A review of advances and challenges in EBSD strain mapping

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Abstract. High sensitivity cross-correlation based analysis of EBSD patterns was introduced by Wilkinson, Meaden and Dingley in 2006 [1, 2]. This paper will describe the basis of the method and the various modifications and improvements that have been made to it over the past few years. Strain sensitivity of ~ 10⁻⁴ is readily obtained and sensitivity to lower strains is achievable if signal to noise ratio in the patterns is improved by simple integration. The method allows maps of local stress and dislocation density distributions to be generated in parallel with information concerning grain orientation, grain boundary misorientation and the presence of other microstructural features. The method is illustrated by example maps from a Ni-based superalloy and deformed Cu.

1. Introduction

Over the past decade dramatic advances have made in developing models capable of simulating the micromechanical response of complex polycrystalline and even multiphase engineering materials to thermal and mechanical loading. The aim is to develop models which successfully capture the detailed grain to grain interactions, and intra-grain variations in deformation that occur. In tackling failure processes (e.g., fracture, fatigue) the driving stress field and consequent material deformation is clearly localized which forces attention to a process zone near the crack tip or crack nucleation site. Furthermore, even when volume averaged responses such as flow stress are of interest the correct micromechanics is important if the effects of changes in microstructure are to be predicted. Experimental methods allowing measurement of stress, strain, and dislocation content at length scales commensurate with the microstructure are of vital importance in this effort in guiding model development and validating predicted responses.

Synchrotron, and neutron facilities have an important role to play in this respect, however, complementary laboratory-based techniques such as digital image correlation and EBSD are also essential. A step change in the sensitivity of EBSD was realized in 2006 by Wilkinson, Meaden and Dingley [1, 2] who introduced a cross-correlation-based analysis of EBSD patterns allowing elastic strain variations to be probed.

The first attempts to use EBSD to study local deformation made use of the loss of contrast and the blurring of the pattern brought about by the increased dislocation content within the diffraction volume [3-5]. The effect is analogous to peak broadening in X-ray and neutron diffraction data but the analysis remains much cruder for EBSD as the kinematic diffraction theory that can be utilized for the X-ray and neutron cases is not applicable for EBSD where the dynamical effects become prohibitive.
The pattern blurring approach was largely dropped after automated analysis of EBSD patterns and orientation mapping became available through the nineties [6-9] as this enabled measurement of the extent of intra-granular lattice rotation. There have now been many studies [10-16] aimed at producing a single simple scalar metric to represent the extent of intra-granular lattice rotations measured over many grains. The metrics are then correlated with macroscopic engineering parameters such as equivalent plastic strain so as to enable assessment of damage development within plant and components extracted from service. It is possible to use the geometrical constructions developed by Nye [17] to estimate the density of geometrically necessary dislocations (GNDs) within the material from the measured lattice curvatures. Coupling this analysis with the higher sensitivity of the cross-correlation based measurements allows GND densities to be found to $\pm 10^{12}$ m$^{-2}$ at 200 nm step size albeit that because the EBSD data is two rather than three dimensional the measured values relate to a lower bound value [18, 19].

Initial studies using the high resolution EBSD technique for strain mapping concentrated on semiconductor structures which offer the advantages of relatively simple well-defined sample geometry, single crystal samples and generally much lower dislocation density than metallics [20-24]. However, applications to deformed metals is now being pursued in earnest and the method has already been used to map stresses near indents [19, 25, 26], at the head of block slip bands [27], near martensite islands in steels [28, 29], and in selected grains of stainless steel during in situ loading [30]. Generally, however where there has been extensive plastic deformation of metals the method has mostly been restricted to assessment of geometrically necessary dislocation (GND) density [1, 18, 19, 27, 31, 32] because large lattice rotations are thought to limit the accuracy with which the smaller elastic strains can be determined [33-35]. Recently, pattern remapping methods have been developed and demonstrated to improve significantly the measurement of small elastic strains in the presence of larger lattice rotations [33, 34] providing the opportunity to study intra-granular stress variations in deformed polycrystalline metals with improved fidelity.

