serious issue, but it does become significant in the transmission Kikuchi diffraction (TKD) technique. Some researchers have used a three-dimensional Hough transform to capture the curvature but such approaches are computationally expensive (Maurice & Fortunier, 2008).

Despite these shortcomings, with some tuning of the governing parameters, such as the pattern size and the butterfly mask, the Hough transform provides robust and rapid detection of the bands. Coupling the band detection with the triplet indexing algorithm provides robust and precise measurements of orientation, even with relatively poor-quality patterns (Ram et al., 2015; Wright et al., 2014).

6.3.3. Indexing reliability. Various metrics can be used to evaluate the reliability of indexing; the two most commonly used are the confidence index (or CI) and the mean angular deviation (MAD) or fit metrics. The confidence index is based on the voting scheme and is given as \( CI = (V_1 - V_2)/V_{\text{IDEAL}} \), where \( V_1 \) and \( V_2 \) are the number of votes for the first and second solutions and \( V_{\text{IDEAL}} \) is the total possible number of votes from the detected bands (Field, 1997). The confidence index ranges in value from 0 to 1. A value of 0 does not necessarily mean the pattern is indexed incorrectly. Consider the case where two solutions were found in the voting scheme such that \( V_1 = V_2 \) but the other solutions received very few votes. In this case, the CI = 0 but there is a 50% chance that the pattern was correctly indexed. Near grain boundaries, the electron beam interaction volume may spread across two grains and the patterns contain a contribution from both lattices within the diffraction volume. Such patterns typically have low CI values, as the votes are shared between solutions for both contributing patterns. Similarly, if two phases produce patterns that are similar then this can also lead to a low CI condition, as discussed in Section 10.2.1.

Some materials produce EBSD patterns from crystallographically distinct orientations that are so similar that conventional indexing is unable to reliably differentiate between the two corresponding orientations, and in this case CI = 0. One condition that leads to this problem is a crystal lattice which is only slightly distorted from a higher symmetry,
such as a tetragonal crystal which is only slightly distorted from a cubic crystal. Patterns from such a crystal in two different orientations related by a 90° rotation about the a axis are difficult to differentiate from each other and thus it is not uncommon to index such crystals as if they were cubic – resulting in the term ‘pseudosymmetry’. Efforts to resolve pseudosymmetry in distorted crystals are described in several papers, including the martensite phase in steel (Ryde, 2006) (resolving the pseudosymmetry in martensite is further compounded by this phase typically producing noisy patterns due to its high dislocation content), geologic materials (Prior et al., 2009), ceramics such as alumina (Al₂O₃) (Nowell & Wright, 2005; Vaudin, 2005), zirconia (ZrO₂) (Nowell & Wright, 2005; Pee et al., 2006; Martin et al., 2012; Ocelík et al., 2017), piezoelectrics (Vaudin, 2005; Farooq et al., 2008), intermetallic γ'-TiAl (Zambaldi et al., 2009) and others.

Another crystallographic phenomenon that leads to pseudosymmetry occurs for particular structures, for instance tetragonal kesterite, Cu₂(Fe,Zn)SnS₄, with a c/a ratio close to 2. In this case, as the copper and tin atoms produce similar scattering, the two atoms are virtually interchangeable in terms of their impact on the diffraction pattern. The structure can, therefore, be considered as essentially a stacked cube structure. Patterns from such a structure mimic a cubic structure, as shown in Fig. 20, and result in pseudosymmetric indexing degeneracy.

Dictionary indexing, discussed in Section 6.5, has shown real progress in resolving pseudosymmetry problems (Nolze et al., 2016; Marquardt et al., 2017; Jackson et al., 2018; De Graef et al., 2019; Pang et al., 2020) as well as an analogous problem that arises in non-centrosymmetric crystals. In principle, EBSD breaks Friedel’s rule which governs conventional X-ray diffraction – (hkl) and (hkl) in non-centrosymmetric crystals should be differentiable from each other. But the only differences in the patterns from different orientations related through centrosymmetry are subtle differences in the intensity, particularly in the neighbourhood of zone axes (Winkelmann & Nolze, 2015). As Hough-based indexing relies solely on band positions and not does not account for subtleties in intensity, advanced techniques, such as dictionary indexing, are required to unambiguously index non-centrosymmetric crystal patterns.

The first step in the computation of the mean angular deviation is to determine where the bands should appear in the pattern based on the indexing solution obtained from the voting procedure. The MAD is the average deviation between the recalculated bands and the detected bands. This metric is sensitive to how well the system is calibrated (Section 2.2) and the performance of the Hough transform in locating the bands in the pattern. This method does not take into account rogue bands (i.e., detected bands that do not match any of the recalculated bands). Rogue bands can occur either because the Hough transform has misidentified them or they may also be bands associated with reflectors that were not explicitly considered during the indexing procedure.

Both the CI and MAD metrics describe the reliability of the indexing solution for an individual pattern. Fig. 21 shows the correlation between the per cent correctly indexed versus the CI and MAD metrics calculated for nickel patterns with artificially added noise (Wright, Nowell, Lindeman et al., 2015). The scatter in the MAD at high MAD values (MAD > 2.5°) is due to low statistics in the 0.1° bins used for averaging. To assess the indexing reliability for a data set, these metrics can be used based on a tolerance. For example, the curves in Fig. 21 would suggest that a conservative estimate of the indexing success rate could be defined as the fraction of points with a CI > 0.2 (Wright, Nowell, Lindeman et al., 2015) or MAD < 1.75°; indexing solutions falling within these tolerances have a high probability of being correct.

6.4. Image processing

EBSD patterns generally exhibit low signal contrast; they consist of a general intensity gradient that is bright near the centre of the pattern and fades to dark at the edges. The actual signal of interest can be less than 10% of the intensity maximum. Fig. 22 shows an example for a pattern from the mineral illmenite; in this case, the foreground signal is approximately 6% of the total signal intensity. As is evident from Fig. 22, it is helpful to remove the overall intensity through some form of image processing. A simple and common approach is to generate a background pattern as
described above. However, for samples containing multiple phases, this approach may not be effective, in particular if the atomic densities of the phases are quite different from each other. In such cases, it would be helpful to apply a dynamic approach based on the pattern itself. This can be achieved by blurring the pattern and then subtracting the blurred pattern from the original as-acquired pattern (Dingley et al., 2005). Band-pass filtering in frequency space can also be used; a low-frequency filter to remove the background intensity and a high-frequency filter to provide some smoothing of the pixel-to-pixel noise is commonly used for HREBSD (Wilkinson et al., 2009). A Gaussian profile can also be used to model the background intensity and then used to create the background pattern (Britton, Goran & Tong, 2018). Adaptive histogram filtering has been found to be particularly useful for dictionary indexing, as discussed in the following section (Singh & De Graef, 2017). One other technique that has shown utility for improving the indexing results is to average patterns from neighbouring points in the microstructure (Wright, Nowell, Lindeman et al., 2015; Brewick et al., 2019).

Various other image-processing techniques can be used to improve the visual quality of the EBSD patterns. These include manipulation of the intensity distribution, such as normalization or equalization to improve the brightness and contrast of the patterns. ‘Salt and pepper’ noise reduction can be achieved through smoothing routines such as convolving the pattern with a smoothing mask (i.e., a Gaussian kernel) or using a median filter. As noted previously, a high-frequency band-pass filter can also be used for smoothing. While smoothing functions are often applied prior to edge detection, owing to the inherent sensitivity of edge detection to noise, it should be noted that the implementation of the Hough transform used for EBSD is not completely focused on the band edges and is relatively tolerant of considerable ‘salt and pepper’ noise.

6.5. Whole-pattern indexing

The relatively limited computational capacity of 1990’s era computers necessitated the introduction of a feature-extraction approach based on the Hough transform to index EBSD patterns, as described in the preceding sections. Modern computational platforms, however, are sufficiently powerful to allow for whole-pattern comparisons between simulated and experimental patterns, without the need for any feature extraction. This requires the ability to compute realistic individual patterns or a complete EBSD master pattern, as described in Section 3.2.2. Two whole-pattern indexing approaches have recently emerged: dictionary indexing (DI) (Chen et al., 2015) and spherical indexing (SI) (Hielsher et al., 2019; Lenth et al., 2019a).

6.5.1. Dictionary indexing. In the dictionary-indexing approach, the cubochoric orientation sampling technique described in Section 5.4 is used to generate a uniform sampling of orientations, \( \{ \rho_i \} \), with \( i \in [1, \ldots, N_d] \), in the Rodrigues fundamental zone for the given sample crystal symmetry. For each of these orientations, a simulated pattern, \( \rho_i \), is generated using the experimentally determined detector geometry. The collection of all patterns constitutes a dictionary \( D = \{ \rho_i \mid i \in [1, \ldots, N_d] \} \); the number of patterns \( N_d \) in the dictionary depends on the RFZ size and the sampling density (Singh & De Graef, 2016); for an average angular step size of 1.4°, there are \( N_d = 8\,000\,000 \) unique orientations for triclinic symmetry, and \( N_d = 333\,327 \) for cubic symmetry.

In the basic DI approach, each experimental pattern \( \mathbf{e}_j \), with \( j \in [0, \ldots, N_e] \) and \( N_e \) the number of experimental patterns in the data set, is compared to each of the \( N_d \) dictionary patterns; as a result, DI is not a real-time indexing algorithm, but rather a post-processing approach. The comparison between simulated and experimental patterns employs a pattern similarity metric; there are many metrics available [e.g., Chapter 2 in Goshtasby (2012)], but for computational efficiency the standard dot product is the preferred metric. After a pattern pre-processing step, each 2D pattern is restructured as a normalized 1D vector, \( \mathbf{e}_j \rightarrow \mathbf{\hat{e}}_j \) and \( \rho_i \rightarrow \mathbf{\hat{\rho}}_i \), and the similarity index is computed as \( d_{ij} = \mathbf{\hat{e}}_j \cdot \mathbf{\hat{\rho}}_i \). For each experimental pattern \( j \), the maximum value in the set \( S_j = \{ s_{ij} \mid i \in [1, \ldots, N_d] \} \) is determined and the corresponding orientation \( \rho_i \) is then assigned to the pattern \( \mathbf{e}_j \), completing the indexing process. The highest dot product value for a given experimental pattern is considered to be the confidence index (CI) for that pattern.

Typical pattern pre-processing steps include high-pass filtering and adaptive histogram equalization, which enhances the contrast in the pattern and spreads the intensity histogram over all available bins. An example of the effect of pre-processing is shown in Fig. 23(a,b); (a) represents a typical 60×60 pixel experimental pattern for Ni at 20 kV and (b) the result of pre-processing. In addition to the CI map [Fig. 23(c)], the pre-processed and normalized pattern vectors \( \mathbf{\hat{e}}_j \) can be used to compute the average dot product (ADP) map, which represents the average similarity index, \( a_j = \sum \mathbf{\hat{e}}_j \cdot \mathbf{\hat{\rho}}_i / 4 \), where \( \nu \) runs over the four nearest neighbour pixels. The ADP is sensitive to the original pattern quality and highlights areas of poor pattern quality (e.g., due to voids or surface grooves or scratches); the map also differentiates between phases and highlights phase/grain boundaries.

In addition to using the confidence index \( CI_j = \max(S_j) \) as the maximum value of the set \( S_j \), one can determine, for every pixel \( j \), how many of the top \( M \) matches in the list of ranked orientations it has in common with its four nearest neighbours; this results in an orientation similarity map [OSM, Fig. 23(e)], which clearly delineates the grain boundaries. For materials with an inhomogeneous deformation across grains, the OSM reveals local fluctuations since the lists of corresponding top matches will be different for neighbouring pixels.

While the DI approach is slow compared to real-time Hough indexing, the whole-pattern nature of the comparison makes DI highly robust against pattern noise; the indexing success rate remains high for noisy patterns for which Hough indexing mostly fails. For overlapping diffraction patterns, often acquired near grain/phase boundaries, the approach will detect the two orientations present and assign a confidence index to each pattern; as a result, inverse-pole-figure maps
resulting from the DI algorithm require, in general, less cleanup than those from the traditional indexing approach.

