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LLNL-JRNL-840753

A Denoising Autoencoder for Improved Kikuchi Pattern Quality and Indexing in Electron Backscattered Diffraction

C. E. Andrews, M. Strantza, N. P. Calta, M. J. Matthews, M. L. Taheri

October 4, 2022

Ultramicroscopy

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1 **Title:** A Denoising Autoencoder for Improved Kikuchi Pattern Quality and Indexing in Electron
2 Backscatter Diffraction

3 Authors: Caleb E. Andrews_A, Maria Strantza_B, Nicholas P. Calta_B, Manyalibo J. Matthews_B,
4 Mitra L. Taheri_{A*}

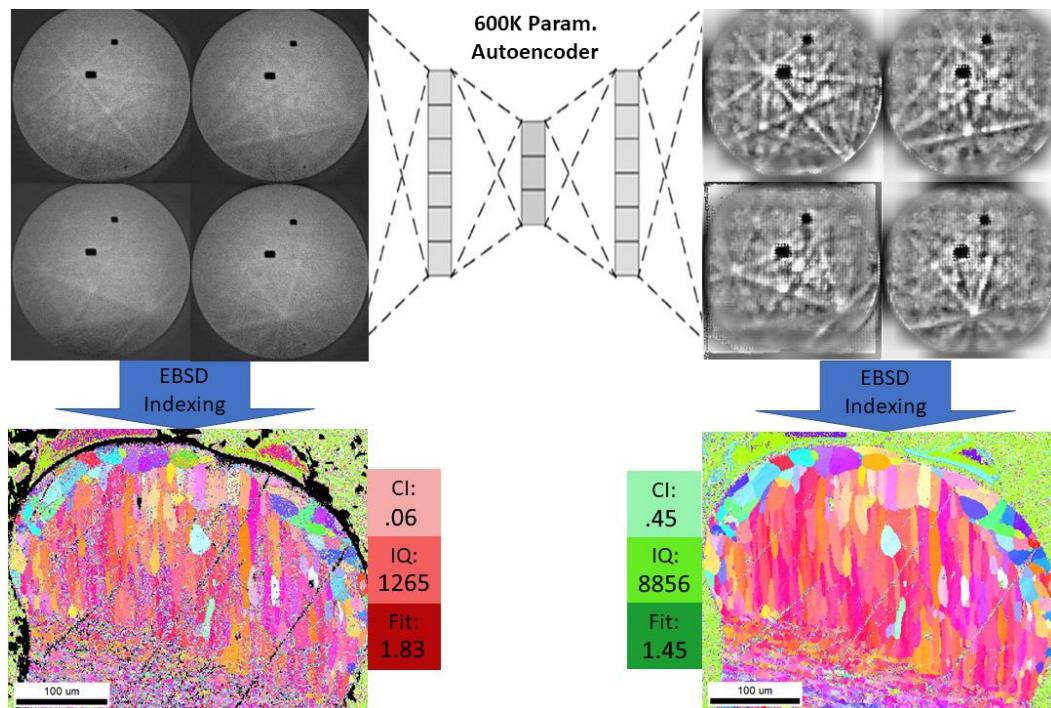
5 A: Johns Hopkins University, Department of Materials Science

6 B: Lawrence Livermore National Laboratory, Materials Science Division

7 *Corresponding Author: mtaheri4@jhu.edu

8 **Abstract:** The rapid collection and indexing of electron diffraction patterns as produced via
9 electron backscatter diffraction (EBSD) has enabled crystallographic orientation and structural
10 determination, as well as additional property-determining strain and dislocation density
11 information with increasing speed, resolution, and efficiency. Pattern indexing quality is reliant
12 on the noise of the collected electron diffraction patterns, which is often convoluted by sample
13 preparation and data collection parameters. EBSD acquisition is sensitive to many factors and
14 thus can result in low confidence index (CI), poor image quality (IQ), and improper
15 minimization of fit, which can result in noisy datasets and misrepresent the microstructure. In an
16 attempt to enable both higher speed EBSD data collection and enable greater orientation fit
17 accuracy with noisy datasets, an image denoising autoencoder was implemented to improve
18 pattern quality. We show that EBSD data processed through the autoencoder results in a higher
19 CI, IQ, and a more accurate degree of fit. In addition, using denoised datasets in HR-EBSD cross
20 correlative strain analysis can result in reduced phantom strain from erroneous calculations due
21 to the increased indexing accuracy and improved correspondence between collected and
22 simulated patterns.

23 **Graphical Abstract:**



25

26 **1) Introduction:**

27 Electron backscatter diffraction (EBSD) is of the most commonly used microstructural analysis
28 tools, and is a widely accessible tool in the materials science and crystallography community. [1]
29 EBSD enables users to obtain a wealth of information from crystalline materials in a
30 conventional scanning electron microscope (SEM) that would traditionally require access to a
31 beamline or similar X-ray techniques: such as crystallographic orientation, distribution of phases
32 within a microstructure, dislocation defect density, and grain size and texture information. [2] In
33 addition to the acquiring crystallographic information, the method enables the measurement of
34 microscale strains in materials with a sensitivity of 10^{-4} through a process of electron backscatter
35 diffraction pattern (EBSP) cross correlation, using high resolution electron backscatter
36 diffraction (HR-EBSD). [3]–[5] Strain determination is accomplished by two different
37 approaches and arrives at two different strain measurements. The first method of relative strain
38 mapping calculates local strain gradients by measuring pattern shifts between two captured
39 patterns, a reference and a test, experimentally this is often preformed such that the reference
40 pattern is that of the grain mean orientation. [6], [7] However, the unknown strain state contained
41 within the reference pattern carries with it uncertainty, and thus this method does not provide a
42 true absolute strain measurement, only relative/deviatoric distortions between the reference and
43 test pattern. [8] The second, more computationally complex method, dynamically simulates a
44 strain free reference pattern for each experimentally obtained pattern and thus determines
45 absolute strain at each point in an EBSD scan. [9], [10] Thus, obtaining an absolute strain
46 measurement relies on the simulation of a ‘zero strain’ reference pattern which closely converges
47 with the experimental one and is limited by two sources of uncertainty: the uncertainty of
48 orientation measurement via Hough transform [1] and uncertainty of pattern center (PC) from
49 conventional SEM calibration techniques which can introduce phantom strains on the order of
50 10^{-3} . [11], [12] Despite advances in improving correspondence between the simulated and real
51 patterns through a gradient-based approach [13] there is still often insufficient correspondence
52 between real and simulated patterns which introduce limitations to this method in obtaining an
53 absolute strain measurement. [1], [14] Although many authors have reported and worked on
54 solutions related to PC shift correction [8], [13], this paper focuses on improving the
55 experimentally collected EBSPs, also known colloquially as Kikuchi patterns, themselves and
56 achieving a higher accuracy measurement of orientation angles and enabling a higher resolution
57 Hough transform indexing procedure and has implications beyond strain measurement.