2. Cross-correlation-based analysis of EBSD patterns

The basis of cross-correlation-based analysis of EBSD patterns is as follows. Elastic strain variations and small lattice rotations within the sample crystal create small shifts in the positions of zone axes and other features in the EBSD patterns. The magnitudes and directions of these shifts vary systematically with position across the EBSD pattern and equations can be written to relate the shifts to the size and nature of the strain and rotation state with the diffracting volume [1, 2]. Within each grain one pattern is selected as a reference pattern and all measurements are made relative to this. Absolute strains can be obtained only in situations where the reference pattern comes from a point on the sample for which the strain is known. When the reference pattern comes from a region with unknown strain then the map show only the relative variation in strain from the unknown reference state and knowledge of the absolute strain values is not possible. However, important information such as lattice curvatures and elastic strain gradients can still be determined in either case and the measured lattice curvatures used to recover the GND density distribution. In polycrystals, multiple reference patterns must be used to capture the strain gradients and lattice curvatures within each grain independently. With the larger datasets that are now studied methods for automatically selecting the reference points have been developed [18]. The issues resulting from the ‘reference pattern’ for EBSD in many ways parallel those resulting from the stress free lattice plane spacing $d_0$ in X-ray and neutron diffraction based methods.

Cross-correlation functions are calculated at a number of square sub-regions dispersed across the patterns from which the shift at each sub-region in the test pattern with respect to the reference pattern is determined. These calculations are performed via the Fourier domain as this is more efficient than direct calculation for the sub-region sizes generally used. We also take advantage of this and apply a band pass filter in the Fourier transforms to remove high frequency noise and low frequency background intensity variations. More details of the image analysis procedures are given in [1, 2].
The original work [1, 2] claimed that pattern shifts in 256 by 256 pixel sub-regions could be measured to ± 0.05 pixels or better and section 3 below will explore how pattern binning and averaging can improve this.

Measurement of shifts in \( x \) and \( y \) at 4 non-coplanar sub-regions of the pattern in principle provide all the information that can be obtained and allow eight of the nine possible degrees of freedom in a general strain and rotation to be calculated. Pure hydrostatic strain accounts for the final degree of freedom which cannot be detected by the technique, as strain of this type does not change any inter-zonal angles and thus does not cause shifts in the sub-regions of the pattern. Instead we rely on some simple mechanics to fully separate the three normal strains. The EBSD patterns originate from the topmost few tens of nanometres of material and allow us in most instances to assume that the local stress state must satisfy the equilibrium conditions for a free surface which must remain traction free. The stress normal to the free surface is thus set to zero and can be written as a linear sum of the elastic strains multiplied by the appropriate elastic constants found by transforming the stiffness tensor to the measured grain orientation.

In practice we tend to use many more than four (typical 50) sub-regions in the analysis so as to reduce noise and bias in the measurements. The use of more than four sub-regions leads to an over-determined set of linear equations to solve for the displacement gradient tensor components (strain and rotation). In the original work this was treated using a conventional least squares error solution [1, 2]. More recently [35] we have made use of the large redundancy in the data when 50+ sub-regions are used and have employed robust iterative solutions in which the influence of sub-regions for which the predicted shifts are furthest away from the measured values are ‘down-weighted’ in the next iterative solution until a convergence criterion is met.

The size and number of datasets obtained using the technique has grown considerably over the last few years and rather rapidly moved to a situation in which it is impossible for the investigator to make a visual check of each EBSD pattern. Thus it has been necessary to implement and use some simple scalar data quality parameters so that the influence of poor quality patterns can be automatically removed from the maps produced. The first of these uses the angular difference between the measured shift and those expected from the best fit solution for the displacement gradient tensor. These differences were simply averaged over all sub-regions in the initial formulation but with the robust statistical analysis the weighted mean angular error is used instead [35]. Where the measured strains and rotations are larger than the mean angular error there is good confidence in the measurement, but where they are smaller they are below the noise limit and must be considered suspect.