6.5.2. **Spherical indexing.** Since the EBSD master pattern represents the intensity distribution on the Kikuchi sphere, one can back-project the experimental patterns onto this sphere and perform a spherical cross-correlation to find the 3D rotation that will bring the pattern into the correct orientation (Hielscher et al., 2019; Lenthe et al., 2019a). Once again, this requires a careful calibration of the detector parameters that are used in the back-projection. The main advantage of the spherical-indexing approach is the fact that no simulated patterns are needed; the spherical harmonic transform of the complete master pattern needs to be computed only once.

The discrete spherical harmonic transform (DSHT) of a function \( f(\theta, \phi) \) on the sphere \( S^2 \) is defined via the expansion

\[
 f(\theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \hat{f}_{\ell}^{m} Y_{\ell}^{m}(\theta, \phi),
\]

where

\[
 \hat{f}_{\ell}^{m} = \sum_{k} f_{k} w_{k} \, \overline{Y}_{\ell}^{m}(\theta_{k}, \phi_{k});
\]

the overbar indicates the complex conjugate, and the spherical harmonic functions are defined as

\[
 Y_{\ell}^{m}(\theta, \phi) = \frac{(2\ell + 1)(\ell - 1)!}{4(\ell + m)!} P_{\ell}^{m}(\cos(\theta)) \exp(i m \phi),
\]

with \( P_{\ell}^{m}(x) \) the associated Legendre polynomial of degree \( \ell \) and order \( m \). If the grid points labelled by \( k \) are chosen as rings of constant latitude \( \theta_{k} \) with equal angular spacing \( \Delta \phi_{k} \) along each ring, then the DSHT can be performed numerically using the fast Fourier transform (FFT) algorithm. Furthermore, the DSHT is exact if the weight factors \( w_{k} \) for each ring are symmetrically chosen about the equator (Sneeuw, 1994) and the latitudes correspond to zeroes of the Legendre polynomial of degree \( N_{r} \), where \( N_{r} \) is the number of rings (Lenthe et al., 2019a). The maximum value of \( \ell \) is known as the bandwidth, and, for the conditions just described, the maximum bandwidth equals \( N_{r} \).

The spherical cross-correlation of two functions \( f \) and \( g \) on the two-sphere can be computed using the Wigner D function:

\[
 (f \ast g)(R) = \sum_{\ell,m,n} \hat{f}_{\ell}^{m} \overline{\hat{g}}_{n}^{m} D_{\ell,m,n}(R),
\]

where \( R \) is a 3D rotation with \( zyx \) Euler angles \( (\alpha, \beta, \gamma) \), and the Wigner D function is defined by

\[
 D_{\ell,m,n}(\alpha, \beta, \gamma) = d_{\ell,m,n}(\beta) \exp(i m \alpha) \exp(i k \gamma),
\]

with the Wigner d function given by

\[
 d_{\ell,k,m}(\beta) = \frac{(\ell + k)!}{(\ell - m)!} \cos\left(\frac{\beta}{2}\right)^{\ell + m} \sin\left(\frac{\beta}{2}\right)^{\ell - m} P_{\ell-m,k+m}(\cos(\beta));
\]

in this expression, \( P_{\ell-k}^{m}(x) \) is a Jacobi polynomial. One can show that this cross-correlation can be computed efficiently as a 3D FFT by leveraging the properties of the \( D \) function. The most likely rotation bringing the experimental pattern into the correct location on the Kikuchi sphere corresponds to the location of the maximum correlation value, and the corresponding Euler angles are then converted to the standard Bunge angles by

\[
 (\varphi_1, \varphi_2) = \left( \alpha - \frac{\pi}{2}, \beta, \gamma + \frac{\pi}{2} \right).
\]

These Euler angles describe the rotation from \( f \) to \( g \). If \( f \) represents the master pattern and \( g \) the experimental pattern, the rotation must be inverted to describe orientations in the standard EBSD convention. The numerical algorithm can be made more efficient by including the crystallographic symmetry of the master pattern directly into the summations of equation (67), so that only non-zero harmonic coefficients are considered. Once the maximum cross-correlation has been determined, a peak refinement can be used to improve the angular accuracy.

To make efficient use of the 3D FFT, the bandwidth \( N_{r} \) must be an integer of the form \( 1 + 3(597^{11})/2 \), where \((p, q, r, s) \in \mathbb{N} \) are small natural numbers. For EBSD patterns of high quality the bandwidth can be taken as low as 53, and the computation time scales as \( N_{r}^{3} \ln N_{r} \). Using multi-threading, the indexing rate can be as high as several thousand patterns per second, which makes this approach competitive.
with real-time Hough-based indexing. With decreasing signal-to-noise ratio, however, the bandwidth must be increased and eventually the computation time becomes similar to or even longer than that of the dictionary-indexing approach. Example applications of the spherical-indexing approach can be found in Lenthe et al. (2019b, 2020).

7. Sample preparation

EBSD is very much a surface-sensitive technique, with the electron beam interaction volume typically penetrating only a few tens of nanometres below the sample surface. Thus, EBSD pattern quality is extremely sensitive to the integrity of the crystallographic lattice at the sample surface. Any disturbance of the crystal lattice will result in more diffuse diffraction bands and a loss of pattern contrast. For this reason, it is imperative to minimize any surface deformation introduced during sectioning and metallographic sample preparation. It is possible to obtain useable EBSD patterns from rough surfaces. Some samples, such as electrochemically deposited metal films, require no preparation prior to analysis. On very rough surfaces such as fracture surfaces, the topography of the surface will often block the diffracted electrons from reaching an EBSD detector, forming shadows in the patterns. While such patterns can be analysed manually, the shadows tend to cause problems for the automated band detection, leading to inconsistent indexing results during orientation mapping. Most samples must be prepared to produce indexable EBSD patterns consistent across the scan area. Proper sample preparation will result in optimal pattern quality and subsequent high-confidence orientation scan data. There are a few journal articles on EBSD-specific sample preparation (Katrukova & Mücklich, 2001, 2002; Koll et al., 2011), but the EBSD vendors (Nowell, 2017; Oxford Instruments, 2019) as well as metallographic preparation equipment vendors (Vander Voort, 2011; Struers, 2019) are a very good resource.

Proper procedures for metallographic preparation are especially critical for EBSD. Good practice seeks to minimize any changes to the sample during preparation due to deformation and/or heat generation. Effects from deformation and/or heat will be particularly evident in EBSD maps compared with standard optical or electron microscopy. While recrystallization and grain growth can lead to higher-quality EBSD patterns, the objective is to image a surface as representative of the bulk of the material as possible. Heating at the free surface can lead to enhanced recrystallization and grain growth as well as phase transformations and precipitation, and must be avoided. Mechanical sample preparation via sectioning, grinding and polishing is generally an abrasive process. Vendors of metallographic sample preparation equipment have specific recommendations for how much force should be used, lubricants, time before the abrasive materials are blunted and so on. These recommendations should be followed closely to reduce the effects of friction on the sample surface. The authors’ experience is that trying to find shortcuts around the vendors’ recommended procedures is rarely, if ever, productive. It is also important to clean the surface well between steps to avoid any residual abrasive material forming scratches during the next step.

7.1. Sectioning

For sectioning the sample, wet abrasive cutting wheels designed for precise and low-damage cutting are recommended. Prior to performing sectioning (and mounting), it is important to ensure that the sample axes are understood, marked and recorded. These axes are generally linked to the forming of the sample such as the rolling, transverse and normal directions in sheet materials, the deposition direction in additive manufactured samples, the drawing axis in wires, or a foliation plane in geological materials. It is also important during the sample preparation process to keep the intended surface as planar as possible so that the absolute orientations measured on the prepared surface are as accurate as possible.

7.2. Grinding

After sectioning, the next step is generally grinding. The goal of every step in metallographic sample preparation is to remove any damage from the previous step. Thus, each step in the grinding sequence uses a less-aggressive abrasive than the previous. This can be observed in local misorientation maps (KAM – see Section 9.4.1) as shown in Fig. 24. Local variations

Figure 24
Local misorientation maps from a cross section of a polished inconel sample after grinding with (a) 240 grit SiC and (b) 1200 grit SiC. The ground surface is to the right.
in orientation are indicative of deformed material. Grinding can be done using fixed abrasives such as silicon carbide, alumina, diamond or cubic boron nitride in the form of papers, films or discs. It is good practice, particularly for EBSD, to use short grinding times with limited force. Grinding times are typically under a minute. One should not be tempted to re-use a grinding paper; even after a short single use, the cutting ability of the fixed abrasives degrades significantly and it is not worth the savings in the cost of consumables. Every effort should be made to produce a planar surface at each successive step in the grinding sequence.

7.3. Polishing

As noted previously, the goal of every step in metallographic sample preparation is to remove any damage from the previous step and thus, like grinding, finer and finer abrasives are used to achieve this goal (Everaerts et al., 2019). Grinding and polishing are conceptually similar, polishing is generally differentiated from grinding in that an abrasive paste or slurry is applied to a supporting medium. In polishing, the abrasive is not fixed to the supporting medium and the medium also provides some shock absorption. As the abrasive material can freely move and the cloth can conform to the topography of the sample more gentle abrasion can be achieved. The softer the cloth, the more the abrasive can move, which will lead to more gentle polishing which, in turn, can lead to more surface relief. For example, a harder phase will ‘rise’ and a softer phase will ‘fall’ due to more rapid polishing of the soft phase relative to the hard phase. While some subtle relief is not a problem for EBSD, it can lead to distortions during imaging due to the high tilt used for EBSD and therefore a planar surface is desirable. Fig. 25 shows the distortions that arise from the surface relief. As opposed to the brief grinding steps, recommended polishing times are generally of the order of 10 minutes.

Vibratory polishing with colloidal silica is a very good method for the final polishing step. It is generally recommended to use low force on samples undergoing vibratory polishing (i.e., the weight of the sample and holder is less than 0.5 kg). The pH of colloidal silica suspensions is typically about 10, which results not only in removal of material due to abrasive polishing but also a chemical–mechanical polish. Vibratory polishing is generally recommended with times ranging from 15 minutes to a few hours. EBSD pattern quality can, in some cases, also be improved by treating the polished surface with a chemical etch (Chou et al., 2005).

7.4. Electropolishing

Electropolishing and electroplating are essentially the same process. In the case of electropolishing, the workpiece is positively charged and immersed in an electrolyte bath. A sacrificial negatively charged cathode is also placed in the bath. This creates an electrochemical circuit and material flows from the surface of the workpiece (the anode) to the cathode. The anodic workpiece is electropolished and the cathode is electroplated. The electrolyte solution is generally acidic and careful control of the operational parameters involved (e.g., temperature, voltage, current) is critical both in terms of safety as well as achieving good results. Selection of the electrolyte composition is important; often solutions are designed to produce surfaces well suited for optical metallography through etching to delineate the grain structure. However, aggressive etching to outline boundaries can lead to surface relief, hampering the ability to get good patterns near grain boundaries and leaving gaps in the EBSD orientation maps at

Figure 25
Polished sample of an aluminium oxide–copper oxide reaction zone containing four phases with differing hardness. (a) Low magnification SE image of the tilted sample showing surface relief, (b) a higher magnification SEM image with the sample flat, (c) the EBSD phase map of the sample obtained at 70° tilt but reconstructed as if it were flat.
those boundaries. There may be preferential etching of certain phases in multiphase materials or even preferential etching due to the crystallographic orientation, leading to steps between grains. It is also important that the electrolyte does not produce a residual reaction product. All of these issues can be mitigated though good process control, and an excellent surface polish producing high-quality EBSD patterns can be achieved (Wynick & Boehlert, 2005). Good grinding of the sample surface should be performed prior to electropolishing and even a certain level of mechanical polishing can also help to achieve the optimal surface for EBSD.

7.5. Ion polishing

Broad-beam ion polishing is a viable alternative to mechanical polishing (Nowell, 2002; Erdman et al., 2006; Nowakowski et al., 2016). Modern ion polishers are generally composed of a specimen vacuum chamber, an ion gun, an optical microscope and a stage. The microscope and stage enable the sample to be positioned to polish a specific region of interest. The ion gun bombards the sample with energetic ions (typically Ar), and the ions remove layers of material at the atomic level. Reducing the angle of the beam to grazing incidence and using lower-energy electrons reduces the depth of penetration, which reduces the induced surface damage. As with electropolishing, proper preparation of the sample through grinding and mechanical polishing prior to ion polishing leads to an optimal surface for EBSD.

