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Supporting Information for

Using crystal lattice distortion data for geological investigations: the Weighted Burgers Vector method

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Contents of this file

Three Appendices describing mathematical background to WBV and error analysis, table of notation and captions to two supplementary figures

Additional Supporting Information (Files uploaded separately)

Wheeler et al. Supplementary Figures S1 and S2 as jpg files

Appendix 1: WBV, numerical aspects and symmetry

We briefly reiterate and extend here the maths in Wheeler *et al.* (2009); for notation see Table S1. We write some equations using vector notation for brevity though we find that index notation (including Einstein summation convention) is most generally useful. We use Greek and Latin indices for sample and crystal coordinate systems respectively otherwise confusion can easily result. For second rank and higher tensors, either can be used, or a "mixed" space. A fundamental concept is the orientation tensor **h** which relates a vector **C** in Cartesian crystal coordinates to its equivalent **V** in sample coordinates

$$V_\gamma = h_{\alpha i} C_i$$

In what follows we assume that there are no elastic strains on the grain scale.

1.1. Differential method

Considering **h** is a mathematical function of position the Nye tensor is defined by

$$\alpha_{i\gamma} = e_{\alpha\beta\gamma} h_{\alpha i,\beta} = \sum_N \rho^{(N)} b_i^{(N)} l_\gamma^{(N)} \tag{A1.1}$$

where **e** is the permutation tensor. If we know only the x and y gradients of **h**, we can still determine 3 out of the 9 components of the Nye tensor

$$W_i = \alpha_{i3} = e_{\alpha\beta3} h_{\alpha i,\beta} = h_{1i,2} - h_{2i,1} = \sum_N \rho^{(N)} b_i^{(N)} l_3^{(N)} = \sum_N \left[\rho^{(N)} l_3^{(N)} \right] b_i^{(N)} \tag{A1.2}$$

The vector **W** encapsulates some but not all of the GND content: the term in square brackets indicates it is weighted towards dislocations lines at a high angle to the map.

EBSD measurements and hence **h** values are determined at a finite number of spaced points. Thus, we must differentiate **h** numerically. For example, to evaluate

$$h_{2i,1} = \partial h_{2i}/\partial x$$

we could choose

$$(h_{2i}(x+u,y) - h_{2i}(x,y))/u$$

where s is step size, or, more symmetrically,

$$(h_{2i}(x+u,y) - h_{2i}(x-u,y))/(2u)$$

Because we are differentiating, we call this "differential" method.

The algorithm requires a minimum of 3 points to get gradients in both x and y (e.g. Fig. 4a)). However, this asymmetric pattern may give biased results, so Fig. 4b)-d) show some more symmetric patterns of nearby points which can be involved in the calculation. Such patterns, used for numerical differentiation in other contexts, are called "stencils". In detail our differential method calculates a "best fit" lattice curvature to the misorientations at each point in the stencil. When high angle boundaries pass through the stencil, the points beyond the boundary are excluded from the fitting. This means that only a subset of the points in the stencil are used. Our "edge preserving" method differs somewhat from that of Humphreys *et al.* (2001).

Crystal symmetry must be accounted for in the calculation. When Kikuchi patterns are indexed, the procedure will give one orientation tensor **h** from each pattern. Because of crystal symmetry there is a choice of **h** values, related by symmetry, all equally valid. Adjacent points which are actually close in orientation may be indexed with different symmetry choices, giving very different numerical **h** components and Euler angles. Numerical differentiation would then give huge and artificial orientation gradients so, rather than calculate gradients directly, the misorientations between points are calculated. The misorientation angle (strictly, "disorientation") is defined as the *minimum* angle needed to rotate one orientation into another (Wheeler *et al.*, 2001), and the misorientation tensors generated are then used to calculate orientation gradients.

1.2. Integral method

Again considering **h** is a mathematical function of position, evaluate the integral of **h** around a closed loop on the map, followed anticlockwise. This gives the *net* WBV of GNDs whose lines cross through that loop, in units of length.

$$B_i = -\oint_{anticl} h_{\alpha i} \, dx_\alpha$$

We generally report the calculation after dividing the net WBV by loop area A, hence delivering a vector **B**/A with units of (length)$^{-1}$. Mathematically the differential and integral methods are precisely equivalent (they are related by a tensor version of Stokes' theorem).

$$B_i = \int W_i dA$$

So **B**/A is just the average value of **W** inside the loop.