The second data quality parameter in use is the geometric mean of the normalized peak heights of the cross-correlation functions calculated for each sub-region. The normalisation is such that cross-correlation of the reference pattern with itself (i.e., auto-correlation) generates a peak height of one. Use of the geometric mean rather than arithmetic mean ensures that poor correlation at only a small number of sub-regions (perhaps due to shadowing) is sufficient to significantly reduce the geometric mean. Typically a threshold value within the range 0.2 to 0.4 is used and points with a geometric mean peak height below this threshold are considered suspect and are ignored in producing subsequent maps and further calculations.

When examining deformed polycrystalline metals Britton et al. [35] noted that the apparent elastic strains measured were often larger than expected and echoed the spatial patterning seen in the lattice rotation. They suggested that the apparent strain were likely to be in error as a result of finite deformation effects due to the lattice rotations which were often an order of magnitude larger than the elastic strain variations. When large lattice rotations are present the mapping between sub-regions on test and reference pattern is not so well represented by a simple linear translation, assumed by the cross-correlation process, and this results in significant errors being induced in the lattice strain variation [35]. To overcome this problem ‘remapping’ algorithms have been developed [33, 34]. Our approach [33] utilizes an initial pass of cross-correlation analysis to estimate the rigid body rotation between the test and reference lattice. This rotation is then used to remap the pattern intensity within
the test pattern so as to bring it in closer (crystal) alignment with the reference pattern. A second pass
of cross-correlation analysis is then undertaken and the elastic strains and a small correction to the
rotation are determined.

3. Measurement sensitivity
The initial 2006 paper reported that using a Si sample the pattern shifts were measured to a precision
of $\pm 0.05$ pixels corresponding to strain and rotation sensitivity of $\pm 8 \times 10^{-5}$ radians at the pattern
centre [2]. The same authors noted an improvement in sensitivity to $\pm 0.02$ pixels and $\pm 4 \times 10^{-5}$
radians in similar measurement from GaAs which they ascribed to the higher signal to noise ratio
obtained from the higher atomic number material [36].

Here we briefly report results of a systematic strain sensitivity study [37] of how the pattern shift
sensitivity is affected by data collection, particularly exposure times and camera binning. Patterns
were recorded using an 11 point line scan with a 10 µm step size along the tilt axis (x-axis),
corresponding to the [110] direction of a Si (001) sample. This was repeated for camera binning levels
of 1x1, 2x2, 4x4 and 8x8 for which corresponding exposure times of 1.04 s, 0.24 s, 0.05 s and 0.02 s
were used. For each condition the line scan was repeated 5 times so that averaging over different
numbers of frames could be used after data collection so as to vary the signal to noise ratio and study
its effect on the shift measurements. Each line scan was treated as 10 pattern pairs with identical
10 µm steps between them. The standard deviation in x- and y-pattern shifts were calculated for these
repeat measurements and these were then averaged over any repeat line scans available and used to
calculate the Euclidian shift which we use as the pattern shift precision. The Euclidian shift is given in
terms of fractions of a raw pixel in the unbinned patterns. For a single EBSD exposure using different
hardware binning (figure 1a) the highest precision, $\pm 0.04$ pixels, was obtained using no binning (1x1),
and as expected the precision worsened significantly as the binning was increased, to $\pm 0.73$ pixels
with 8x8 binning.