With the advent of SEMs coupled with focused ion beam (FIB) columns, EBSD samples can be prepared using FIB milling and polishing (Matteson et al., 2002; Michael & Kotula, 2008). FIB samples will be limited in size, although with plasma FIB milling the practical limit for size over conventional FIB is much larger. High-voltage (~30 kV) ion milling can produce a significant damage layer. To remove the damage layer induced by milling, the sample is tilted (after lift-out) to a glancing angle relative to the ion beam (~6°). The sample can then be polished by lowering the FIB voltage to within the range 2–5 kV. Just like abrasive sample preparation, the more aggressive the FIB settings, the faster material can be removed but greater damage is imparted. The exact conditions are generally material dependent.

7.6. Coating

For SEM applications, the sample must be grounded (unless a low-vacuum SEM is used). Electron charge can build up even on grounded samples, particularly when the samples are poor conductors, leading to drift of the sample under the beam. Such samples should be coated with a thin layer of a conductive material such as carbon or gold. This surface coating should be very thin (1–5 nm) and as uniform as possible. Thicker coatings may require increased voltage to obtain usable EBSD patterns. On non-conductive samples it is generally good practice to image the area to be scanned for a few minutes prior to EBSD investigation to reach a steady-state condition to minimize drift due to charging. Most drift due to charging can be eliminated by coating and proper grounding of the sample, but in cases where it is a concern working quickly can alleviate drift. Patterns do not have to be perfect but just of high enough quality for reliable indexing. It is recommended to configure the SEM and EBSD system on an area of the sample away from the intended field of view. Once the settings are optimized, then the EBSD scan can be performed on the region of interest.

7.7. In situ plasma cleaning

While not actually sample preparation, in situ plasma cleaning (Postek & Vladař, 2012) can be helpful for EBSD work. As the sample is imaged under the electron beam, the surface will undergo hydrocarbon contamination. Generally, the level of contamination is not an obstacle to EBSD work, but there are instances where it can be a problem. In situ plasma cleaning can remove the contamination so that pristine surfaces can be imaged.

8. Software

8.1. Free software

There are several EBSD-relevant software packages available; the most notable of these are listed below. Unless noted, these tend to be platform-independent software packages.

* **Dream.3D** is a software package designed to reconstruct three-dimensional microstructures from two-dimensional serial section EBSD data. It has many contributors and is managed by BlueQuartz software (http://dream3d.bluequartz.net).

* **MTEx** is a MATLAB toolbox for analysing and modelling crystallographic textures by means of EBSD or pole-figure data. It is managed by Ralf Hielscher at the Institute of Mathematics, TU Chemnitz, Germany (https://mtex-toolbox.github.io).

* **EMsoft** is an open-source package for the simulation of electron microscopy – both imaging and diffraction. The library has core routines for crystallography, symmetry, dynamical scattering, Monte Carlo simulations and others. The package is managed by Marc De Graef at Carnegie Mellon University (https://github.com/EMsoft-org/EMsoft).

* **OpenXY** is a MATLAB-based tool for performing cross-correlation analysis of EBSD patterns using both experimental and simulated patterns. This software package is managed by David Fullwood at Brigham Young University (https://github.com/ BYU-MicrostructureOfMaterials/OpenXY).

* **ATEX** is a set of analysis tools for both electron and X-ray diffraction. The software is Windows-based and developed and managed by Jean-Jacques Fundenberger and Benoit Beausir at the University of Lorraine in France (http://www.atex-software.eu).

* **Merengue2** is software designed for the reconstruction of parent grains from the daughter variants after a phase transformation. The software is the product of Lionel Germain at the University of Lorraine in France (http://lionelgermain.free.fr/merengue2.htm).
AstroEBSD is a set of MATLAB-based tools for indexing EBSD patterns. The software is managed by Ben Britton’s research group at Imperial College London in the UK (https://github.com/benjaminbritton/AstroEBSD).

STABiX is a MATLAB toolbox for analysing slip transmission through grain boundaries (Mercier et al., 2015). The software can import EBSD data in a wide variety of formats (https://stabix.readthedocs.org).

The Berkeley Texture Package BEARTEX provides a set of Windows-based programs for analysing preferred orientation in polycrystals. It can be used to process neutron, synchrotron X-ray and electron diffraction data and is managed by Hans-Rudolf Wenk at the University of California Berkeley Texture Laboratory (https://eps.berkeley.edu/~wenk/TexturePage/beartex.htm).

There are several other freeware packages that have been available in the past but are no longer supported or have been folded into some of the packages in the list above or even into the commercial packages listed in the following section. A search of GitHub for ‘EBSD’ will result in a variety of EBSD-related projects, generally with very specialized functionality.

8.2. Commercial software

The commercialization of EBSD technology began with David Dingley at the University of Bristol; he created a company (DingleSoft) to commercialize his EBSD hardware and software named COS. The core of this was implemented into a commercial product named EBSD and sold through Link Analytical (now Oxford Instruments) in 1986. In 1990, Niels-Henrik Schmidt founded HKL to sell EBSD systems. TexSEM Laboratories (TSL) was founded in 1994 by Dingley and Brent Adams, whose research team developed the first fully automated EBSD system, which they named Orientation Imaging Microscopy or OIM. DingleSoft was folded into TSL, but the sale of automated systems quickly supplanted the manual systems. Other commercial EBSD ventures include Jarle Hjelen at the Norwegian University of Science and Technology, who focused on the NORDIF series of EBSD cameras, and Robert Schwarzer, formerly of the Technical University of Clausthal, who focused on software (ACOM). Some of Joe Michael’s phase-identification work at Sandia National Laboratory formed the basis of a system sold through Noran named PhaseID and then later Schwarzer’s ACOM software (Dingley, 2020; Maitland & Sitzman, 2006; Camus, 2020).

Currently, there are four commercial vendors of EBSD systems selling both hardware and software. The software capabilities include control of the EBSD detector unit, integration with the control software for the SEM, a pattern indexing engine, and data processing and visualization. Some of the early suppliers of EBSD technology were acquired by established microanalysis companies. These are noted below to avoid confusion with past vendors.

EDAX is a business unit of the Material Analysis Division of Ametek. In 1999 EDAX acquired TexSEM Laboratories (or TSL). Ametek acquired EDAX in 2001 (https://www.edax.com/).

As noted, Oxford Instruments has been involved with EBSD since the early manual systems. Oxford acquired HKL Technology A/S in 2005 (https://www.oxinst.com/).

Bruker entered the EBSD market in 2008 (https://www.bruker.com/).

Thermo Fisher Scientific’s roots in EBSD are with Thermo Noran (https://www.thermofisher.com/).

Other commercial EBSD-relevant software includes: CrossCourt by BLG Vantage. CrossCourt is focused on HREBSD – the measurement of strain using cross-correlation of EBSD patterns at nearby points in the microstructure (http://www.hreb.com/wp/crosscourt/).

Labosoft’s focus is on crystallographic texture analysis via X-ray diffraction, but their software can also use individual orientation measurements as acquired by EBSD as input (http://www.labosoft.com.pl/).

9. Output forms
9.1. Data recorded

A wealth of data is collected during automated scanning. The rawest form of data for EBSD work is the EBSD pattern prior to any image processing. Patterns can be recorded directly to disk during automated scanning – this has become more common in the last decade. For indexing, some level of image processing (see Section 6.4) is performed, generally background correction and histogram normalization. Besides the pattern itself, several other forms of data are recorded at each point of the scan grid:

(i) Descriptive parameters associated with the pattern itself. Various descriptions of the pattern quality are used in the literature, the most common ones being image quality (IQ) (Wright & Nowell, 2006), band contrast (BC) and band slope (BS) (Maitland & Sitzman, 2006; Kang et al., 2013). Other metrics have been proposed (Tao & Eades, 2005; Krieger Lassen, 1994) but have not seen widespread use. The intensity of individual pixels in the pattern or sets of pixels can also be recorded (Wright, Nowell, de Kloe et al., 2015).

(ii) Data associated with indexing of the pattern, most notably the crystallographic orientation, but also various parameters providing an indication of the reliability of the indexing solution (see Section 6.3.3).

(iii) Data collected simultaneously from other detectors. For example, intensities from the SE detector, intensities from a BSE and/or forward-scatter electron detectors, spectra or simply counts within specific energy ranges from an XEDS detector.

Such data can be statistically analysed and correlated. The data can be used: (1) as raw numerical data in file formats that can be ported to various other software for analysis; (2) to generate plots in graphical representation, such as pole figures and inverse pole figures. In addition, since the data are recorded at each point in the scan grid, microstructural visualizations can be reconstructed from the data by assigning...
9.2. Numerical data

9.2.1. .ang file format. The .ang file format has been in use since the very first automated systems and is the text export format used by EDAX EBSD systems. It has been extended since, but the core elements have remained the same. The basic format is that the first few lines are header lines with various information. These lines all begin with the # character. The header can contain any information, but there are some standard pieces of information exported by the EDAX systems that can be important, in particular crystallographic phase information. After the header lines, each row corresponds to a point in the scanning grid and contains at least the following columns:

1. Euler angle $\varphi_1$ in radians;
2. Euler angle $\Phi$ in radians;
3. Euler angle $\varphi_2$ in radians;
4. $x$ coordinate in microns;
5. $y$ coordinate in microns; and

Newer versions may also contain the following additional columns (see EDAX’s documentation for specifics):

7. confidence index (CI): a value of $-1$ indicates an unindexed point, $-2$ indicates a skipped point;
8. phase index: an integer identifying the phase, 0 for single-phase scans, 1, . . . , n for multiphase scans;
9. detector intensity: generally from the SE detector but depends on how the system was configured at the time of data collection;
10. fit: mean angular deviation between the detected location of the bands in the pattern relative to their location as prescribed by the Euler angles (in degrees);
11. PRIAS values: integrated intensities from a small rectangle at the top of the detector, a square at the middle of the detector and/or a rectangle at the bottom of the detector (Wright, Nowell, de Kloe et al., 2015); and
12. EDS data: counts on the EDS detector at specified energy ranges.

9.2.2. .ctf file format. The .ctf or ‘channel text file’ is the text export format used by Oxford EBSD systems; it also has a header with a specific format. Those interested in such information should contact Oxford for assistance. After the header, each row corresponds to a point in the scanning grid and contains at least the following columns:

1. phase: an integer identifying the phase, where zero indicates an unindexed point;
2. $x$ coordinate in microns;
3. $y$ coordinate in microns;
4. bands: the number of bands used in indexing;
5. error: zero indicates a well indexed point;
6. Euler angle $\varphi_1$ in degrees;
7. Euler angle $\Phi$ in degrees;
8. Euler angle $\varphi_2$ in degrees;
9. mean angular deviation (MSD) in degrees;
10. band contrast: a measure of pattern quality; and

9.2.3. HDF5 file format. In recent years, EBSD vendors have started to support the open-source Hierarchical Data Format, commonly known as HDF5 (The HDF Group, 1997–2020). This file format allows for the user to create an internal file layout that resembles a computer file system, with data sets (files) and groups (folders) as well as attributes for each component. HDF5 libraries are available for all major computer languages as well as several data-processing packages, including MATLAB (MATLAB, 2019) and the Interactive Data Language (L3Harris Geospatial, 2020). There is generally no need to provide a detailed description of the internal file structure for any given application since the format is user-discoverable, i.e., there are several tools available, both via the command line ($h5dump$) and using a graphical user interface ($HDFView$), to inspect the file structure. Thus, users can import EBSD data directly from HDF5 files for various post-processing applications, including whole-pattern indexing. The HDF5 format also provides an easy path to data sharing between user groups, since no proprietary vendor software is needed to access the data.