58 All EBSD methods rely on the correct identification and indexing of bands appearing on the
59 EBSP which represent the crystal lattice planes, determining the positioning and angles between
60 these bands, and from this the orientation of the local crystal lattice can be measured. [15]–[17]
61 The most commonly used method of indexing EBSPs utilizes band detection via Hough
62 transform, whereby each Kikuchi line in detector space is a 2D point of accumulation (a peak of
63 high intensity) in transform space. [18] Thus, in transform space the distance and angle between
64 these peaks can be measured trivially and the relationship between the planes in detector space
65 elucidated to determine crystallographic orientation. [15], [19] This method has been integrated

66 into many commercial systems and has seen widespread use and improvement over the past
67 several decades, however this algorithm's performance degrades with increasing noise input. The
68 Hough transform method suffers from poor indexing, fit, and confidence index (CI) in EBSPs
69 featuring increasingly high noise levels, with noise primarily manifesting as low pattern contrast,
70 Gaussian noise, or lack of clear band definition. [2], [20], [21] This noise can originate from
71 sample preparation, the detector, microscope, and camera settings utilized (i.e. poor exposure),
72 localized strain/deformation within the sample area, and improper utilization of large step sizes
73 with fine-grained materials. [22]–[24] Various indexing algorithms have been introduced which
74 aim to address these issues, each introducing their own advantages and drawbacks. Spherical
75 indexing methods utilize a forward model to generate a spherical master EBSP from which
76 collected patterns are projected onto and correlated via a spherical harmonic transform (SHT),
77 resulting in higher indexing quality with EBSPs that would be difficult to index with traditional
78 Hough techniques. [25] The dictionary indexing method (DI) has demonstrated the ability to
79 index samples with greater accuracy and correctly index patterns with high noise [24], [26], but
80 the size of the simulated pattern dictionary increases with decreasing crystal symmetry; meaning
81 that indexing a cubic material will take six times less computation time than indexing an
82 orthorhombic one. [25] Computation time is the largest drawback of the DI method, with an
83 indexing speed of ~12 points per second and larger datasets taking days to process when
84 including orientation refinement. [27] For context, both the Hough method and SHT method are
85 capable of processing hundreds to thousands of points per second and are limited more by EBSD
86 detector speed and exposure settings than execution time. [25] Refinements and optimization to
87 the DI method have been forwarded to improve execution time, with Fourier domain based
88 pattern matching enabling more rapid orientation refinement and requiring a smaller pattern
89 dictionary to parse. [28]

90 While introducing the subject of noise and its implications towards EBSD indexing, we must
91 also briefly discuss the quantification of EBSD data quality metrics. Quality in an EBSD context
92 can refer to two things, the quality of the diffraction pattern itself and the quality of the indexing
93 solution of that pattern to a crystal system. Quality at the pattern level is a measurement of how
94 well defined the Kikuchi bands are relative to the background, with higher quality patterns
95 featuring bands of high intensity and sharp band edges. [29] This is often defined as image
96 quality (IQ), a measure of the average height of the Kikuchi band peaks in Hough space, and is
97 effected by local lattice strain, the atomic scattering factor of the material being analyzed, surface
98 preparation and/or topology, and other microstructural features like grain boundaries which
99 would result in low IQ. [30], [31] As indexing and/or SEM parameters will often induce changes
100 to IQ irrespective of the microstructure, relative values between points are used to describe
101 microstructural features and an absolute measure of IQ is not particularly useful in this regard.
102 [30] Indexing success rate (ISR) is a general term for describing the fraction of patterns
103 successfully indexed in an EBSD scan, and this is defined differently depending on the EBSD
104 detector manufacturer. At time of writing Oxford and Bruker systems describe this as the
105 fraction of zero solutions, or points with no indexing solution to the corresponding pattern, while
106 EDAX systems utilize a triplet voting method, defined as a confidence index (CI), to provide a
107 measure of how reliable the indexing solution would be on a scale of 0 to 1. [24], [32] A 'vote'
108 in this context is an orientation solution for a set of Kikuchi band triplets, the more well fit that

109 solution is the more votes it receives, and the CI is calculated as the difference in votes between
110 the most likely solution (determined by number of votes) and the second most likely, divided by
111 the number of total band triples available. [19], [32], [33] CI is impacted by the number of bands
112 present in a pattern, with more bands resulting in a greater number of correct solutions, but a
113 lower average CI due to conflicting votes; experimentally this results in ~90% of the orientation
114 solutions being correct with a CI=0.1. [34] Degree of fit is another ISR metric, and defines the
115 degree of angular deviation between the observed crystallographic orientation of the EBSP and
116 the ideal solution provided by the indexing software. [35] There is no one single quality metric
117 which can fully describe an EBSD dataset due to the physics of diffraction, for example a highly
118 strained sample would result in lower IQ than a relaxed one but could still feature high ISR. In
119 addition, different detector manufacturers will use different image collection, processing, and
120 measurement methods all of which impact these metrics which is beyond the scope of this study.

121 Machine learning (ML) methods have been recently introduced as an alternative to the discussed
122 algorithms as a method of indexing EBSPs. [36] Deep learning methods, such as the use of
123 convolutional neural networks (CNNs) trained with simulated EBSPs, have indexed
124 polycrystalline nickel with decreased disorientation error when compared to DI methods. [37]
125 Refinements and improvements to the CNN indexing method, including EBSP preprocessing and
126 use of disorientation error as its own loss function, resulted in a model fast enough for real-time
127 indexing but performed slightly worse at indexing noisy patterns. [38] These improved indexing
128 methods offer reduced orientation fit error over the conventional Hough methods, which is key
129 for cross-correlative strain determination and accurate indexing of strained materials. [1], [37]

130 Image processing algorithms which aim to denoise the EBSPs themselves, rather than addressing
131 noise at the indexing stage, have also shown utility. The commercially available Neighbor
132 Pattern Averaging & Reindexing (NPARTM) algorithm averages neighboring patterns above a CI
133 threshold, which has shown improved Hough indexing and enables the collection of data at
134 higher speed with more noise. [24], [39] NPAR functions as a virtual pattern averaging function
135 which can be done post-process, as it averages patterns across space it is inherently lossy with
136 spatial resolution, and NPAR is less effective with larger step sized scans and fine grained
137 materials. This method has been refined using a non-linear smoothing kernel (NLPAR) to weigh
138 patterns based on their similarity of quality, rather than their spatial proximity, and results in
139 further improved results including gains over the DI method. [22] These are inherently post-
140 process methods, but demonstrates that when using the conventional Hough indexing method,
141 the quality of orientation mapping and index success rate can be improved through EBSP
142 preprocessing and denoising.

143 Utilizing a denoising autoencoder (DA) approach to preprocess EBSPs prior to indexing should
144 lead to indexing improvement, without needing to alter the indexing process itself. Autoencoders
145 are a type of feedforward neural network model consisting of two functions: an encoder which
146 translates the input into latent space, and decoder, which attempts to reconstruct the input from
147 this latent space representation. [40] The goal of a DA model is to learn to reconstruct a noise-
148 free output from a noisy input. [41] Using DAs for image denoising has shown utility in
149 removing Gaussian noise and undesired features from image data. [42] Stacked convolutional

150 DAs have been able to denoise medical mammogram and X-ray images with very small training
151 datasets, and reconstruct images from incredibly noisy datasets. [43], [44] Thus, there is
152 evidence that utilizing DAs at the stage of EBSP collection or prior to indexing could reduce
153 noise within the EBSPs themselves which would result in erroneous or poor indexing.

154 In this paper, by synthesizing both ML and conventional image processing methods, we
155 introduce a convolutional DA framework for EBSD denoising which has shown to significantly
156 improve indexability of poor quality EBSPs and improve the fit accuracy of the Hough transform
157 method with DA-processed patterns. By addressing noise at the EBSP level, we are able to
158 improve the CI, image quality (IQ), and degree of fit both among individually noisy patterns and
159 across the whole dataset. In addition, this DA framework reduced the contributions of ‘phantom
160 strain’ in dynamically resolved absolute HR-EBSD strain measurement because of this improved
161 fit accuracy. By improving the pattern quality and Kikuchi band edge fidelity, the accuracy of
162 interplanar angle measurement of the Hough indexing procedure was improved. Because of this
163 we observe increased correspondence between experimental EBSPs and simulated ones used for
164 strain cross correlation. EBSPs denoised by the autoencoder often demonstrate a sub-1° of fit,
165 with indexing metrics showing improvement over and compatibility with existing EBSP image
166 post-processing methods. In addition to improving HR-EBSD absolute strain determination, this
167 allows for noisier EBSD datasets to be collected and indexed with conventional Hough-based
168 indexing and thus enables higher speed and higher resolution EBSD experiments in general.