The numerical version of the integration is written as follows. For a square grid of points, we assume that a particular orientation measurement $h_{\alpha i}^{(p)}$ applies to a square region around the point p at which it was taken. In numerical integration, then, the "dx" term becomes a vector $x_\alpha^{(p)}$ spanning this square region, horizontally, vertically, or diagonally (at corners). Then:

$$B_i = -\sum_{p=1}^{L} h_{\alpha i}^{(p)} x_\alpha^{(p)}$$

where L is the number of points included in the loop.

1.3. Symmetry

When a crystal has symmetry, there is more than one choice for the orientation tensor **h**. If **h** is a valid description, then so is **hS** where **S** is any symmetry operator expressed in crystal coordinates. Because **h** is non-unique, so is $\alpha_{i\gamma}$ and so is the WBV in crystal coordinates: hence it is plotted on the usual IPF segment. However, we now show that if the first index is transformed to sample coordinates, the tensor is unique. In sample coordinates

$$\alpha'_{\delta\gamma} = h_{\delta i} e_{\alpha\beta\gamma} h_{\alpha i,\beta}$$

Let us replace **h** by the symmetric equivalent **hS**, so then **α**' becomes

$$\alpha'_{\delta\gamma} = h_{\delta p} S_{pi} e_{\alpha\beta\gamma} \left(h_{\alpha q} S_{qi} \right)_{,\beta} = S_{pi} S_{qi} h_{\delta p} e_{\alpha\beta\gamma} h_{\alpha q,\beta} = h_{\delta i} e_{\alpha\beta\gamma} h_{\alpha i,\beta} \qquad (A1.3)$$

because **S** is a rotation tensor and so $S_{pi}S_{qi}$ is the identity tensor. So **α'** has a unique value when both coefficients are in sample coordinates, and so does the WBV.

Appendix 2: Derivations of model Nye tensors

Since we have chosen olivine as our example mineral, we have designed models so that distortion can be expressed by GNDs with [100] and [001] vectors. The distortions are gradational but we use the same nomenclature as that for subgrain walls.

2.1. Tilt

Our tilt model is in essence 2D - there are no distortions in the 3rd dimension – so we begin with a completely general 2D model ın which lattice orientation is defined by a single angle as a function of position θ(x, y), with anticlockwise rotation positive. Then the orientation tensor is

$$h_{\alpha i} = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

So

$$h_{\alpha i,\beta} = q_{\alpha i}\theta_{,\beta}$$

where

$$q_{\alpha i} = \begin{pmatrix} -\sin\theta & -\cos\theta & 0 \\ \cos\theta & -\sin\theta & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

From eqn (A1.1) we obtain, considering the zero values in **e** and **q**

$$\alpha_{i\gamma} = e_{\alpha 1\gamma}q_{\alpha i} + e_{\alpha 2\gamma}q_{\alpha i}\theta_{,2} = e_{21\gamma}q_{2i}\theta_{,1} + e_{12\gamma}q_{1i}\theta_{,2}$$

So setting γ = 3 the WBV is, in crystal coordinates

$$\boldsymbol{W} = (-\cos\theta\,\theta_{,1} - \sin\theta\,\theta_{,2}, \sin\theta\,\theta_{,1} - \cos\theta\,\theta_{,2}, 0)$$

and in sample coordinates

$$\boldsymbol{W} = -(\theta_{,1}\,\theta_{,2}, 0)$$

This simple result tells us that orientation variations in the x direction relate to Burgers vectors with an x component (in sample coordinates) and similarly for y: a rigorous version of what we discussed in the introduction.