9.3. Orientation plots

There are several ways to graphically represent crystallographic orientation data (Kocks et al., 1998). One approach is a pole figure, which shows the orientation of a selected plane normal (pole) with respect to the sample reference frame. Imagine a unit sphere surrounding a crystal; the pole will intersect the circumference of the sphere at a specific location. There are a few different ways in which this location in three-dimensional space can be projected onto a two-dimensional plane. Fig. 26 shows the stereographic projection, and Fig. 27 shows two pole figures for a hexagonal crystal, the [0001] and
The poles marked by solid circles appear in the upper hemisphere and those marked by open circles appear in the lower hemisphere. Metallurgists tend to show the pole in the upper hemisphere, whereas geologists have a preference for the lower hemisphere (‘into the ground’). Note that there are two markers for the {0001} pole and three for the {10T0} pole. This is reflective of the symmetry of the hexagonal crystal: (0001) and its inverse (000T) for the basal poles and (10T0), (1T00), (01T0) and their their inverses for the prismatic poles.

The inverse pole figure is complementary to the pole figure. While pole figures show the orientation of a selected pole with respect to the sample reference frame, an inverse pole figure shows the orientation of a selected sample direction with respect to the crystal reference frame. Fig. 28 shows an example for three different orientations of a cubic crystal for two different sample directions – one aligned with the sample normal and the other with the ‘1’ direction. It may be more intuitive to think of inverse pole figures as showing which crystal directions are aligned with a specific sample direction (most commonly the sample normal). Because of crystal symmetry, it is not necessary to show the full circle as is done for pole figures. Only an asymmetric portion of the circle is needed.

Pole figures and inverse pole figures are useful representations of orientation, but they provide only a partial description of orientation. Consider the (0001) pole figure shown in Fig. 27; while the pole figure prescribes the orientation of the (0001) pole, the rotation of the crystal about the (0001) pole remains unknown. A second pole figure, e.g., (1010), is needed to completely describe the orientation. The same is true for an inverse pole figure. When the orientations of many crystallites are displayed in a PF or IPF, it becomes impossible to ascertain the full three-dimensional orientation of each crystallite, and other plotting schemes are needed. One approach involves sections (or essentially bins) through a three-dimensional space according to a specific representation of crystallographic orientation, for example, the space described by Euler angles or one described by Rodrigues vectors. Once again, owing to the inherent crystal symmetry, the full orientation space need not be considered but only the fundamental zone. Fig. 29 shows 49 000 discrete orientations from rolled copper in Euler space, Rodrigues space and in a (111) pole figure and a normal direction inverse pole figure.

As with orientations, it is useful to plot misorientations both in terms of individual discrete misorientations or as distributions in sections (or bins) through a three-dimensional misorientation space. Fig. 30 shows examples in both axis–angle and Rodrigues vector space for a distribution of misorientations obtained from a copper thin-film sample. The highest peak in the misorientation distribution is at a 60° rotation about the (111) axis due to the prevalence of recrystallization twins in this material. The shaded portions in these plots are outside the fundamental zones for misorientation for cubic symmetry.

9.4. Mapping

Mapping is an integral part of EBSD analysis; in general, some parameter associated with a point in the scan data is assigned a colour through some kind of systematic coding scheme. There are a myriad of ways in which this can be accomplished. To simplify the description, we will group the maps into two types: (1) orientation based and (2) non-orientation scalar based. In addition, a subsection on boundaries in maps will also be included. Recall that maps are reconstructed from EBSD data collected at individual points in regular scan grids. Often, the term pixel is used as a synonym for these grid points. However, the pixels in a bitmap do not have a one-to-one relationship with the grid points, in particular when a hexagonal grid is used for scanning. It is not uncommon for two different parameters to be mapped in the same image. One common example is to map the orientation in colour, such as the inverse pole figure (IPF) map, and the
pattern quality in a grey-scale map. The colour map is overlaid on the grey-scale map creating an image where the orientation and the pattern quality can be linked together.

**9.4.1. Orientation maps.** As EBSD provides point-specific crystallographic orientation data, the ability to visualize such data provides unique information about microstructures. Often, the first map made after collecting the data is an inverse pole figure (IPF) map in the normal direction. In this map, each point is coloured according to the crystal direction parallel to the sample normal. The colour scheme is that given by a so-called ‘colour triangle’. However, this is a very loose description as the shape of the colour coding diagram is a function of crystal symmetry and will only approximate a triangle for selected symmetries. Since the inception of EBSD colour mapping various colour mapping schemes have been proposed, each with their own advantages and disadvantages (Nolze & Hielscher, 2016). As an IPF map only shows the crystal direction aligned with a selected sample direction, a IPF map provides no information on alignment within the plane normal to the selected sample direction. One way to resolve this ambiguity is to use a second IPF map in a direction normal to the first sample direction. Other approaches use colouring schemes based on Euler angle space, Rodrigues vector space or other parametrizations of orientation. These come with their own sets of advantages and disadvantages as well. An example of an IPF map is shown in Fig. 31(a) for a

![Figure 29](image-url)

**Figure 29**
Orientations measured on rolled copper. (a) Sections through Euler angle space. (b) Sections through Rodrigues vector space. (c) 111 pole figure: RD indicates rolling direction and TD indicates transverse direction. (d) Normal-direction inverse pole figure.
copper thin film. In this example, the majority of the material has a (111) pole aligned with the sample normal, as can be observed in the accompanying (111) pole figure.

As EBSD provides quantitative measurements of orientation, it is helpful to use colour mappings of orientation to reflect the quantitative nature of the orientation data. The alignment of the (111) crystal axes with the sample normal can be shown by assigning a colour based on the deviation of the (111) axes from the normal direction, as shown in Fig. 31(b). Note that only the rotation about the (111) axis is considered, not the full orientation.

Fig. 31(c) shows a map where points within 15° of two specific orientations are coloured according to their angular distance from the two reference orientations. This is very helpful in texture component analysis (see Section 10.1.3). In doing such analysis for multiple reference orientations (or texture components), two components may overlap in orientation space when large tolerances are used for the deviations. In this case, a measurement point could belong to multiple components or the analysis could be performed so that a measurement point will belong to only one component, i.e., the closest (in orientation space) component (Kang et al., 2008).

Property maps. Other maps can be derived from orientations, for instance property maps for the fourth-rank elastic stiffness tensor, $C_{ijkl}$. Hooke’s law states that the strain is proportional to the applied stress, which can be written in tensor form as

$$\varepsilon = C_{ijkl}\varepsilon_{kl}. \quad (71)$$

If the single-crystal elastic constants are known, then, for a given orientation, the stiffness tensor can be brought into coincidence with the sample axes by rotating the single-crystal stiffness tensor as follows:

$$C_{ijkl}' = g_{ip}g_{jq}g_{kr}g_{lt}C_{pqr}. \quad (72)$$

where $g_{ij}$ is the orientation in matrix form and $^T$ denotes the transpose. Using this approach a component of the elastic stiffness tensor or some derivative quantity can be mapped; this can be applied to any material property that can be expressed as a tensor.

Taylor-factor and Schmid-factor maps (Birosca et al., 2014; Telang et al., 2016; Jiang et al., 2015; Cicaleò et al., 2002; Livescu et al., 2015) can also be generated based on the point orientations. These two factors predict the propensity for a material’s grains to slip based on their crystallographic orientations, the characteristic slip system (slip plane and direction of slip) and the imposed strain gradient. The Schmid factor is a geometrical factor based on the direction of the principal stress with respect to a given slip plane and direction. The Taylor factor is similar to the Schmid factor but takes into account slip on multiple systems (Kocks et al., 1998).

Local orientation variation maps. Another series of maps focuses on local variations in orientations instead of the orientations themselves. Such maps provide an indication of plastic strain within the microstructure (Wright et al., 2011). These maps can be point-based or grain-based. For brevity, we review only three of the most common map types.

The first is the kernel average misorientation (KAM), which is a point-based metric. For a given point, $i$, in the scan, the KAM is given by

$$\text{KAM}(i) = \frac{1}{N} \sum_{n=1}^{N} \omega_n, \quad (73)$$

where $N$ is the number of neighbouring pixels (6 for orientations collected on a hexagonal grid and 4 or 8 for data collected on a square grid) and $\omega_n$ is the misorientation angle between the point $i$ and its neighbours. This methodology can be extended to larger kernels; for example, a second-order kernel would include the next-nearest neighbours. For a KAM map, a colour is assigned to each pixel based on its KAM value. One often adds an additional criterion to the KAM calculation, namely that when the misorientation angle exceeds some tolerance value, this misorientation angle is excluded from the averaging calculation.

The grain orientation spread (GOS) is a grain-based metric and is given by

$$\text{GOS}(j) = \frac{1}{N(j)} \sum_{n=1}^{N(j)} \omega_n, \quad (74)$$

where $N(j)$ is the number of pixels in grain $j$ and $\omega_n$ is the misorientation angle between the average orientation of grain $j$ and each of its constituent pixels. For a GOS map, a GOS...
value is calculated for each grain, thus all the pixels in a grain will be assigned the same colour. KAM and GOS have been compared in several deformation studies (Allain-Bonasso et al., 2012; Cruz-Gandarilla et al., 2016).

These two ideas are coupled to generate a grain reference orientation deviation (GROD) map. The reference orientation is typically the average orientation for a grain. This is a point-based map, where the GROD value at point $i$ in the scan grid is given by

$$\text{GROD}(i) = \omega(i, \bar{g}(i)).$$  \hspace{1cm}(75)$$

where the function $\omega(i, \bar{g}(i))$ denotes the misorientation between the orientation at point $i$ and the average orientation of the grain to which point $i$ belongs. This map then shows the deviation within the grain with respect to the average orientation of the grain. Different reference orientations for each grain can be used (Wright et al., 2016).

An example of these three metrics for a low-carbon steel sample strained uniaxially in situ to 10% is shown in Fig. 32; the data have been post-processed to remove rogue points (0.6% of the orientations were modified using grain dilation) (Wright, 2006).

In the last decade, high-resolution EBSD (HREBSD) has been playing a more significant role in EBSD-based deformation studies (Wilkinson & Dingley, 1991; Wilkinson & Britton, 2012). Instead of indexing a pair of patterns and calculating the misorientation between the two measured orientations, HREBSD uses cross-correlation between the
two patterns directly to calculate the misorientation, leading to much higher angular resolution. This technique can be used to estimate a displacement gradient tensor from which the elastic and inelastic strain tensors can be derived. Maps can be generated from individual components of these tensors. Both standard EBSD and HREBSD are used to characterize the density of geometrically necessary dislocations.

**Boundaries.** Since the orientation at each point on the grid is known, it is possible to reconstruct the boundary network from the orientation measurements. The boundaries can be coloured according to the misorientation angle or misorientation axis, or both together (Patala et al., 2012). Fig. 33 shows an example for an aluminium thin film where the boundaries are overlaid on a grey-scale map generated from the secondary-electron detector intensity. Early studies of grain boundaries using EBSD focused primarily on the misorientation angle (Goyal et al., 1997) or coincident-site-lattice (CSL) boundaries (Lin et al., 1995). CSL boundaries are boundaries where a specific fraction of atoms at the boundaries are shared between the neighbouring grains and as such special properties are attributed to CSL boundaries (Thaveeprungsi & Was, 1997; Randle & Brown, 1989; Lehockey et al., 2004; Schuh et al., 2003). More recently, the importance of the role of the grain boundary plane has been recognized (Adams, 1986; Field & Adams, 1993; Davies & Randle, 2001; Rohrer, 2011).

9.4.2. Scalar maps. Maps can be generated from non-orientation parameters, or at least parameters indirectly related to orientation; the most common of these are metrics describing pattern quality. The pattern quality is affected by many different things: phase (atomic density), strain, grain boundaries, cracks, voids and even orientation. Pattern quality can be defined in multiple ways (Section 9.1), but in general it is a measure of pattern contrast and sharpness. If the electron beam interaction volume contains a distorted lattice, then the pattern quality is diminished; strained areas will thus tend to

![Figure 32](image1.png)

**Figure 32**
Maps from a 10% uniaxially strained low-carbon steel. The tensile direction is horizontal. (a) IPF, (b) KAM, (c) GOS and (d) GROD.