169 **2) Sample Preparation and EBSP Acquisition Methods:**

170 Two HR-EBSD datasets were utilized to build and demonstrate the DA, both captured from the
171 cross-sectional surface of a Ti-5553 melt bead. First, an ‘ideal’ EBSD dataset was taken from a
172 well-polished, scratch free, surface captured using 4x frame averaging resulting in slow capture
173 rates but high quality orientation data; the EBSPs from this dataset would ultimately not be used
174 in any following analysis, but the orientation data from this scan would be used to generate and
175 simulate patterns for DA training. These Ti-5553 surfaces were then heat treated to relieve any
176 internal residual stresses in a Across TF1700 tube furnace at 300°C for 2 hours and allowed to
177 cool at 2 °C/min under .5L/min of argon to prevent oxidation. We then collected a second,
178 demonstrative, HR-EBSD dataset from a scratched, poorly prepared, surface. This dataset was
179 chosen specifically because of the presence of multiple surface defects, lackluster pattern quality,
180 poor indexing metrics, and represents the experimental “as-collected” data being denoised and
181 reindexed. Both of these HR-EBSD datasets were collected on a ThermoFisher G4 UC
182 DualBeam FIB/SEM equipped with an EDAX Velocity EBSD camera, while the resulting data
183 from the “as-collected” surface was indexed with TSL OIM Analysis Version 8.1. 2x2 binning
184 was used on the detector representing a EBSP resolution of 235x235 pixels. Note that our
185 detector featured two dead zones along the phosphor screen, these are present visually as two
186 dark rounded rectangles in the EBSPs shown in Figures 2 and 3. These dead zones were caused
187 by a sample crash from a prior user, and served to demonstrate a ‘worst case’ scenario of
188 detector damage induced noise on pattern collection. Collected data was then processed through
189 the DA and reindexed in TSL OIM Analysis software to understand the effects of EBSP

190 denoising on indexing metrics. Model training and the theory behind that training is described in
191 section 3.1.

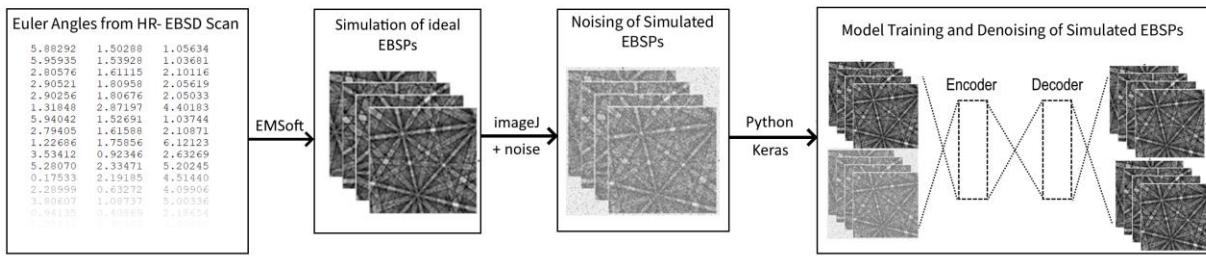
192 Seeking to extend the improvements from indexing towards HR-EBSD dynamic strain
193 measurements, the original as-collected data and DA-processed reindexed data was analyzed
194 using the open source EBSD cross correlation software OpenXY. [45] Dynamically simulated
195 reference patterns were used in cross-correlation utilizing the EMSSoft method described in
196 section 3.1 and 3.2. Mutual image information between simulated, zero-strain, EBSPs and the
197 experimental, as-collected, EBSPs was calculated with each iteration of cross-correlation for
198 both input datasets. No pattern centering (PC) calibration was performed in OpenXY, and a
199 radial region of interest (ROI) pattern was utilized with a total of 48 ROI's across each EBSP
200 being utilized in the shift calculations which is described in section 3.2.

201 **3) Theory and Calculation:**

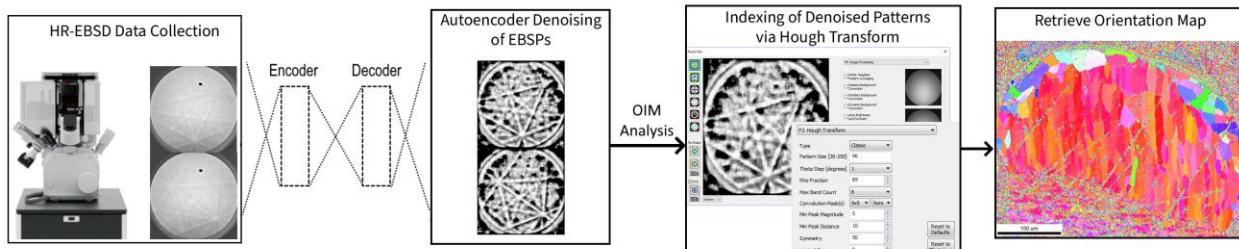
202 *3.1) Dataset Generation and Training the Denoising Autoencoder*

203 To generate EBSPs to train the model, a representative noise free dataset was generated using the
204 Monte Carlo-based EBSP simulation suite, EMSSoft [46], from the crystallographic orientation
205 information from the ‘ideal’ EBSD dataset mentioned in the Methods section. First, an EBSP
206 master pattern file was generated for β -titanium matching the energy conditions used in the
207 microscope. This method uses the Bethe Continuous Slowing Down Approximation
208 implemented in Fortran, along with the scattering cross sections determined by Rutherford
209 scattering, to produce distributions of the depth, direction, and energy of billions of back-
210 scattered electrons (BSEs) as reflected from a simulated β -titanium surface to produce simulated
211 EBSPs from these reflection conditions. [47] Using the Euler orientation data from the first
212 ‘ideal’ dataset, the microscope conditions/geometry, and the simulated electron diffraction
213 distributions, 37,135 simulated EBSPs were generated to construct a training dataset of noise
214 free simulated EBSPs. A matching noisy dataset was then constructed from these simulated
215 EBSPs, artificially noised with Gaussian noise ($\mu=0$, $\sigma=25$) and their contrast levels reduced in
216 imageJ to closely resemble low contrast found in the as-collected experimental EBSPs. Thus, the
217 autoencoder is trained via simulated EBSPs entirely and learns to reduce noise and enhance
218 contrast to what an idealized EBSP should look like regardless of orientation, crystal system, or
219 indexing solution. The autoencoder was programmed in Python utilizing the TensorFlow
220 libraries and trained with the simulated images. The model was trained for 10 epochs, a batch
221 size of 64, utilizing the ‘adam’ optimizer, and the mean square error loss function; resulting in a
222 final loss value of .0022. TensorFlow was not compiled or optimized for GPU utilization, and all
223 code was run on the CPU of a commercially available workstation. After training, the model was
224 validated with the simulated EBSPs such that the DA was able to accurately reconstruct noise-
225 free output from noise-free input as well as denoised output from noisy input. A schematic of
226 this process and where the DA fits in the HR-EBSD indexing procedure is described in Figure 1,
227 while a more in-depth flowchart of the autoencoder network and workflow is given in the
228 supplemental. The code utilized, the autoencoder model, and its weights are available at the
229 sourced Github. [48] A figure describing the training workflow, the architecture of the
230 autoencoder, and the denoising workflow is shown visually in the Supplemental Figure S1.

Dataset Generation and Model Training



Real EBSP Denoising and Indexing Workflow



233 **Figure 1: General workflow describing the autoencoder training methodology and its use**
 234 **within the EBSD indexing procedure.**

235 *3.2) Denoising, Re-indexing Patterns, and Strain Cross Correlation*

236 The noisy, as-collected, experimental EBSPs from the heat treated surface were stored in the
 237 proprietary EDAX *.up2* format, a single file storing every EBSPs in the scan as a 16-bit unsigned
 238 binary file with a mixed bit-depth header. This raw image file was separated into individual files
 239 such that the model could encode/decode each individual image rather than loading the entire
 240 image dataset into memory, or needing to build a method to parse the large proprietary datafile.
 241 Each EBSP was then processed through the trained DA using Keras' forward prediction
 242 functionality. Optional in this process is the use of contrast limited adaptive histogram
 243 equalization (CLAHE) as implemented in the CV2 library for either pre-processing or post-
 244 processing of EBSPs alongside DA-processing, and in this case CLAHE was applied post-DA-
 245 process to produce the results shown in section 4. The directory of loose images is then
 246 repackaged into the *.up2* format for analysis and re-indexing in TSL OIM Analysis v8. Dataset
 247 background correction and/or automatic brightness and contrast (auto B/C) was utilized when re-
 248 indexing to examine how the DA-processed EBSPs could be further enhanced by common image
 249 processing methods and how they compare with them. The same methods were utilized on both
 250 the as-collected patterns and DA-processed patterns to allow a direct comparison.