Now we design a specific 2D model: a tilted crystal so that rotations are around [001], perpendicular to the map, and [010] is parallel to rays from the centre of curvature. Then, let x and y in map view be measured relative to the centre of curvature, r be the distance from the centre so the misorientation of [100] relative to the x axis is:

$$\theta = -\text{atan}\left(\frac{x}{y}\right)$$

so the gradient vector is

$$\theta_{,\beta} = \frac{1}{r}(-\cos\theta, -\sin\theta, 0)$$

so in sample coordinates

$$\boldsymbol{W} = \frac{1}{r}(\cos\theta, \sin\theta, 0) \qquad\qquad \text{(A2.1)}$$

And in crystal coordinates

$$\boldsymbol{W} = \frac{1}{r}(1, 0, 0)$$

2.2. Twist

Misorientation is around the [010] axis, running parallel to x. Let the misorientation relative to the y axis be an arbitrary function of x. This allows us to deal with a linear function (constant distortion) or a quadratic function (increasing distortion)

$$\theta = \theta(x)$$

and

$$h_{\alpha i} = \begin{pmatrix} 0 & -1 & 0 \\ \cos\theta & 0 & \sin\theta \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}$$

So

$$h_{\alpha i,\beta} = q_{\alpha i}\theta_{,\beta}$$

where

$$q_{\alpha i} = \begin{pmatrix} 0 & 0 & 0 \\ -\sin\theta & 0 & \cos\theta \\ -\cos\theta & 0 & -\sin\theta \end{pmatrix}$$

And the gradient vector

$$\theta_{,\beta} = \left(\frac{d\theta}{dx}, 0, 0\right)$$

From eqn (A1.1) we obtain

$$\alpha_{i\gamma} = e_{\alpha 1\gamma}q_{\alpha i}\theta_{,1} = e_{21\gamma}q_{2i}\theta_{,1} + e_{31\gamma}q_{3i}\theta_{,1}$$

$$= \frac{d\theta}{dx}\begin{pmatrix} 0 & -\cos\theta & \sin\theta \\ 0 & 0 & 0 \\ 0 & -\sin\theta & -\cos\theta \end{pmatrix}$$

and in crystal coordinates (setting $\gamma = 3$)

$$\boldsymbol{W} = \frac{d\theta}{dx}(\sin\theta, 0, -\cos\theta) \qquad\qquad \text{(A2.2)}$$

To transform **W** sample coordinates, calculate **hW** to find

$$\boldsymbol{W} = \frac{d\theta}{dx}(0, 0, -1).$$

So in sample coordinates the WBV (= $\alpha_{\beta 3}$) is a vector parallel to z.

Appendix 3: Error analysis

3.1. Standard deviation of WBV

We undertook numerical modelling to assess how errors in orientation measurements propagate. To generate figures S1 and S2, we took the two models of Fig. 2 and added orientation errors by imposing small additional rotations. Each additional rotation matrix was generated using a unit vector rotation axis selected at random, and a rotation angle selected at random from the range 0 to 0.01 rad. We then calculated the WBV using various methods. The calculations are undertaken in sample coordinates, meaning the theoretical and calculated WBVs have unique values as shown in eqn. (A1.3). and implying that crystal symmetry does not enter into the calculations. For that reason, although the models are for olivine, we assert that the results will apply in any crystal system, because we are applying equations which do not involve symmetry operations. For display we find IPFs are easier to understand even though calculations are undertaken in sample coordinates.

First row. Fig. S1 a)-c) show IPFs for three different stencil sizes, and d)-f) for three different tile sizes. The noise has led to larger scatter in WBV direction for small stencils and tiles.

Second row. To understand this in more detail, we compare the theoretical WBV of eqn (A2.1), denoted here as $\mathbf{W}_c$, with the calculated WBV, defining an error vector $\mathbf{E}$ as the difference between the two. Fig. S1 g)-i) show the magnitudes of the error vectors (blue cloud) for three stencil sizes. Errors do not seem to be correlated with WBV size and to quantify this, we must use the statistics of vectors. Any error vector $\mathbf{E}$ has a covariance matrix given by

$$C_{ij} = mean(E_i E_j)$$

We find that the covariance, a second rank tensor, is somewhat anisotropic in our models but rather than consider that detailed complexity, we assume isotropy

$$\mathbf{C} = \frac{1}{3}\sigma^2\mathbf{I} \,,$$

where I is the identity tensor, and then

$$\sigma^2 = trace(\boldsymbol{C}) = mean(E_1^2 + E_2^2 + E_3^2)$$

Here σ can be thought of as a standard deviation for the vector $\mathbf{E}$. We calculated it for the entire W range, and also for binned intervals of W to discover whether W had a strong effect on σ. For each particular model, e.g. Fig S1g), the cyan line shows the average values of σ in bins of width 0.002. We do not see a strong correlation with W (bearing in mind the vagaries of such numerical experiments) so we propose that σ should be considered independent of W. In contrast, σ clearly decreases from g) to i) so the idea that larger stencils will reduce directional errors is confirmed. Although directional errors are reduced, the larger stencil size means that a larger region of microstructure is contributing to the calculation, so it is less obvious where the contributing GNDs are. In Fig. S1j)-l) we repeat this analysis for tiles of different sizes.