![Figure 33](image2.png)

**Figure 33**
Secondary-electron image map from an aluminium thin film overlaid with boundaries coloured by (a) misorientation angle, (b) misorientation axis and (c) a colouring scheme based on both the misorientation angle and axis.
produce lower-quality patterns than recrystallized areas where the lattice contained in the interaction volume is pristine. In the immediate vicinity of a grain boundary the interaction volume will contain two crystal lattices and will thus produce poor-quality patterns. Many of these effects can be observed in the pattern quality map shown in Fig. 34. Scratches from sample preparation can be observed in a soft phase, phases are evident in terms of general intensity, cracks and voids are visible, grain boundaries are clearly delineated and even orientation contrast can be observed in the grain-to-grain grey-level differences of Fig. 34. The fine grains appear dark because they are near the spatial resolution limit – in effect, a high density of mixed orientation interaction volumes.

Metrics derived directly from the patterns themselves can be mapped. Generally, the idea is to construct a virtual dark-field image from the patterns recorded at each point in the scan. A virtual aperture can be prescribed on the EBSD field image from the patterns recorded at each point in the domain where the orientation of the crystal lattice is the same and (c) background correction of the patterns was performed, whereas in (b) it was not. The primary contrast mechanism for the three maps in Fig. 35 is (a) topographic, (b) phase and (c) orientation.

10. Selected applications

If one were to survey the scientific literature for materials-science papers published in the early 1990’s where EBSD was used, one would obtain a listing of just a few papers; in these early papers, ‘EBSD’ nearly always appeared in the title of the paper. As EBSD has matured, the term ‘EBSD’ has moved from the title to the abstract and is now usually hidden within the body of the paper. A search for ‘EBSD’ in one of the journal paper search engines will now result in a listing containing thousands of entries over a very wide array of topics. Several books have appeared reviewing EBSD and its applications (Schwartz et al., 2000, 2009; Brissett, 2015). As the underlying crystallography affects the evolution of microstructure in nearly every process (deformation, recrystallization, solidification and so on) as well as the behaviour (i.e., anisotropy), EBSD has and is being used to better understand the evolution of microstructure as well as to better predict the performance of a component in use. For example, with the advent of additive manufacturing (AM), EBSD has been shown to be a useful tool for understanding how the processing conditions inform the highly oriented microstructures obtained in additive manufactured materials (Seifi et al., 2016). AM holds promise for generating microstructures specifically tailored to optimize performance of components in engineering applications. EBSD has enabled the development of microstructure design to find processing paths to reach a desired microstructure (Adams et al., 2012; Fullwood et al., 2010). Rather than review the full gamut of materials applications of EBSD or even focus on a few particular applications, we focus on a few of the analyses that are often performed.

10.1. Texture analysis

10.1.1. Introduction. Polycrystalline materials are typically composed of many grains. A grain (in most cases) describes a domain where the orientation of the crystal lattice is the same or at least very nearly the same. A grain boundary is then an interface between two crystal lattices of different orientation. If a polycrystal is composed of grains with very similar orientations, then the material is considered textured. The term ‘texture’ is used to describe the statistical distribution of grain orientations within a polycrystalline material. The metallurgical community uses the terms ‘crystallographic texture’, ‘orientation texture’ or simply ‘texture’, whereas the geological community employs the terms ‘lattice preferred orientation’ (LPO) or ‘fabric’.

Why does texture matter? Many properties of materials vary with direction, that is they are anisotropic. The anisotropy will be most evident in a single crystal. If a polycrystal is composed of similarly oriented grains (in terms of lattice orientation not grain shape, i.e., not elongated grains aligned along an axis), then the properties of the polycrystal would mimic the inherent anisotropy of the single crystal. Conversely, if the polycrystal lacks any texture (also referred to as having a ‘random’ texture) then the properties of the polycrystal would not reflect the anisotropy of the constituent crystals, but would be isotropic (i.e., the properties would not vary with direction, at least for low-rank tensors). Real polycrystals vary between these two extremes depending on the processes used to form the material. For mechanical proces-
material processing, deformation is imparted into the material during forming. As materials deform, orientation gradients can arise within individual grains, and grains can even fragment into subgrains. The variation in orientation within grains can be so severe in heavily deformed materials that it may be difficult to define the grains. The distribution of orientations within a grain is sometimes labeled ‘microtexture’.

As nearly all materials-forming processes produce textured materials, the characterization of texture is an important element to understanding the relationship between microstructure and properties as well as the evolution of microstructure during processing. There are several good texts that delve into texture analysis in detail (Bunge, 1982; Kocks et al., 1998; Field, 2004; Wright & Hielscher, 2016; Chateigner et al., 2019). EBSD is well suited for characterizing texture as well as microtexture. Texture analysis was established by the measurement of pole figures using X-ray diffraction. While standard X-ray diffraction techniques can inform us that a measurement of pole figures using X-ray diffraction. While standard X-ray diffraction techniques can inform us that a large fraction of the grains in the material have a preferred orientation, they are unable to pinpoint which grains have that orientation and how they are arranged spatially in the microstructure. EBSD enables the correlation of crystallographic orientation with specific features in the microstructure.

### 10.1.2. Orientation distribution function (ODF)

The basis of texture analysis is the orientation distribution function or ODF. The ODF is a probability density function describing the probability that a grain with an orientation, \( g \), is present in the volume of the sample. The ODF can be used to estimate the fraction of material of a given orientation through the following integral relationship:

\[
\frac{V_{(g_0 + \Delta g)}}{V} = \int_{f(g_0 + \Delta g)} f(g) \, dg. \quad (76)
\]

The quantity on the left is the volume fraction of material oriented within \( \Delta g \) of \( g \) and the function \( f(g) \) is the ODF. The following normalization condition must hold:

\[
\int f(g) \, dg = 1. \quad (77)
\]

An ODF value of 3 for a specific orientation means that grains of such an orientation are three times more likely than expected for a polycrystal with a random distribution of orientations. An ODF may be represented as a sum of generalized spherical harmonics \( T_{\ell}^{m}(g) \) weighted by coefficients as follows:

\[
f(g) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} C_{\ell m}^{n m} T_{\ell}^{m n}(g). \quad (78)
\]

The \( C_{\ell m}^{n m} \) coefficients contain the texture information. Carrying out the numerical summations is computationally intensive and is generally performed only up to a maximum rank of \( \ell = 34 \). However, recent algorithms, which make use of fast Fourier techniques, allow for the rapid evaluation of the series expansion up to \( \ell = 200 \), reducing truncation errors (Potts et al., 2009; Kalidindi et al., 2009).

A pole figure can be derived through integration of the ODF along a specific path in orientation space:

\[
P_{\text{h}}(y) = \frac{1}{2\pi} \int_{h||y} f(g) \, d\chi, \quad (79)
\]

where \( P_{\text{h}}(y) \) is the pole figure, \( h \) represents the pole of interest, \((hkl)\), and \( y \) is a vector in the sample reference frame. The integration is carried out along the path, \( \chi \), where \( h \) and \( y \) are coincident. Given equation (78), a pole figure can be calculated using symmetric spherical surface harmonics \( (k\eta(y)) \) in the following form:

\[
P_{\text{h}}(y) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} C_{\ell}^{m n} k_{\ell}^{m n}(h)k_{\ell}^{n n}(y). \quad (80)
\]

The objective of texture analysis is to process the individual orientation measurements to determine the ODF. Consider, for a moment, that orientations are one-dimensional quantities and can be displayed on a number line as shown schematically in Fig. 36. A histogram can be constructed by allocating a set of bins between the endpoint of the line and the number of orientations in each bin counted as shown. A curve can then be fit to the histogram. It would be equally valid to describe the distribution using other curves, as shown in Fig. 37 using larger or smaller bins. The choice of bin size will depend on the property being studied. For example, a smoother curve would be appropriate for elastic anisotropy, whereas piezoelectricity is more

![Figure 36](image)

**Figure 36**

A schematic of the calculation of the ODF from individual orientation measurements.

![Figure 37](image)

**Figure 37**

Schematic showing lower- (dotted line) and higher-order (grey line) descriptions of the simplified texture in Fig. 36.
dependent on the details in the texture and would thus be better served by an intermediate curve. This conceptual binning approach can be extended to three dimensions and applied to EBSD data. However, to calculate the $C_{\ell m}'$ coefficients used in equation (78) requires the following formulation:

$$C_{\ell m}' = \frac{2 \ell + 1}{N} \sum_{i=1}^{N} K_{\ell} T_{\ell m}'(g_{i}),$$  \hspace{1cm} (81)

where $g_{i}$ represents one orientation from a set of $N$ individual orientation measurements. If the orientations are measured grain-by-grain as opposed to point-by-point on a regular sampling grid, then a weighting factor proportional to the grain area (or ideally the volume) must also be introduced. $K_{\ell}$ is a smoothing factor:

$$K_{\ell} = \exp(-\ell^2 \omega^2/4) - \exp(-(\ell + 1)^2 \omega^2/4) - \exp(-\omega^2/4).$$  \hspace{1cm} (82)

$\omega$ is the Gaussian half width. The choice of the degree of smoothing is somewhat arbitrary. Generally, it is assumed that a sharper texture requires less smoothing (a smaller Gaussian, $\sim 1$–$2^\circ$), whereas larger values ($\sim 5$–$10^\circ$) are suggested for more random distributions. Other studies suggest that the more orientations measured the smaller the Gaussian should be (Wagner et al., 1981). Early comparisons between X-ray data and EBSD data suggested a value of 7.5$^\circ$; however, with the increased speed in modern EBSD systems, larger data sets are being measured and therefore values of the order of 0.1$^\circ$ are now more appropriate.

When estimating the ODF from individual measurements it is important that enough measurements are collected to ensure statistical reliability (Hielscher, 2013; Wright et al., 2007). Note that it is the number of grain orientations sampled that is the key criterion for statistical reliability and not just the number of orientations measured.

10.1.3. Examples. In some materials like thin films, the texture occurs by the alignment of a particular crystallographic axis with the sample normal but without any in-plane crystallographic alignment. Fig. 38 shows a (111) pole figure for an aluminium thin film that exhibits such a texture. The sharp peak at the centre of the texture correlates to (111)
poles aligned with the normal direction. The outer ring is due to symmetry-equivalent (111) poles; if a cubic crystal has a (111) pole aligned with the sample normal then there must be three other (111) poles 70.5° away from the pattern normal. The fact that these equivalent poles lie in a ring denotes the lack of in-plane alignment. Some properties (such as mean time-to-failure in microelectronic devices) can be sensitive to the sharpness of the fibre texture. The ODF can be used to analyse the sharpness of the central peak, as shown in Fig. 38.

Early on, texture analysis was applied most often to rolled aluminium sheet. The texture must be well controlled in order to produce stock that is suitable for deep-drawing beverage cans. Typical (111) pole figures for aluminium sheet are shown in Fig. 39. The majority of orientations in rolled face-centred cubic materials typically lie within a ‘fibre’ in Euler space, as shown in Fig. 40. In order to simplify the analysis of this material, components associated with key locations along this fibre have been identified. Instead of tracking the entire ODF across a matrix of samples, a researcher can focus solely on the ODF intensities for just these few key components.

Texture is important in predicting anisotropic behaviour. Consider for example the Young’s modulus, which is one metric for describing elastic anisotropy. Fig. 41 shows the Young’s modulus for several different grains and an average Young’s modulus for the scan area after enforcing orthotropic sample symmetry. Using the tools of texture analysis coupled with EBSD measurements enables the Young’s modulus for the bulk material to be estimated.

10.2. Phase identification

Phase identification is an important EBSD application arena. However, it can be a difficult process to perform reliably and is thus under-utilized. With the advances in dynamic pattern simulation there is now more momentum to make this a more fruitful application for EBSD. Phase identification is a broad term that can be broken down into three different levels: (1) phase differentiation, (2) phase ID and (3) unknown determination. Phase differentiation has become routine when the phases are crystallographically distinct, whereas phase ID and unknown determination are still not widely used within the EBSD community. Phase differentiation can be used during automated collection of EBSD scan data, whereas phase ID and unknown determination require user interaction and are used on individual patterns or small sets of patterns.