251 Quantifying residual strain in the datasets was performed with the open-source software package
 252 OpenXY [45], utilizing the dynamically simulated pattern configuration for absolute strain
 253 determination. Specifically, the stable 'UPfile' branch of OpenXY was utilized as it gives the
 254 ability to load and quickly work with the *.up2* file format. The absolute cross-correlation process
 255 dynamically simulates an ideal, strain-free, reference EBSP through EMSoft for each orientation

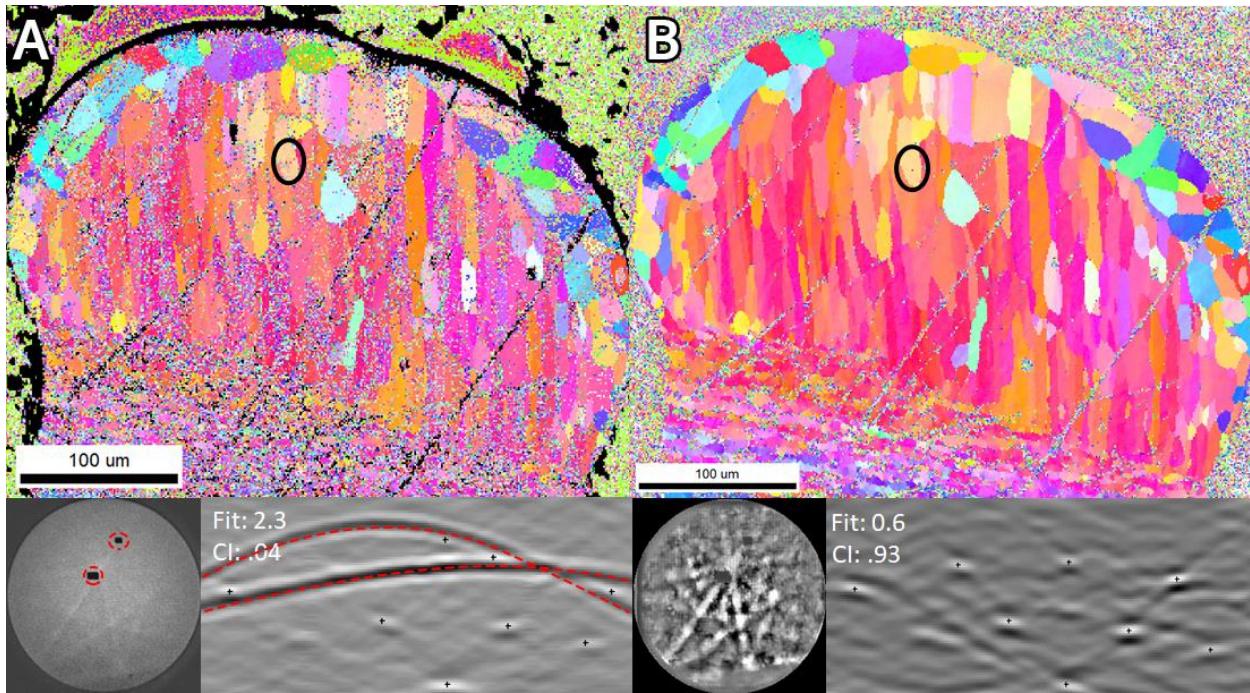
256 point and EBSP in the experimental datasets. At each point of cross-correlation an ROI screen is
257 then applied to both the reference and experimental pattern, and the shifts in EBSP features
258 within those ROIs is utilized to calculate the elastic distortion tensor: $\beta=F-I$. The full
259 deformation gradient tensor, $F=R^*U$, is split into a rotational (R) and strain (U) component, with
260 the strain component given by $U=I+\epsilon$. Thus, by comparing shifts between experimental and
261 dynamically simulated strain-free reference patterns, the deformation gradient tensor and
262 absolute strain within the experimental pattern can be determined by solving $F=R^*U$ from the
263 measured shifts in the elastic distortion tensor β and the identity matrix I . [8], [45], [49]

264 A detailed workflow showing all the steps utilized in EBSD data capture, image processing,
265 indexing/re-indexing, EBSD data cleaning, and where the DA fits within this workflow is given
266 in the Supplemental Figure S2.

267 **4) Results:**

268 *4.1) Pattern Quality and EBSD Indexing Improvement*

269 The model trained on simulated datasets was able to correctly identify that band contrast and
270 Kikuchi line intersections were of visual importance, leading to local enhancement of the
271 Kikuchi lines relative to the background, and resulting in more easily identifiable and
272 pronounced peaks in Hough space. This is clear in Figure 2, which shows the IPF map of the as-
273 collected EBSD data in contrast to the IPF map of the DA-processed data with examples of their
274 respective EBSPs in real and Hough space. The denoised EBSPs show greater peak contrast in
275 Hough space, and as a result the OIM Hough transformation and indexing algorithm produces a
276 higher fit accuracy and confidence index. A full comparison of image processing and reindexing
277 parameters between the as-collected and denoised EBSPs across the entire sample area is shown
278 in Figures 4 and 5, with IQ, IPF, and fit maps given, and a table of indexing quality metrics
279 shown in Table 2 to more quantitatively compare results with different re-indexing parameters.
280 The total time for the model to load and denoise the entire dataset (124658 EBSPs) utilizing only
281 the CPU was 3 hours and 19 minutes, translating roughly to a post-processing latency of 10.4
282 patterns/second.