Third row. In Fig. S1m)-r) we display the angular errors. The magenta lines indicate the points below which 95% of the data lie (for binned ranges of W). The red lines are discussed below.

In Fig. S2 we show the same error analysis for a smooth twist structure as in Fig. 2, using the theoretical WBV given by eqn. (A2.2). The same patterns in error are shown: again, the magnitude of the error vector is not dependent on W, so the angular error is less for larger W; again, larger stencil sizes give smaller errors.

These graphs are not intended as a universal guide as to how orientation measurement errors will affect WBV directional errors, because many different types of 3D orientation gradients may exist, but they serve as a preliminary indication. We quantify the link between standard deviation of W with dimensionless stencil size S or tile size T. For each of the 12 models (6 tilt, 6 twist) we calculate the value of σ across the entire range of W (in essence averaging the values shown by the blue lines). We then did a best fit of log σ versus log S or log T, finding an exponent of -0.99 for stencils and -0.718 for tiles. An outline algebraic analysis under development for tiles suggests the exponent is -3/4; for stencils we rounded it to -1. A best fit using these exponents then gives:

$$\sigma_S = 0.0247 S^{-1}/u \tag{A3.1}$$

where u is step size, and with the dimensionless area T of a tile:

$$\sigma_T = 0.0081 T^{-3/4}/u . \tag{A3.2}$$

3.2. Angular errors from standard deviations

To link these standard deviations to directional statistics we assume a Fisher distribution in which the directions are distributed in accordance with a probability density function F

$$F = \frac{\kappa}{4\pi \sinh \kappa} \exp(\kappa \cos \psi)$$

where ψ is the angle from the mean direction, and κ is known as a "concentration" parameter (Watson, 1982). When κ is large the distribution is very focussed around the mean direction and that would be expected to relate to small values of standard deviation σ of **W**. To quantify that, we refer to section 2 of (Watson, 1982) and note that the definition of σ there is equal to our definition divided by $\sqrt{3}$. Watson defines a parameter m = W$\sqrt{3}/\sigma$ (in our notation) and then shows how it relates to κ via his eqn. (30). Having κ we calculate the 95% confidence angle by integrating F to obtain the proportion of the distribution within an angle θ, and then rearranging to find the angle within which 95% of the distribution lies:

$$\alpha_{95} = \mathrm{acos}\left(1 + \frac{1}{\kappa}\ln(1 - 0.95(1 - \exp(-2\kappa))) \right)$$

To help to understand the errors, this equation can be related back to the inset cartoons in Fig. 4. When κ is large and errors are small

$$\alpha_{95} \cong \mathrm{acos}\left(1 + \frac{1}{\kappa}\ln(0.05) \right) \cong \mathrm{acos}\left(1 + \frac{1}{m^2}\ln(0.05) \right) \cong \frac{1}{m}\sqrt{2\ln(20)}$$

$$= \frac{\sigma}{W}\sqrt{2\ln(20)/3} = 1.413\frac{\sigma}{W}$$

where we have used the Watson eqn. 30 for large κ and the power series expansion of cos. Although there is now a constant of proportionality, the basic link between vector and directional errors in Fig. 4 is confirmed. For binned ranges of W, we plot the calculated

values of α_{95} as red lines in the bottom rows of Figs. S1 and S2. These are comparable to the magenta lines which are calculated directly from the model data (particularly for the twist models), suggesting that our statistical analysis is adequate. We note our models are based on "noise" up to 0.01 radian. We expect that eqns (A3.1) and (A3.2) will scale with the level of noise but assessing angular noise levels is not a straightforward procedure and is a topic for future research.