10.2.1. Phase differentiation. In phase differentiation, the phases in the sample are known. The objective then is to identify which of the known phases best fits a pattern from the sample. A good example is duplex steel, which contains both ferrite [a body-centred cubic (b.c.c.) phase] and austenite [a face-centred cubic (f.c.c.) phase]. As these two phases are crystallographically distinct, it is relatively straightforward to differentiate the two phases. The process is simply to index the pattern assuming it is ferrite and then assuming it is austenite. The indexing result that best fits the pattern is then deemed

Figure 41
Texture component map overlaid on an image-quality map. The Young’s modulus at four selected points in the map as well as the average Young’s modulus for the full map area (orthotropic sample symmetry enforced) are shown.

![Texture component map overlaid on an image-quality map. The Young’s modulus at four selected points in the map as well as the average Young’s modulus for the full map area (orthotropic sample symmetry enforced) are shown.](image-url)

Figure 42
Phase differentiation example for a duplex steel containing ferrite (b.c.c.) and austenite (f.c.c.). (a,b) EBSD patterns from the steel sample, (c) pattern (a) indexed as austenite, (d) pattern (b) indexed as austenite, (e) pattern (a) indexed as ferrite, (f) pattern (b) indexed as ferrite.
the identified phase. Fig. 42 shows an example of this process for a pattern from ferrite and a pattern from austenite along with a map showing results of the phase differentiation process. The phase differentiation process is reliable when the phases are crystallographically distinct. It is also assumed that the structures are well understood, such that the reflectors associated with the most prominent bands in the pattern have been optimized for reliable indexing.

When the structures are not crystallographically distinct, the indexing process can become unreliable. Steel, once again, provides a classic example of this challenge. In steel samples composed of both ferrite (b.c.c.) and martensite [body-centred tetragonal (b.c.t.)], it is difficult to ascertain the phase associated with a pattern based solely on the indexing. Martensite is only slightly tetragonal, typically less than 2%. The degree of tetragonal distortion is a function of the amount of carbon in the crystal structure. The distortion generally amounts to only sub-pixel shifts in the EBSD pattern; thus, it is difficult to differentiate these two phases based on indexing alone. Some of the phases in steels are not crystallographic in nature and require a morphological approach for differentiation (Wilson et al., 2001; Nowell et al., 2009; Zaefferer et al., 2008; Gazder et al., 2014).

There is also the case where the phases are crystallographically similar but very different in chemical composition. Consider, for example, three f.c.c. phases: copper, nickel and iron. For a given pattern from any three of these phases it is very difficult to correctly identify the diffracting phase, since the difference between them lies not in the geometry of the bands in the pattern but rather in their width. The difference in band width is generally small, just a few pixels in a very high resolution pattern (e.g. 1024 x 1024 pixels). In addition, the Hough-transform method for band detection is not well suited for accurately detecting the band widths. Thus, it is practically impossible to differentiate these three phases from each other using conventional rapid indexing techniques. The problem is easily solved when XEDS data are collected simultaneously with the EBSD pattern. It is trivial to differentiate these three phases using the XEDS data (Nowell & Wright, 2004).

10.2.2. Phase ID. The term ‘phase ID’ generally refers to the approach when the phases contained within a sample are not known. Once again, an approach based on the goodness-of-fit of indexing is used, but, instead of differentiating between a small set of known phases, the pattern is indexed from a large set of phases such as that found in a crystallographic database (Michael, 2000; Wright, 2000), for example, the PDF4+ file from the International Centre for Diffraction Data, the Inorganic Crystal Structure Database (ICSD) from FIZ Karlsruhe or the American Mineralogist Crystal Structure Database (AMCSD). These are large databases containing thousands of phases. Attempting to index a given pattern using the crystallographic structure data for each of these phases is impractical. Thus, the first step in the phase ID process is to measure the chemistry via XEDS at the same point in the microstructure for which the EBSD pattern is obtained. The chemical signature is used to dramatically reduce the number of phases in the database to a tractable list of candidate phases. It should be noted that some elements such as hydrogen and carbon are difficult to catch using XEDS, therefore the search of the database based on chemistry should be expanded beyond the XEDS identified elements to include these XEDS ambiguous elements. Once the reduced candidate list is obtained, the same procedure as previously outlined for phase differentiation (Section 10.2.1) can be applied. The basic premise behind indexing is to correlate the bands in the pattern with planes in the crystal lattice. Thus, some knowledge of the crystal structure is required; namely, the point-group symmetry, the lattice parameters and the Miller indices of the strongest diffracting planes. In the large databases cited, this information is typically obtained using X-ray powder diffraction. The highest-ranking planes (i.e. by X-ray intensity) do not always match the intensity ranking of visually observed bands in EBSD patterns. This discrepancy is simply due to differences in the scattering between X-rays and electrons. When the atom positions are known, a better correlation with the observed EBSD band intensities can be obtained via a kinematical calculation of structure factors for the atomic planes (Krieger Lassen, 1994). In some structures, the kinematical model does not accurately describe the interaction between the electron beam and the crystal structure. In these instances, the calculated scattering factors do not correlate well with the observed EBSD band intensities, and an operator will need to manually optimize the selection of reflectors in order to achieve reliable indexing of the diffraction patterns. This is typically an iterative process with the X-ray intensities or the calculated structure factors providing a starting point. This can be a difficult process requiring both a thorough understanding of the parameters associated with the band detection (i.e., the Hough transform, Section 6.3) as well as the underlying crystallography of the phase being investigated. For these reasons, the phase ID process is not nearly as simple as the phase differentiation process, where the reflector optimization has already been performed. Recent progress in reflector optimization using dynamic simulation of EBSD patterns (Wright et al., 2019) has been achieved, which may alleviate some of the challenges associated with the phase ID process, but these calculations are computationally intensive and, as of yet, the phase ID process remains limited in application. Alternative approaches to the phase ID process based on unit-cell volumes have been proposed but have been only limited application (Michael, 2000; Michael & Goehner, 1999).

10.2.3. Unknown determination. The third level of phase identification is the case where the phase ID process described previously fails. This may be due to a failure in the identification process, i.e., the indexing, or may simply be due to the phase of interest not being present in the databases. In this case, the challenge is to determine the crystal structure directly from the pattern itself. A few ab initio procedures have been proposed (Dingley & Wright, 2009; Li & Han, 2015; Kaufmann et al., 2019), but their use has not yet gained any traction outside their individual research groups.
10.3. Grain analysis

In an optical or SEM micrograph, a grain is commonly understood as a domain of pixels with similar intensities surrounded by a boundary usually of darker intensity. In EBSD data, a grain is usually defined as a domain of scan points having similar crystallographic orientation. For each point in an EBSD scan data set, each neighbouring point is checked to see if the difference in orientation is within a tolerance angle. If this criterion is met, then the two points are assumed to belong to the same grain. Fig. 43 shows an example for data collected on a hexagonal grid; for data collected on a square grid, the decision must also be made whether or not points on the diagonal are considered as neighbours. Using this approach, the point-to-point misorientation in a grain will be quite small, but the spread of orientation among all points in the grain could be relatively large. Another governing parameter that can be used in defining grains is the minimum number of points needed to define these domains of similarly oriented points as a grain; in this way, rogue points (i.e., mis-indexed or non-indexed) points can be excluded from any grain analysis.

The grains can be analysed in various ways to study size (Day & Quested, 1999; Humphreys, 1999; Bowles et al., 2004; Gao et al., 2005; Mingard et al., 2009; Wright, 2010) and shape, and correlate such features with crystallographic orientation. However, as in conventional metallography, it is important to remember that grains are three-dimensional and that a cross section of a grain is observed when measured on a plane. The tilt of the EBSD measurement plane must be well known, as any uncertainty relative to the tilt can have large impacts on measurements of grain size and shape (Nolze, 2007).

10.4. Strain

Characterizing strain in crystalline materials is one of the most common application areas of EBSD. Strain is not only important in and of itself, but is also a critical element in studies of recrystallization (nucleation), grain growth and phase transformations, as the distribution of localized strain in the microstructure is often the driving force behind these phenomena.

Elastic and plastic strain present themselves differently in EBSD patterns. Elastic strain is generally associated with a distortion of the lattice, which produces subtle shifts of the locations of the zone axes within the EBSD patterns. These shifts are typically of the order of sub-pixels even in high-resolution EBSD patterns. In unconstrained single crystals, plastic deformation via slip produces no change in crystal orientation; however, constraining the deformation requires that slip be accompanied by local changes in lattice orientation to realize the imposed deformation (Dieter & Bacon, 1976; Jiang et al., 2016). In polycrystals, regardless of whether the deformation is constrained externally, the local deformation is constrained by surrounding grains and thus plastic strain generally results in a rotation of the crystal lattice. The lattice rotations cause small movements of the bands in the EBSD pattern relative to a pattern from the pristine pre-deformation state. Within an individual grain, the orientation change can create significant orientation gradients. Thus, point-to-point measurements of orientation within the grain can provide information on strain within the crystal. For elastic deformation and a small degree of plastic deformation, the effect on the patterns is too small to reliably measure using standard Hough-based indexing approaches. A branch of EBSD analysis known as high-resolution EBSD or HREBSD has...
been developed to measure the subtle changes in the patterns (Wilkinson & Britton, 2012); ‘high resolution’ indicates high angular resolution and should not be confused with high spatial resolution.

HREBSD uses cross-correlation techniques to compare patterns; Fig. 44 shows a schematic of the process. A pattern from a non-strained point in the material is compared with a pattern from a strained point. The comparison uses many regions of interest (ROIs) – typically many more overlapping ROIs than shown in the figure. Pairs of ROIs are compared with each other using fast-Fourier-transform-based cross correlation and a displacement vector is fitted to each ROI pair (note these vectors are often less than a pixel in length and not drawn to scale in the schematic). The vectors are then combined together to determine a displacement gradient tensor. The displacement gradient tensor can be decomposed into its symmetric and antisymmetric parts; the symmetric part is the elastic strain tensor and the antisymmetric part describes the rotations associated with plastic flow in the material:

$$e_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$  \hspace{1cm} (83)$$

and

$$\omega_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right).$$  \hspace{1cm} (84)$$

It should be noted that the patterns for HREBSD must be of high quality, both in terms of the signal-to-noise ratio and also the number of pixels in the pattern. Thus, pattern-acquisition times are typically much longer than those needed for basic orientation mapping. In addition, post-processing is also relatively computationally intensive. Both a high band pass and low band pass filter are applied to the patterns prior to processing. Other methodologies based on digital image correlation have also been applied to extract strain information from the patterns (Vermeij & Hoefnagels, 2018).

For the plastic strain measurement, patterns from two points in the microstructure can be compared to determine the plastic strain gradient between the two locations. Using neighbouring points in the microstructure in both the vertical and horizontal direction allows for the geometrically necessary dislocation (GND) density to be determined (Pantleon, 2008; Wilkinson & Randman, 2010; Field et al., 2012). Geometrically necessary dislocations are the dislocations needed to accommodate the lattice rotation from one point to another in the microstructure. It should be noted that the GND density only describes the dislocation density associated with the measured rotations. It does not capture the full dislocation density, as the material will also contain accumulated dislocations that do not contribute to the measured rotations (e.g., opposite dislocation pairs will cancel each other’s rotations). Such dislocations are referred to as statistically stored dislocations. This approach to measuring dislocation density is very sensitive to the distance between the pairs of points from which the EBSD patterns are obtained (Field et al., 2012).

For the elastic strain measurements, a non-strained reference pattern is needed. With the advent of dynamic pattern simulation, approaches for using a simulated reference pattern are being explored to alleviate this difficulty (Tanaka & Wilkinson, 2019; Jackson et al., 2016).

The cross-correlation approach can be used to precisely characterize the strain (both elastic and plastic) in crystalline materials based on EBSD patterns. Conventional EBSD measurements of crystallographic orientation can also be used to characterize the strain (Wright et al., 2011). In this case, the full strain tensor is not measured, but rather the focus is on the magnitude of the local misorientations within the microstructure, i.e., the orientation variation within grains as previously described in Section 9.4.1. When the rotation is small, the axis of rotation is not well defined; nonetheless, there have also been EBSD-based strain studies performed that consider the angle as well as the axis of rotation (Chun & Davies, 2011; Michels et al., 2015). The strain analyses described here focus on strain being accommodated through dislocations. However, strain can also be accommodated in combination with grain boundary sliding (Han et al., 2017) and/or twinning (Yu et al., 2014; Gutierrez-Urrutia et al., 2010). It should be noted that even in severely deformed materials or in materials deformed at high rates (i.e., shock), it is possible to obtain EBSD patterns of high enough quality to get useful results (McNelley et al., 2009; Bingert et al., 2009).