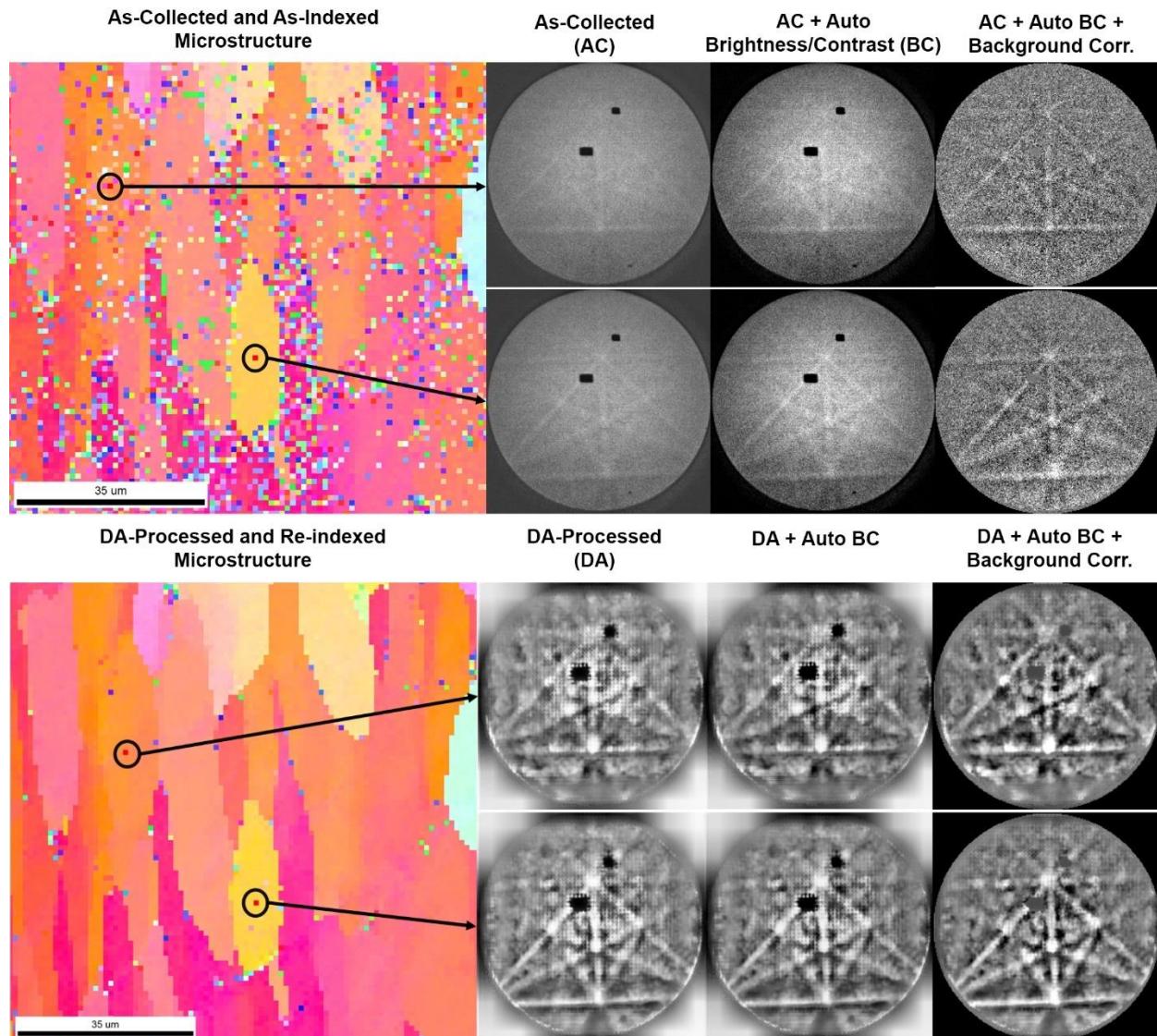


283 **Figure 2: IPF map of the indexed as-collected EBSPs (A) and the DA-processed EBSPs (B),**
 284 **with respective EBSPs and resulting Hough transformation from a single point within the**
 285 **circled grain. The indexed fit and CI are given for each pattern, while detector dead**
 286 **zones are highlighted in both real and Hough transform space.**

287 Figure 2 summarizes the overall improvements to indexing that patterns denoised with the
 288 autoencoder provided, showing the effect the autoencoder had on the EBSPs, their resulting
 289 Hough transformation, and improvement towards CI and degree of fit. Figure 2.A shows the IPF
 290 from the as-collected data without any further post-processing or re-indexing, with significant
 291 orientation noise visible within the scan. Figure 2.B shows the IPF generated by indexing the
 292 DA-processed EBSPs with background correction and auto B/C enabled as image processing
 293 during reindexing, it is identical to Figure 5.F. This highlights the best performing dataset,
 294 patterns which have been DA-processed and conventional image processed, alongside the worst
 295 performing dataset, the raw as-collected data. It is shown enlarged here for context to highlight
 296 how improvements to individual EBSPs processed by the DA result in an overall the reduction of
 297 noise visible in the orientation map. Note the effect of background correction on the dead zones
 298 highlighted in 2.A, and how these dead zones impact the quality of the initial Hough transform
 299 solution in comparison.

300 Examining the changes that both the autoencoder and conventional image processing techniques
 301 have on the diffraction patterns themselves, both in comparison and in combination, Figure 3
 302 shows a cropped selection of the microstructures shown in Figure 2 and two diffraction patterns
 303 from the same grain for both the DA-processed patterns and the as collected patterns. The as-
 304 collected patterns and DA-processed patterns are shown both independently, and in combination
 305 with the common image processing options often used in post-collection re-indexing; the effects
 306 of which we show quantitatively in Table 2. There are distinct differences in the contrast and

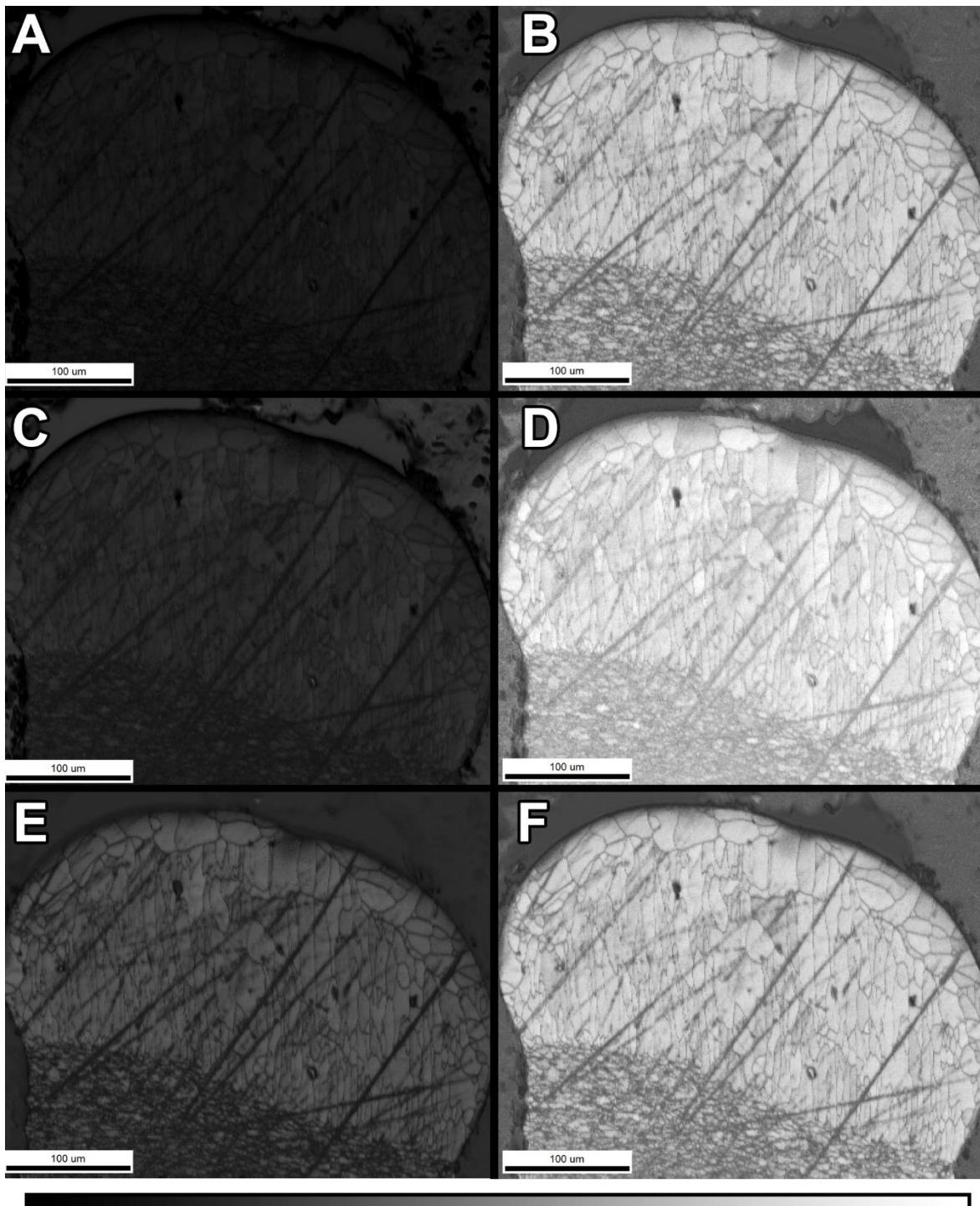
308 band definition when comparing the as-collected and DA-processed patterns, and differences in
309 how these image processing options impact the final image quality of each. Background
310 correction in both cases leads to the infilling and correction of the effects of the detector dead
311 zone. It is not the DA-process which infills this detector damage noise, however there is less
312 observable Gaussian-type noise introduced via background correction to the DA-processed
313 patterns than the as-collected ones. In general, the definition of the Kikuchi lines and their
314 intersection points are better defined against the background when comparing the DA-processed
315 patterns to the as-collected patterns.