Software binning was used to generate patterns at different binning levels but similar exposure
times. Patterns at the same positions in the five line scans obtained at 1x1 binning were averaged and
then software binned and figure 1b shows that at 1x1 and 2x2 binning similar precision of $\pm 0.018$ and
$\pm 0.019$ pixels respectively were obtained, while with greater binning the precision deteriorates.
Notably even for 8x8 binning the precision is better than $\pm 0.05$ pixels once frame averaging has
improved the signal to noise sufficiently. The similarity of the 1x1 and 2x2 binning results suggests
that there is in fact little real gain in information content afforded by the additional pixels for this
detector. Finally, the detector binning was fixed at the highest resolution 1x1 binning and the effect of
software integration for increasing total exposure times was examined. Figure 1c shows that the
precision improved with increasing exposure time but the response was non-linear with an ultimate
precision of $\pm 0.019$ pixels with five seconds exposure. Sensitivity gains beyond this would require
drastic increases in total exposure time and would not realistic for mapping operations. The
$\pm 0.019$ pixels reported here for Si corresponds to an angular resolution at the pattern centre of
$\pm 4 \times 10^{-5}$ radians.

4. Two illustrative applications

4.1. Thermal residual strains near a carbide in a superalloy
We have used the cross-correlation-based EBSD method to study the thermally induced deformation
around carbide precipitates in a nickel-based superalloy (Mar-M-002). The final step of the heat
treatment was ageing for sixteen hours at 870 °C and cooling to room temperature. The difference in
thermal expansion coefficients between the matrix and carbides, of order $10^{-5}$ K$^{-1}$, should lead to
significant thermal residual strains, of order $10^{-3}$. A JEOL JSM6500 FEG SEM equipped with TSL
digiview II based EBSD system was used to acquire EBSD patterns on a square grid with a 500 nm
step size, which is well above the spatial resolution of the method. The strain-free reference point was
selected toward a corner of the map in a position remote from the carbide.
Maps of the data quality parameters in the matrix region surrounding the selected carbide are shown in figure 2. The cross-correlation peak height map in figure 2a indicates a good match (peak height above 0.8) between the test patterns and the reference pattern throughout the Ni matrix, while the different pattern generated in the large carbide toward the centre of the frame results in low values of 0.3 and below. There are a number of localized low values toward the bottom right of the map which correspond to a group of smaller carbides. The carbide is also obvious through large values in the mean angular error map (figure 2b) while throughout the matrix regions the angular errors are below \( \sim 3 \times 10^{-4} \). Data within the matrix region was considered good and shown in subsequent analysis if the peak height was above the threshold value of 0.4.

The thermally induced strain field (figure 3) around the large central carbide particle is far from symmetric presumably due to the complex particle shape and the distribution of fine carbides around it both in and below the section plane. The normal strain \( \epsilon_{11} \) along the horizontal \( x_1 \) axis is compressive to the left and right of the carbide and tensile above and below it, while the \( \epsilon_{22} \) strain along the vertical axis shows strains with the opposite sign. This is broadly consistent with a radial compressive strain and tensile hoop strain that is expected to develop during cooling as the matrix contracts more strongly than the carbide it surrounds. The in-plane shear strain \( \epsilon_{12} \) distribution shows maximum positive and negative values at \( \sim +45^\circ \) and \( \sim -45^\circ \) around the carbide, which is again generally in accord with
expectation. The two out of plane shear strains remain close to zero in accord with the expectation that the corresponding out of plane shear stresses should be zero to comply with the traction free surface condition. Fuller analysis and related crystal plasticity modelling is available [38-41].

4.2. Tensile deformation of a polycrystal
The second example concerns residual strains, lattice rotations and dislocation density with a Cu polycrystal deformed in tension to 6 % plastic strain. We focus on the distribution within a selected grain that is close to the cube orientation which is shown with its immediate neighbourhood in figure 4a. The reference pattern was taken from a point toward the middle of the grain (for which the strain is unknown) and where the mean angular error measured for a first pass of the cross-correlation analysis is low (figure 4b). However, the considerable orientation spread within the grain (figure 5a) causes a noticeable increase in the mean angular error toward the left and right hand ends of the grain. The higher mean angular errors were reduced by remapping the intensities in the test patterns so as to affect a virtual rotation of the crystal back to the reference orientation and then applying a second pass of the cross-correlation analysis (figure 4c). This remapping algorithm is described briefly at the end of section 2, and in more detail by Britton and Wilkinson [33].