3.3. Angular errors and crystal symmetry

Our calculation of α_{95} does not consider crystal symmetry. The error cone should be the same in crystal coordinates but there are some subtleties to consider. If α_{95} was for example 3° then this could help specify a narrow cone of directions, displayed as a small circle, within which the true direction lay on a PF or an IPF. However, if α_{95} was 40° in, for example, the cubic crystal system, then the error cone would overlap several symmetric equivalents and be difficult to interpret; it might cover most of the IPF. In general, the error cone would be sliced up by symmetry operations and would be represented by several small circle arcs on an IPF; it is beyond the scope of this contribution to consider this in detail. Nevertheless, we find our estimates of α_{95} are always informative.

3.4 Summary

In summary, and adding practical detail, errors are evaluated as follows. In bold are the quantities which enter into the calculation.

1. Assume a particular range of orientation **measurement errors** in the EBSD measurements (we give an example where we assume errors go up to 0.01 rad).

2. We use a particular **stencil or tile area** for WBV calculation and calculate the standard deviation in W from eqn (A3.1) and (A3.2) which also requires the **step size.**

3. To get an overview of errors in WBV PFs and IPFs when looking at a range of WBVs, we want the maximum relevant α_{95} so we select a **minimum WBV length** which then allows calculation of m, then κ, then α_{95}.

Supplementary Table S1. Notation.

Symbol	Meaning	Units, if dimensional
A	Area of integration loop on map	$(\text{length})^2$
B	Net Burgers vector sum for dislocations threading a particular loop	length
e	Permutation tensor (3rd rank)	-
h	Orientation tensor (2nd rank)	-
K_i	i^{th} coefficient for writing **W** in terms of lattice basis vectors	$(\text{length})^{-2}$
$\mathbf{L}_i$	i^{th} lattice basis vector	length
S	Area of stencil in pixels	-
T	Area of tile in pixels	-
W	Weighted Burgers Vector	$(\text{length})^{-1}$
W	Magnitude of **W**	$(\text{length})^{-1}$
W_t	Characteristic W used in precision analysis	$(\text{length})^{-1}$
$\mathbf{W}_c$	Theoretical value of **W** in noise-free model	$(\text{length})^{-1}$
E	Error vector in value of **W** in noisy model = **W** – **W**$_c$	$(\text{length})^{-1}$
$\rho^{(N)}$	Density of Nth type of dislocation	$(\text{length})^{-2}$
$\boldsymbol{b}^{(N)}$	Burgers vector of Nth type of dislocation	length
$\boldsymbol{l}^{(N)}$	Unit line vector of Nth type of dislocation	-
u	Step size	length
X, y, z	Cartesian coordinate system	length
α_{95}	Angle related to precision of a direction. 95% chance that the true direction of a vector is that angle or less from the calculated direction	-
$\boldsymbol{\alpha}$	Nye Curvature tensor (2nd rank)	$(\text{length})^{-1}$
$\boldsymbol{\kappa}$	Curvature tensor (2nd rank)	$(\text{length})^{-1}$
κ	"concentration" parameter in spherical statistics (Appendix 3)	-
σ	"Standard deviation" of a vector, assuming isotropic covariance (Appendix 2)	Same as vector
σ_S	Standard deviation of **W** when calculated using stencils	$(\text{length})^{-1}$
σ_T	Standard deviation of **W** when calculated using tiles	$(\text{length})^{-1}$

Captions for supplementary figures

Figure S1. Analysis of errors in the noisy tilt model.

a)-f) For the noisy model, IPF plots for WBV calculated for three stencil sizes (left) and three tile sizes (right) with a W threshold of 0.001 $(\mu m)^{-1}$.

g)-l) Errors (magnitude of $\mathbf{W_e}$) versus W for the various stencils and tiles in a). In each graph, individual values are plotted as a blue cloud and the cyan line indicates the average value of error for binned ranges of W.

m)-r) Directional errors (angle between $\mathbf{W}$ and $\mathbf{W_c}$) versus W for the various stencils and tiles as in upper rows. In each graph, individual values are plotted as a blue cloud and the magenta line indicates the points below which 95% of the data lie (for binned ranges of W). The red line indicates predicted α_{95}. The W minimum thresholds used in displays in a) are shown by stars.

Figure S2. Analysis of errors in the noisy twist model, organised as in Fig. S1.