316
317 **Figure 3: Pattern level comparison of DA-processing and common image processing**
318 **techniques utilized in re-indexing.**

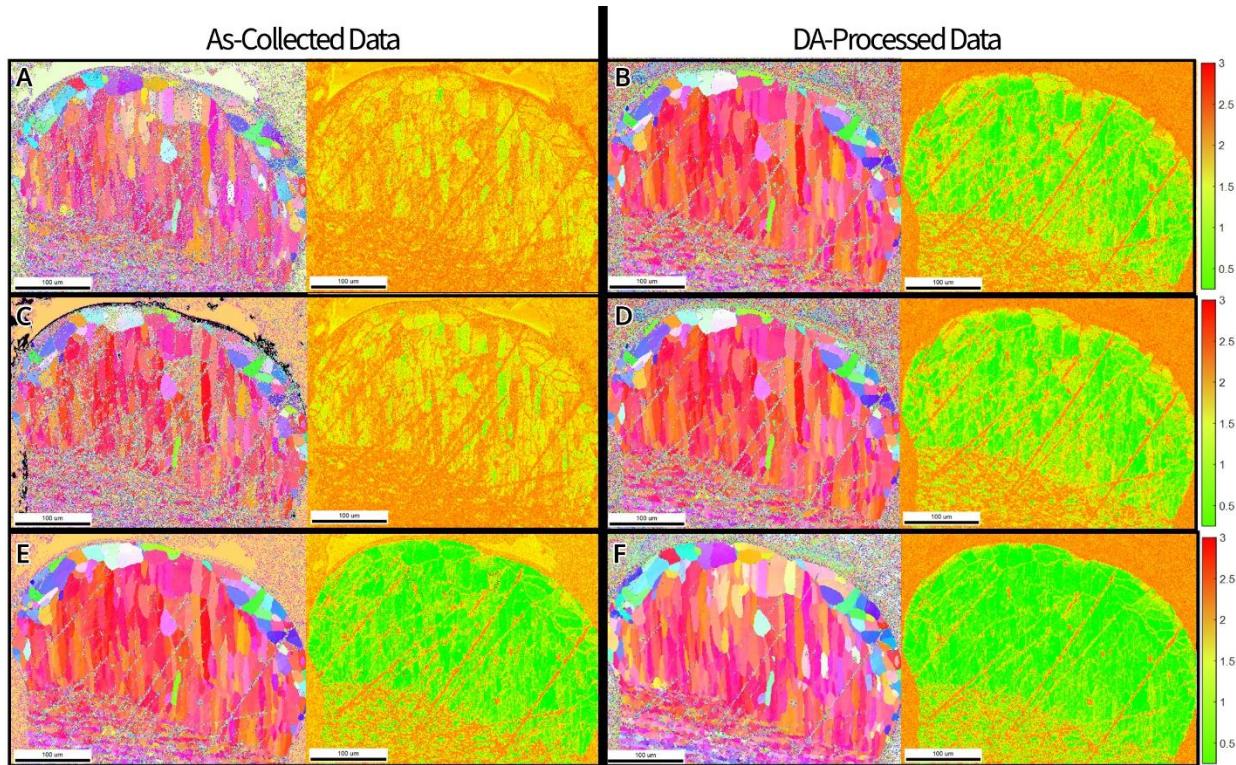
319 Examining the IQ maps of each of these conditions in greater detail, the improvements shown at
320 the pattern level can be observed across the whole microstructure dataset. Figure 4 shows the IQ
321 maps of the same image processing conditions shown in Figure 3, allowing a comparison of IQ

322 improvements between both conventional image processing and novel DA-processing pathways.
323 Although improvements to IQ can be observed with the as-collected patterns using conventional
324 image processing techniques, greater improvements to IQ are obtained through DA-processing,
325 and these increases are further improved by subsequent image processing while reindexing. Note
326 that scratches and pores remain relatively low in IQ as no diffraction would be expected in these
327 regions.



328

329 **Figure 4: IQ maps of the EBSD dataset utilizing the as-collected patterns (A, C, E) and the**
330 **DA-processed patterns (B, D, F). The IQ maps for both of these datasets re-indexed with**
331 **automatic brightness and contrast enhancement are shown in (C) and (D), respectively,**
332 **with the addition of background correction shown in (E) and (F).**



333

334 **Figure 5: IPF (left) and degree of fit (right) maps of the as-collected and DA-processed**
 335 **datasets, with no additional image processing performed in re-indexing (A,B), with auto**
 336 **B/C adjustment preformed while re-indexing (C,D), and both auto B/C and dataset**
 337 **background correction preformed while re-indexing (E,F). The scalebar reads 100μm.**

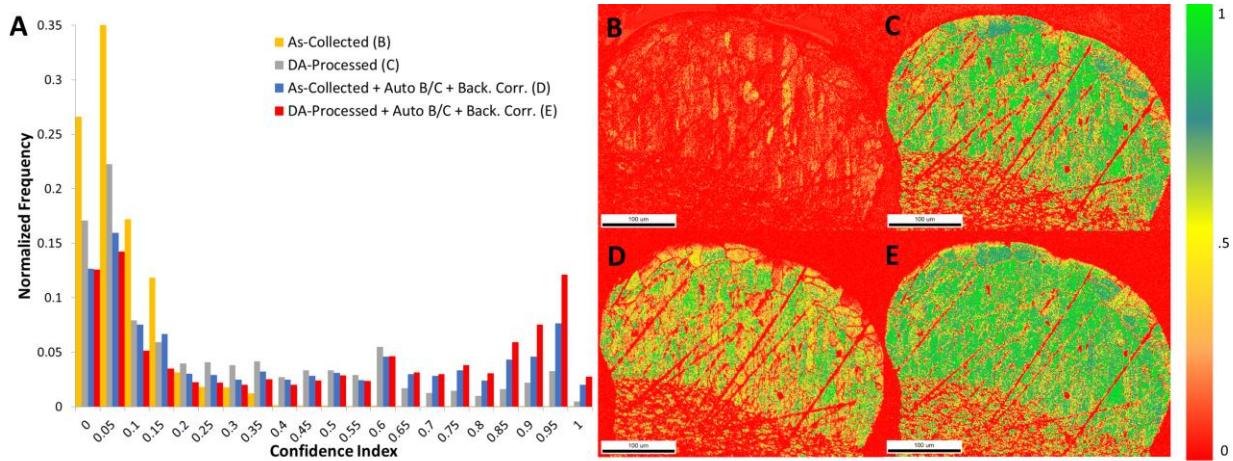
338 Figure 5 visually demonstrates the denoising performance of the EBSPs processed through the
 339 autoencoder (B,D,F) with the as-collected EBSPs (A,C,E) combined with commonly used EBSD
 340 post-processing techniques used in re-indexing: auto B/C and background noise correction.
 341 Figure 5.C shows that auto B/C alone is insufficient, showing minimal improvements to fit
 342 accuracy and orientation noise, while Figure 5.E indicates that incorporating background
 343 correction in re-indexing alongside auto B/C can improve fit and indexing quality, but is
 344 outperformed by the DA when combined with the same image processing conditions as shown in
 345 Figure 5.F. The DA-processed data shown in Figure 5.B resulted in significantly less orientation
 346 noise and a higher degree of fit accuracy when indexed compared to the as-collected patterns,
 347 both with and without auto B/C image processing shown in Figure 5.C and 5.A respectively.
 348 Combining the DA-processed patterns with a combination of image processing while re-indexing
 349 resulted in the best performance, with superior indexing metrics shown for all DA-processed data
 350 relative to as-collected data, resulted in higher IQ in all cases, reduced orientation noise, and
 351 significantly improved indexing properties when quantitatively compared in Table 2.