Problems with the first pass of the cross-correlation analysis are also suggested in figure 5. The lattice rotations (represented by a single component $\psi_{12}$ in figure 5a) are generally much larger than the elastic strains (again represented here by the in plane shear strain $\varepsilon_{12}$ in figure 5b). There is also some suggestion that the elastic strains are mimicking the spatial pattern shown by the rotation field, and are taking very large values over appreciable areas. Application of the pattern remapping
Algorithm and a second pass of the cross-correlation analysis reduces many artefacts from the elastic strain map (figure 5c). At the left and right hand ends of the grain it is seen that the large magnitude of the shear strains is significantly reduced and the sense of the shear is inverted. The histogram of shear strain distribution (figure 5d) as calculated at the first and second pass of cross-correlation analysis also show the reduction in shear strain magnitudes brought about by the remapping. On this plot the green line represents the elastic strain calculated after remapping following a simple (infinitesimal deformation theory) linear decomposition of rotation and strain for the second pass of cross-correlation. For the blue line the deformations extracted at both passes of the cross-correlation are combined and a multiplicative polar separation (finite deformation theory) into a finite rotation tensor and a Green’s strain tensor. In most instances we have examined including this particular instance there is very little difference between these two results.

**Figure 5.** a) In plane lattice rotations in the selected grain. Comparison of in plane elastic shear strain variations from b) single pass of cross-correlation analysis, and c) after pattern remapping and a second cross-correlation analysis. d) Histograms comparing shear strain distributions from first and second pass analyses. e) Map of the GND density.
The gradients of the lattice rotations can be used within Nye’s dislocation tensor framework to form a lower bound estimate of the dislocation density at each point in the map. The analysis is given in full in [19] which also includes some discussion of numerical methods employed. Regions of high dislocation density are seen to correspond well to regions in which the lattice rotation varies most rapidly. There is an obvious tendency for dislocations to accumulate in high density regions separated by regions of low dislocation density. For this section through this grain the high GND density regions are arranged in thin wall-like features that span across the grain and tend to emanate from triple junctions or the end of narrow twins. Correlations between the spatial variations of GND density and elastic strains are much less obvious and to understand these will require much more detail analysis, including the dislocation types and the tensor nature of the stress field.0

5. Summary and outlook
High resolution EBSD provides a useful bridge between X-ray and neutron techniques on the one hand and very localized transmission electron microscope methods on the other. The example applications given here illustrate the considerable potential of the method for studying structural metallics. The main strengths of the technique are (i) that all components of the 3D strain and rotation tensors are obtained in parallel, (ii) the use of an electron beam allows very small volumes of material to be probed, and (iii) the equipment required is rather widely available. The detailed information shown in the examples can be acquired with 1 - 2 hours of SEM time and of course much larger, richer and more microstructurally representative datasets can be obtained with overnight scans. A disadvantage is that the depth probing capabilities of X-ray, in particular synchrotron methods, are clearly not available.

The major challenge in further developing the technique is the need for a reference pattern. In situations where the strain is generated at some localized feature (such as the carbide particle in section 4.1) then a reference may be obtained by moving the probe away from the centre of strain. However, in the more general cases (e.g., polycrystal deformation in section 4.2) it is not possible to identify a position on the sample at which the strain state is known. In these cases the strains reported must either be relative to the reference position or show the variation from the grain averaged strain state. The reference pattern issue has many parallels with the need for stress free lattice parameters in X-ray and neutron diffraction studies. Dynamical diffraction based simulations of EBSD patterns such as those undertaken by Winkelmann [42] may eventually resolve this issue, however, current methods of determining the detector geometry are not sufficiently accurate and can induce errors as large as 10⁻² [43].

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