EBSD can also be combined with other characterization techniques to provide a more complete description of the accommodation of strain within the microstructure. This includes techniques at higher spatial resolution, such as the imaging of individual dislocations using the transmission electron microscope and/or at the same SEM spatial resolution using electron channelling contrast imaging (ECCI) (Ruggles et al., 2020). Another SEM-based technique is digital image correlation (DIC) (Kammers & Daly, 2013; Harte et al., 2020). The advantage of the SEM-based techniques is that they can be directly correlated with the EBSD measurements. As EBSD is a surface-focused characterization technique, it can also be illuminating to compare EBSD results with three-dimensional results obtained by high-energy X-ray diffraction (HEDM) (Nygren et al., 2019), i.e., obtained at synchrotron beamlines.

10.5. Grain boundaries

Since the first automated EBSD maps were generated, it was quickly realized that the grain boundary structure could be reconstructed from the EBSD data, and many studies have been performed using EBSD to investigate the grain boundary network. However, it is important to recall that the character of a grain boundary is a five-dimensional entity; three parameters are needed to describe the misorientation between the neighbouring grains separated by the boundary and two parameters are needed to describe the orientation of the boundary plane. For an EBSD scan on a single two-dimensional surface, the misorientation can be fully described but only the trace of the boundary plane can be extracted, not
the full orientation; hence, a three-dimensional data set is needed to fully capture the boundary plane orientation. Thus, the majority of EBSD-based grain boundary studies have focused on the misorientations. Examples include studies for grain boundary engineering (Palumbo et al., 1998), stress corrosion cracking (Lehockey et al., 2004), void formation (Nucci et al., 1997), recrystallization and grain growth (Lens et al., 2005), surface roughness (Stoudt et al., 2011), superplasticity (Pérez-Prado et al., 2003), slip transmission (Bieler et al., 2014), deformation (Mishra et al., 2009), and others.

EBSD characterization of the misorientation of grain boundaries can focus solely on the magnitude of the rotation, the axis of rotation or on the full axis/angle description. As an example, consider the formation of tensile and compression twins in titanium. In the example shown in Fig. 45, two types of tensile twins are shown and two types of compression twins are highlighted in a bend specimen. Note that the twins are dominated by the 94.8°@<T210> tensile twins and the 64.3°@<T100> twins. However, there is no propensity of tension twins to form in regions associated with the bulk state of tension (i.e., on the left side of the map) nor for compression twins to form in the region where the material is macroscopically in compression (i.e., on the right side of the map). This shows that twin formation is much more sensitive to the local stress state than the imposed general stress state.

As previously mentioned, the misorientation is only a portion of the grain boundary character that can be obtained from 2D EBSD measurements. Some sense of the role of the boundary plane can be derived from the two-dimensional measurements (Wright & Larsen, 2002). Fig. 46 shows an example for deformation twins in zirconium. Two specific boundaries are investigated using pole-figure analysis. The first meets the misorientation criterion to consider the boundary a 34.8°@<T100> twin and the second a 94.8°@<T210> twin. However, if the pole figure for the plane associated with the twins is plotted ([1121] for the 34.8° twin and [1012] for the 94.8° twin), then it is evident that the first (34.8° twin) is not a coherent twin boundary as the twin plane is not aligned with the boundary trace, whereas in the second case (the 94.8°) the twin is coherent. Coherency has been shown to be an important part of the sensitivity of grain boundaries to attacks such as grooving (Skidmore et al., 2004).
More recently, the study of grain boundaries in the full five-dimensional space has been performed (Rohrer & Randle, 2009); much of this work has focused on characterizing grain-boundary energies. Increasing our understanding of grain-boundary energy (Beladi et al., 2014; Ratanaphan et al., 2019) is important as it will help the scientist better understand microstructural evolution during processing as well as better predict the material behaviour of engineered components in service.

10.6. Phase transformations

Phase transformations are an active area of study using EBSD (Gourgues-Lorenzon, 2009), in particular the study of the orientation relationship between the parent and daughter phases. Considerable work has been done to reconstruct the parent microstructure from EBSD measurements of the daughter microstructure after transformation (Germain et al., 2012; Miyamoto et al., 2009; Brust et al., 2020). The majority of this work has focused on steels, but it has also been applied to other systems, such as titanium- and zirconium-based alloys.

10.7. Geological applications

Many of the application areas for materials science are also relevant for geological materials, but there are some specific areas of particular interest to earth scientists. Texture analysis of geological materials has long been a topic of interest in the earth sciences (Wenk & Van Houtte, 2004). Geologists tend to use the terms fabric, crystallographic preferred orientation (CPO) or lattice preferred orientation (LPO) instead of ‘texture’. One reason for the difference in terminology is that in many cases it is not so much the area or volume fraction of grains with a specific orientation that is important but rather the number of individual (mineral) grains with a specific orientation, especially when multiple deformation or orientation forming events are superimposed in the rock. EBSD’s ability to make spatially specific measurements of lattice orientation have provided additional insight into relationships between microstructure and fabric compared with measurements of the bulk LPO based on X-ray or neutron diffraction. Rather than trying to give a comprehensive overview, we highlight a few examples; for a fuller review of such analyses see Prior’s review on EBSD applications in geological materials (Prior et al., 2009).

Rock and mineral samples for microstructural analysis tend to be polyphase and the ability of EBSD to both identify phases (Section 10.2.2) and differentiate phases during the scanning process (often in concert with simultaneous EDS characterization for chemical composition) is crucial (Section 10.2.1). The application of dictionary indexing to minerals (Marquardt et al., 2017) has shown potential in recent years to overcome some of the misindexing challenges inherent to some of the key geologic materials, as noted in Prior’s review (Prior et al., 2009).

EBSD can be used to gain understanding of the geology of features at the Earth’s surface (or near surface), for example the strain history of geologic features of interest. Rock formation, deformation, compaction, recrystallization etc. all leave traces in the microstructure of materials undergoing natural earth-forming processes. Through analysis of the fabrics in these materials (along with other aspects of the microstructure such as chemical composition) the geologist can deduce the conditions behind the resulting microstructure or at least some of the constraints surrounding it (Wheeler et al., 2012; Cross et al., 2017). Comparison with fabrics formed during deformation in the laboratory setting can aid such forensic analysis (Heidelbach et al., 2003; Muto et al., 2011; Katayama et al., 2004). For example, dislocation creep systems can be constrained by comparing CPO data with numerical models of crystalline slip. Easy slip planes tend to align with foliation (i.e., the repetitive layers in metamorphic rocks) and easy slip directions tend to align with the lineation direction within the foliation planes. As the CPO can provide the distribution of easy slip planes within the microstructure, we can deduce the forces at play during the forming process (Mehl & Hirth, 2008; Skemer et al., 2006).

To understand the geology of the Earth’s interior we have to use a combination of indirect measurements based on seismic waves and the study of pieces of the upper-mantle material that can be found on the Earth’s surface (Mainprice, 2010; Worthington et al., 2013; Zhong et al., 2014; Mitroi et al., 2019). These pieces can be in the form of large chunks of mantle rocks that have been brought up during orogenesis (mountain building) or in xenoliths that have been brought up with molten rock (magma or lava) in a volcanic environment. From the study of seismic waves it is clear that the Earth’s mantle is highly anisotropic (Spakman et al., 1993; Rawlinson et al., 2014), and in order to refine our picture of its structure we need to know how the CPO of mantle rocks affects the seismic wave propagation. To understand that correlation, both acoustic (seismic) experiments (Wang et al., 2015; Duffy & Anderson, 1989) and texture analyses have been done on materials obtained at various depths in the crust and mantle. Synthetic rocks are also used to derive ‘standard’ or ‘reference’ signals that can be used to extrapolate these experimental values to earthquake-derived signals and image the Earth’s interior (and thereby also providing hints of the deformation processes occurring in different places).

The microstructures of metallic meteorites have been explored to gain understanding of the impact histories of the meteorites. The impacts on their parent bodies can cause deformation, heating and phase transformations, much of which is recorded in their microstructures. EBSD (along with other microstructural characterization techniques) has been used to deduce information on their thermal and shock history (Yang et al., 2011) along with studies of local texture (or fabric) in stony meteorites, or chondrites, which are among the oldest materials in the solar system. The fabrics of chondrules (igneous spherules in chondritic meteorites) offer evidence on environmental conditions surrounding the formation processes of the first solids in the development of our planetary system (Bland et al., 2011; Libourel & Portail, 2018).

The study of biominerals is of interest because of the insight it gives into natural evolutionary processes as well as what can
be learned to improve the forming of synthetic materials for specific engineering applications (Cusack, 2016). One example is the study of cross sections of avian egg shells (Dalbeck & Cusack, 2006). Ostrich egg shells show a strong alignment of the $c$ axes with the shell surface normal, while chicken egg shells show a weaker alignment. Similar analysis of fossilized dinosaur egg shells gives insight into dinosaur taxonomy (Eagle et al., 2015). Another fascinating example is the study of trilobite eyes. Trilobites are fossilized marine arthropods with hard exoskeletons. They had two compound eyes each with tens to hundreds of lenses, as seen in Fig. 47(a). These lenses were made from crystalline calcite ($\text{CaCO}_3$). Calcite allows light transmission, but a double image will be formed in directions not aligned with the $c$ axis and therefore extraordinary organic crystallographic control was required in their formation. The crystallography of the lenses as seen in Fig. 47(b,c) gives insight into the light-gathering ability of the eyes. The many subgrains in each lens may have acted as ‘light guides’, making each lens its own compound eye (Torney et al., 2014). Other biominerals have been investigated by EBSD, including sea shells (Casella et al., 2018) and corals (Cusack et al., 2008). Ice is another material studied by earth scientists; EBSD measurements can now be performed relatively routinely (Prior et al., 2015) and studies of sea ice (Wongpan et al., 2018; Weikusat et al., 2017) and glacial ice (Monz et al., 2019) have been performed.

10.8. Three-dimensional (3D) EBSD

EBSD is inherently a 2D surface-characterization technique. However, there are many cases when a three-dimensional characterization of a sample volume is critical to understanding how microstructure evolves during a material-formation process or the role microstructure plays in a material’s response. 3D-EBSD-based characterization can be achieved through serial sectioning (Zaefferer et al., 2015). Serial sectioning is a destructive technique comprised of the planar removal of a layer of material followed by a 2D characterization of the newly exposed surface. The 3D structure can be reconstructed from stacks of recorded 2D data. There are many examples of materials-science studies performed using 3D EBSD, including characterization of grain boundaries. Recombination of 2D section planes into a 3D microstructure allows for the determination of the true grain boundary normal. When combined with the misorientation between the two grains, one can generate a 5D distribution, sometimes referred to as the grain boundary character distribution or GBCD. In fact, quantities such as boundary curvature, or perhaps chemical composition or strain state in the near vicinity of the boundaries, can be correlated with the GBCD using 3D EBSD measurements (Zhong et al., 2017). Another example is the characterization of the 3D grain shape. When the grain shape is more complex than a simple straight-sided polygon, it can be difficult to extract the true shape from a single 2D planar section or even from a few different cross sections of the microstructure. EBSD is well suited to reconstructing grains based on orientation measurements, and is hence well suited to reconstructing complex grain shapes; in addition, this can even provide insight into some of the crystallographically related features in the grain shapes (Rowenhorst et al., 2020). Fig. 48 shows an example of the complex grain structures formed in an additively manufactured 316L stainless steel sample (Rowenhorst et al., 2020). In this example, a cluster of grains grown from one of the pores in the microstructure is displayed.