352 **Table 2: Comparison of indexing metrics between the as-collected (AC) EBSPs and DA-**
 353 **processed EBSPs with common re-indexing post-processing settings: automatic brightness**
 354 **and contrast correction (auto B/C) and dataset background correction (back. corr.)**

	As Collected (AC)	DA Processed (DA)	AC + auto B/C	DA + auto B/C	AC + auto B/C + back. corr.	DA + auto B/C + back. corr.
Average CI:	0.06	0.25	0.04	0.27	0.37	0.45
CI > .2 [%]:	5.29	42.85	7.86	45.02	54.18	62.30
Average Fit (°):	1.83	1.68	1.96	1.64	1.50	1.40
Fit < 1° [%]:	0.03	9.27	0.1	23.73	19.28	36.44
Average IQ:	1265	9804.54	2145	9682	3130	8856

355

356 The DA framework for denoising EBSPs resulted in higher CIs, fit, and IQ than the as-collected
 357 patterns when normalized across the different re-indexing image processing conditions,
 358 outperformed auto B/C image processing alone, and combining the DA with re-indexing image
 359 processing resulted in the best indexing performance. Although improvements can be observed
 360 with the as-collected EBSPs enhanced by combining both auto B/C and dataset background
 361 correction, it is important to note that these gains are only further enhanced through the use of
 362 the DA to process the EBSPs prior to re-indexing and that the DA results in significant
 363 improvements to fit, IQ, and CI on its own. Examining the CI distributions in greater detail, we
 364 find that the autoencoder results in high CI points with greater frequency than just using post-
 365 processing and re-indexing alone, and that the DA is not falsely generating indexable features
 366 from pure noise. This is clear when visualizing the CI as shown in Figure 6, in that regions we'd
 367 expect to be indexed with zero confidence (i.e. scratches, mounting compound surrounding the
 368 melt bead, and surface defects) are not artificially improved simply by parsing the patterns
 369 through the DA, and the CIs in these regions remains low. Instead, the DA results in increased
 370 frequency of high CI points ($CI > .5$) and reduced frequency of low CI points ($CI < .2$) compared
 371 to the as-collected data both with and without post-process re-indexing. Examining the CI
 372 distribution leads to a similar result described in Figure 5 and Table 2, where the DA-processed
 373 data shows large improvements over the as-collected data, and is further enhanced by using
 374 dataset background correction as image post-processing in re-indexing.



375

376 **Figure 6: A comparison of CI values from indexed EBSPs as shown via histogram (A) and**
 377 **visually with a colormap. The CI maps from the as-collected data is shown in (B) while DA-**
 378 **processed data is shown in (C). Examining the effect of image processing while re-indexing,**
 379 **the CI maps for the as-collected (D) and DA-processed (E) EBSPs re-indexed with**
 380 **additional post-processing is shown in (D) and (E), respectively.**

381 *4.2) Autoencoder Denoising and Dynamic Strain Cross-Correlation*

382 Generally speaking, two inputs are required in the dynamic cross-correlative strain measurement
 383 process: the experimental EBSPs which contain the local strain and orientation information and
 384 the corresponding map of indexed Euler angles. Examining how improvements to the EBSP
 385 pattern quality driven by the DA would impact the dynamic strain cross-correlation process, we
 386 find that the mutual information within the cross correlated regions of interest (ROI) is higher
 387 between DA-processed EBSPs and the simulated zero strain EBSP than with the as-collected
 388 EBSPs. Mutual information between two images is defined as the difference of the signal
 389 entropy between the two, normalized by the sum of their frequency histograms; in other words
 390 the DA-processed EBSPs feature greater ROI correspondence to and image likeness with
 391 simulated EBSPs when compared to as-collected EBSPs. [50] The distribution of the mutual
 392 information across the datasets is shown in Figure 6.A, showing the shift of the distribution to
 393 higher mutual information with the DA-processed EBSPs and DA-reindexed Euler angles.
 394 Examining if simply improving the degree of fit and providing more accurate Euler angle input
 395 to the cross-correlation process would result in more accurate strain measurement, Figure 7.B
 396 shows the resulting strain map when using the as-collected EBSPs but the DA-reindexed Euler
 397 angles for generating the simulated patterns. Better fit Euler angles combined with as-collected
 398 EBSPs results a noisy strain map with an order of magnitude of higher strain that does not trend
 399 with the other datasets, indicative of a poor absolute cross-correlation result. The strain maps
 400 using as-collected EBSPs and as-indexed Euler angles is shown in Figure 7.C, while the strain
 401 maps using the DA-processed EBSPs and DA-reindexed Euler angles is shown in Figure 7.D.
 402 The strain results indicate that using both the DA-processed images and the DA-reindexed Euler
 403 angles as cross-correlation input results in the clearest strain map, with reasonably low strain
 404 values for an annealed sample, and higher correspondence between the experimental pattern and
 405 the simulated one.

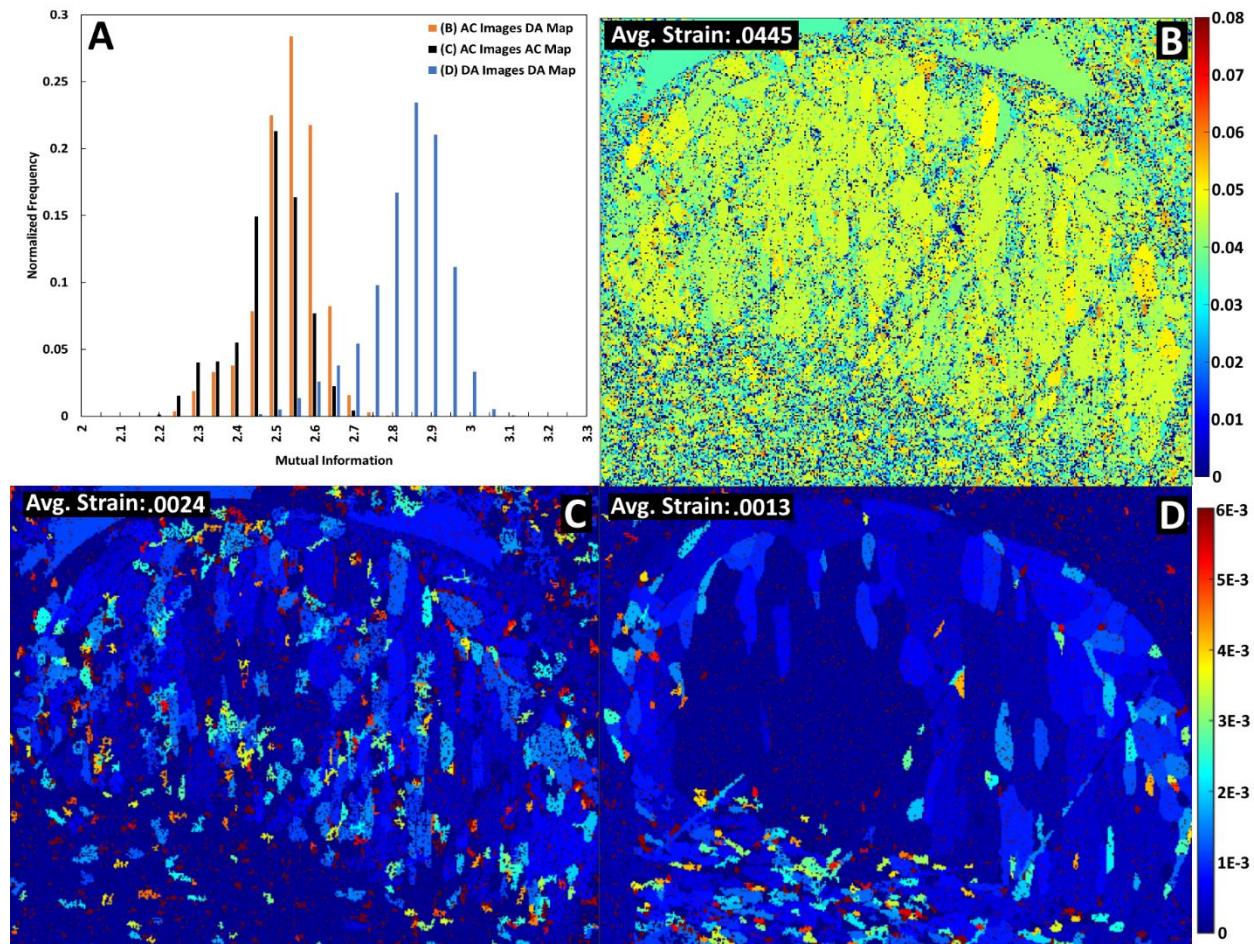
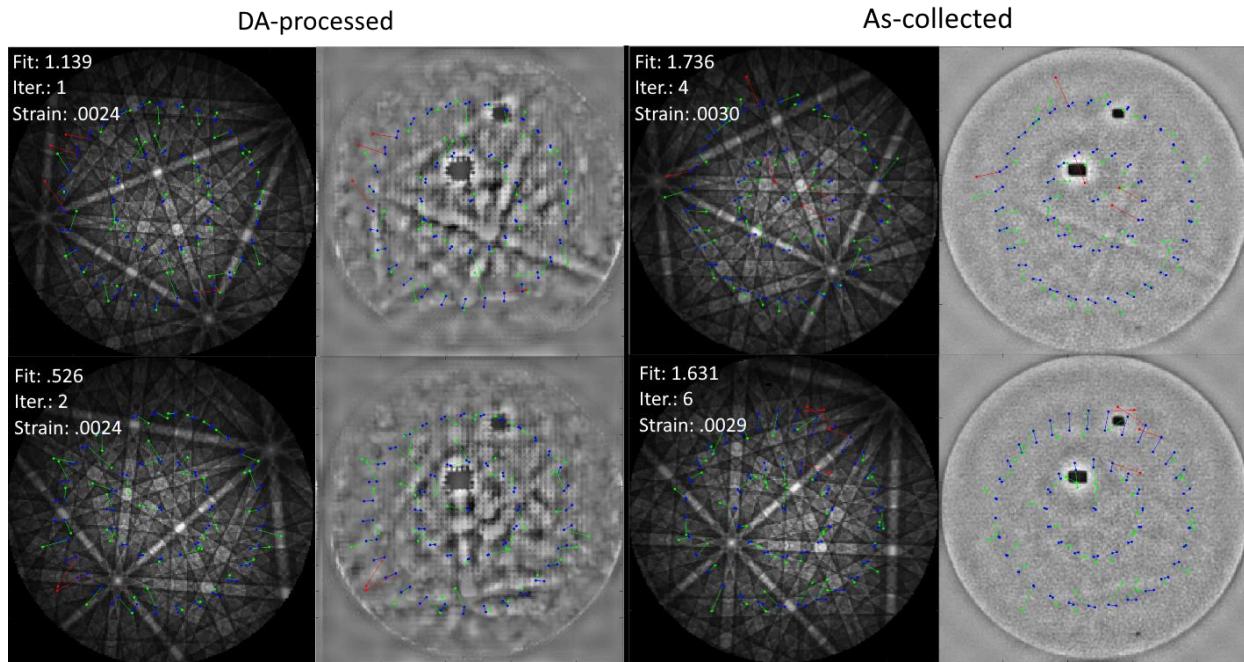