For 3D EBSD characterization via serial sectioning, there are several different approaches to controlled removal of material. One significant challenge in all of these approaches is registering the exposed surfaces with respect to one another, which is often best achieved using fiducial markers. This is

Figure 47

EBSD results from (a) one lens in a compound trilobite eye. (b) Top-down view of the crystallographic orientation within the lens and (b) cross section view of the lens with the orientation of individual $c$ axes outlined in yellow.
critical so that the same area is repeatedly scanned with the electron beam in focus.

10.8.1. FIB/SEM. Given that EBSD is an SEM-based technique, the most common method for material removal is to use a combined focused ion beam (FIB)/SEM instrument. The impact of the FIB beam (typically Ga⁺ ions) on the sample leads to localized sputtering of the target material. Thus, a FIB can be used to cut into the material with cut widths of just a few nanometres. This enables material to be removed precisely so that the FIB can be used to mill a series of planar sections with distances between sections of tens of nanometres to several microns with a precision in the nanometre range. If the material is milled too aggressively, the microstructure of the sample can be disturbed. But, if grazing incidence is used and/or the energy of the beam is reduced, then the beam can be used to essentially polish the material, leaving a surface with minimal radiation damage well suited for EBSD characterization (Groeber et al., 2006; Zaefferer et al., 2007). The amount of material removed is relatively small and redeposition within the specimen chamber is generally not an issue.

10.8.2. Plasma FIB/SEM. The plasma source FIB provides high xenon-ion currents enabling very high material removal rates, exceeding those of conventional Ga⁺ sources by a factor of 20 to 100. The plasma FIB enables larger areas (and volumes) to be prepared for EBSD characterization (Burnett et al., 2016). As with the conventional FIB, it is important to minimize surface damage both for obtaining EBSD patterns of good quality but also for reducing any disturbance of the microstructure to be characterized. As more material is removed than in the FIB, some effort may be needed to manage the re-deposition within the SEM chamber.

10.8.3. Laser ablation. 3D serial sectioning can also be performed by mounting a femtosecond laser onto a FIB/SEM (Echlin et al., 2012) and using the laser beam for sectioning. Excellent results have been obtained on a variety of materials and imaging modalities, including EBSD. Like the FIB/SEM approach, care must be exercised to avoid unintentional modifications of the microstructure by the laser beam, and to manage the deposition of the laser-removed material. In some materials, it may be necessary to clean the laser-milled surface by polishing the surface using the ion beam to reduce surface damage. The workflow for the TriBeam, as the system is called, is highly streamlined and is very well suited for 3D EBSD characterization of larger 3D volumes using serial sectioning.

10.8.4. Broad ion beam (BIB). Broad beam ion etching is a proven method for preparing surfaces well suited for EBSD (Section 7.5). BIB milling has been used for 3D serial sectioning (Winiarski et al., 2017) in conjunction with EBSD. This is a laborious manual approach that involves moving the sample back and forth between the SEM and the BIB, with all the requisite alignments being performed for each cycle. However, experiments with a BIB mounted inside a cryogenic SEM chamber have been explored, which, given the right geometry, could enable a more automated approach to serial sectioning and subsequent characterization using EBSD or other SEM-based imaging modalities (Desbois et al., 2013). One concern with an in-chamber system is the amount of sputtered material that would be re-deposited in the microscope; thus, some shielding of sensitive equipment, such as the EBSD detector, may be required. Assuming such issues can be resolved, an in-chamber system shows promise for larger volumes than can be tractably achieved with a FIB/SEM approach, but with less resolution between slices (~300 nm).

10.8.5. Mechanical polishing. Relatively precise amounts of material can be removed through carefully controlled mechanical polishing and electropolishing (Rowenhorst et al., 2006). Robotic systems have been developed to automate the series of tasks needed to achieve automation for serial sectioning: removing the sample from the SEM, transferring it to the polishing system and then returning it to the SEM after polishing for characterization (Uchic et al., 2013). The advantage of the mechanical polishing approach is that large areas can be characterized with relatively large lengths in the third dimension as well.

10.9. In situ experiments

As with other SEM-based materials characterization techniques, it is possible to use EBSD during in situ heating and/or deformation experiments in the SEM (Seward et al., 2002; Wright & Nowell, 2009; Wakita & Suzuki, 2017). As EBSD is typically done at sample tilts near 70°, good geometric compatibility between the SEM, EBSD detector and heating or deformation stage is required. There can be deleterious effects on the EBSD detector (and other SEM detectors) from...
the heat generated, so the material heated should be very much localized. Nonetheless, temperatures exceeding 1000°C have been achieved. The high speed of modern EBSD detectors is also helpful to capture the dynamic changes of the microstructure during an in situ experiment. As with any other surface-based characterization technique, the fact that only a free surface can be characterized during the in situ experiment must be considered when interpreting results from such analyses. In situ heating EBSD studies have been used to characterize recrystallization and grain growth (Takajo et al., 2019; Jin et al., 2014; Brisset et al., 2013) as well as phase transformations (Hata et al., 2016). Tensile stages in conjunction with EBSD have been used to track changes in orientation and the microstructure during deformation (Wright et al., 2016; Wang et al., 2018) as well as crack propagation (Mingard et al., 2013).

11. Summary and future prospects

11.1. Summary

Since the introduction of commercial automated EBSD systems in the early 1990’s, EBSD systems have become relatively commonplace in materials- and earth-science microscopy facilities worldwide. While EBSD is still very much a research tool, more and more industrial research laboratories have adopted the technique. The number of papers in peer-reviewed journals has increased 100-fold over the last three decades, showing both a tremendous increase in the number of researchers using EBSD as well as growth in the variety of applications. Professor Anthony D. Rollett has noted that EBSD has ‘democratized’ some of the principles of texture analysis and crystallography, making those fields more accessible to those studying polycrystalline materials (Rollett & Pauza, 2021). While this is certainly a positive development, it also means more researchers working in these arenas are less familiar with the details of these fields and more likely to make errors in their application. There are two common pitfalls that are worth noting.

11.1.1. Sample preparation. EBSD places more demands on sample preparation than general microscopy. Careful sample preparation of the surface is often required to get indexable EBSD patterns (Section 7). However, getting good EBSD patterns is not the only objective in sample preparation. EBSD is very much a surface-sensitive technique, so too much disturbance of the surface in order to get good EBSD patterns can lead to a measured microstructure that may not be representative of the actual state of the material. In some cases different phases and/or orientations may be over- or under-represented owing to preferential polishing or chemical attack during the preparation process. It is also important to remember that whenever the microstructure is characterized at the surface using any microscopy technique, it may not be representative of the bulk material. This principle is true for general microscopy as well, but in some cases surface effects can be more prevalent in EBSD-based measurements.

11.1.2. Statistics. With modern EBSD systems it is possible to measure 10 000 000 individual orientations in under an hour. This makes EBSD measurements helpful for statistical characterizations of microstructure such as texture analysis. If a small scanning step size is used, it is possible to reconstruct a high-fidelity visualization of the structural aspects of the microstructure. However, this may not be the best way to capture the statistical nature of any preferred orientation or texture (Section 10.1). While 1 000 000 EBSD measurements in 100 grains will provide an aesthetically pleasing colour map of the microstructure, it is inadequate for capturing the texture. Distributing the 1 000 000 points over 100 000 grains to average ten points per grain would provide a much better characterization of the texture. For measuring average grain sizes and shapes, a balance must be achieved between the number of points needed to reliably capture a grain and its shape, and the number of grains measured, as well as the time to make measurements (Section 10.3).

11.2. Future prospects

It is always dangerous to try to forecast the future, but there are some recent developments within the microscope arena that are gaining more traction in the EBSD community. Some of these have already been alluded to in previous sections of this article.

11.2.1. Direct electron detection. While the application of direct electron detectors to EBSD is underway at individual laboratories (Wilkinson et al., 2013; Vespucci et al., 2015), such detectors are now becoming commercially available and the expectation is that such detectors will enable high-resolution and high-speed applications (Wang et al., 2020). The increased sensitivity and clarity provided by direct electron detection coupled with the lack of need for a lens is expected to improve HREBSD measurements of strain. The increased sensitivity also shows promise for improved low-voltage imaging of EBSD patterns, which is helpful for the characterization of beam-sensitive materials and should also improve spatial resolution, as the interaction volume decreases with decreasing beam voltage. The quality of the direct electron detector EBSD patterns coupled with the capabilities of dynamic pattern simulation can be used to resolve indexing ambiguities in non-centrosymmetric crystals (Winkelmann & Nolze, 2015).

11.2.2. Smart sampling. Ideas for smarter sampling for EBSD measurements were proposed shortly after EBSD was automated within the framework of a conventional fixed sampling grid (Yang et al., 1999). In recent years, more sophisticated approaches no longer requiring a grid have been proposed (Tong et al., 2019; Godaliyadda et al., 2017). However, adoption of such techniques will require improvements to the scanning hardware currently used for controlling the electron beam during scanning as well as architectural changes to the software used for visualization and post-processing of the EBSD data.

11.2.3. Machine learning. Machine learning has been used for segmentation of metallographic images (DeCost et al.,...
2018; de Albuquerque et al., 2009) and is now being applied to EBSD. Examples include crystal symmetry determination from EBSD patterns (Kaufmann et al., 2020), separating phases (Kaufmann & Vecchio, 2021; Goulden et al., 2017) and identifying correlations between microstructural characteristics that lead to twinning (Orme et al., 2016). Some specific examples of algorithms applied to segmentation problems in microstructural images including those obtained by EBSD are graph-cutting (Brust et al., 2019) and expectation maximization/maximization of posterior marginals (EM/MPM) (Simmons et al., 2008). It is anticipated that such techniques will become more mainstream within the EBSD community for a wide variety of problems.

11.2.4. Correlative microscopy. Correlative microscopy is the combination of multiple imaging modalities to create a more comprehensive description of the microstructure and its inherent link to properties than can be extracted from an image provided by a single microscopy technique. Correlative microscopy is used in both the life sciences (Verkade & Collinson, 2019) and materials science (Burnett & Withers, 2019). For example, EBSD and EDS can be collected simultaneously in the SEM and used to correlate the crystallographic structure with chemical composition (Nowell et al., 2009). While it is straightforward to correlate simultaneously collected EBSD and XEDS data, more advanced correlation techniques are required to register and analyse EBSD maps with other non-simultaneous imaging modalities. There are many examples of EBSD being correlated with other microscopy techniques. The following are the few examples: EBSD linked with electron-beam-induced current measurements (EBIC), conductive atomic force microscopy (c-AFM), variable-temperature Kelvin probe force microscopy (KPFFM), scanning capacitance microscopy (SCM) and Raman microspectroscopy for the study of photovoltaic materials (Stoffers et al., 2015; Sadewasser et al., 2011; Schmid et al., 2015); EBSD coupled with scanning Kelvin probe force microscopy (SKPFFM) and AFM for analysing corrosion (Örnek & Engelberg, 2016; Gray et al., 2006); EBSD in conjunction with electrochemical mapping for studying microelectrochemical behaviour (König & Davepon, 2001); and EBSD correlated with HREBSD, TEM imaging, electron channelling contrast imaging (ECCI) and digital image correlation (DIC) for studying deformation (Ruggles et al., 2020; Kammers & Daly, 2013; Harte et al., 2020). No doubt the inclusion of EBSD with other imaging modalities for increased understanding of the link between crystallographic orientation and materials properties will continue to expand. As EBSD already produces large amounts of data, correlating EBSD with other data-rich imaging methodologies will only increase the already-demanding data analysis needs for post-processing of EBSD data. Thus, big-data techniques will need to be employed to fully capitalize on the benefits that correlative microscopy can bring to materials science (McAuliffe et al., 2020).

11.2.5. Forward modelling. As noted in Section 6.5.1, the application of forward modelling for dictionary indexing is gaining more traction. Adding orientation refinement to dictionary indexing appears to be the most likely way forward to resolving pseudosymmetry issues as well as potentially differentiating domains in non-centrosymmetric crystals. The extension of this approach using spherical indexing (Section 6.5.2) shows particular promise for accelerating the dictionary indexing process. The use of simulated patterns in improving HREBSD measurements (Section 10.4) has also been cited as a promising arena of future improvements. Pattern simulation coupled with the new direct electron detectors (Section 11.2.1) may also provide new insights into the fundamentals of the interaction between the incident electron beam and the crystal lattice.

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