Figure 7: Histogram (A) of the mutual information between the experimental and simulated patterns used in HR-EBSD cross correlation, each distribution matching the dynamic strain analysis shown in the following plot. (B) shows the strain that results when correlating the as-collected patterns to patterns simulated using the Euler angles from the DA-reindexed fit, (C) is the strain resulting from as-collected patterns and the originally indexed Euler angles, and (D) shows the strain resulting from the DA-processed images correlated against patterns simulated from the DA-reindexed fit.

Further analyzing the mechanisms of how the EBSPs impact the dynamic pattern simulation and cross correlation process at the individual pattern generation and deformation gradient calculation level, Figure 8 shows the same two indexed EBSPs from the DA-processed and as-collected datasets alongside the simulated zero-strain EBSPs generated for both. The simulated EBSPs are overlayed with the ROI shift required to fit the two patterns, the magnitude of these shifts is used to calculate the deformation gradient tensor and thus strain between the zero-strain simulated reference and strained experimental EBSP. Figure 8 shows that the DA-processed images and better fit DA-reindexed Euler orientation results in a simulated EBSP with greater convergence with the experimental pattern, reduced local strains, and less computational

424 iteration required to arrive at a solution. The simulated EBSP generated from the DA-processed
 425 orientation data more closely correspond to the experimental EBSP, and although subtle, this
 426 results in less rotational and positional deviation from the experimental pattern when compared
 427 to the as-collected dataset. Comparing the overlayed ROI shifts, the magnitude of these shifts is
 428 reduced when using the DA-processed data while the number of outliers is also reduced.



429
 430 **Figure 8: Comparison of the cross correlated ROI shifts between the simulated and**
 431 **experimental EBSP when using DA-process (left) and the as-collected and originally**
 432 **indexed data (right) from the same two points. Experimental EBSPs are shown to the right**
 433 **of their matching simulated EBSP. Annotated above each pair is the degree of fit, strain,**
 434 **and number of iterations required to arrive at the solution. The EBSPs are overlayed with**
 435 **ROI shifts: the green lines represent the shifts used to calculate the deformation tensor,**
 436 **red lines represent outliers ignored by the calculation, and blue lines are the shifts predicted by**
 437 **the final deformation gradient tensor.**

438 **5) Discussion**

439 *5.1) Improvements to EBSD Orientation Indexing*

440 Utilization of a denoising autoencoder as an image preprocessor for EBSPs prior to indexing is a
 441 good solution for indexing noisy EBSD datasets, and especially when used in tandem with
 442 existing image processing like background correction and auto B/C, as usage of the autoencoder
 443 leads to a higher accuracy Hough indexing procedure than simply re-indexing with these options
 444 alone. Table 2 shows commonly described indexing metrics used to qualify EBSD scans (IQ, CI,
 445 fit), while Figure 2 and 3 describes at the pattern level the mechanism by which these
 446 improvements are derived. The accuracy of the Hough procedure, whereby the orientation of the
 447 crystal is determined by the angle and distance between the Hough peaks, rapidly deteriorates

448 with image noise and especially band contrast. This lack of contrast results in low IQ, visible in
449 the as-collected datasets in Figure 4. The low band contrast results in the Hough peaks shown in
450 Figure 2.A being difficult to detect from the background, and are even skewed or overshadowed
451 by a dead zone in the detector screen. In Figure 2.B we see that the autoencoder is able to
452 enhance band contrast in the EBSPs and thus peaks in Hough space, and when combined with
453 background correction also leads to infilling of dead zones on the detector. The improvements to
454 band contrast across the whole dataset becomes clear when comparing the IQ maps in Figure 4,
455 as the IQ of the whole dataset is improved, while relative differences in IQ values between grains
456 are still maintained. These improvements are derived from how the model was trained. The
457 simulated EBSPs generated by EMSoft contained no noise and perfect band contrast, and served
458 as the training target. By artificially noising them to near-experimental levels and using this as
459 the noisy training input, the autoencoder learns to reproduce high quality EBSPs from noisy
460 ones. Although one single metric (IQ, CI, or fit) alone cannot alone describe the quality of an
461 EBSD dataset due to the convolution of factors which cause noise in electron diffraction
462 patterns, usage of a convolutional autoencoder leads to improvements to all metrics
463 simultaneously. When utilized on noisy experimental patterns the model results in both visual
464 and quantitative improvements to the IPF and degree of angular fit maps in Figures 5 while also
465 improving the whole distribution of CI across the dataset as shown in Figure 6. Thus, the DA
466 model improves both the fit of the orientation solution and the confidence in the accuracy of that
467 solution simultaneously. Importantly, the degree of fit is improved with utilization of the DA
468 prior to re-indexing, with Table 2 showing that ~36% of the data had a fit parameter of less than
469 1° of misorientation from the indexing solution. The improvements made using denoised EBSPs
470 prior to Hough indexing results in orientation maps of similar quality to those demonstrated with
471 the DI and SHT based indexing methods when indexing noisy datasets, but we note a full
472 quantitative comparison between different indexing methods would require additional analysis as
473 we are using an entirely different dataset and material system. [25], [51]

474 This denoising model is an inherently generative one, so it is critical we ensure the DA is not
475 generating new information from pure noise or encoding new Kikuchi bands and EBSP features
476 from non-existent data. The fit and CI values as mapped in Figures 5 and 6 are critical in
477 assessing this. Scratches, defects, or a high density of grain boundaries on the imaged surface
478 would result in EBSPs of high noise due to lack of coherent diffraction and would result in near
479 zero CI and low fit accuracy within these regions. In the noisy as-collected dataset we see this is
480 true, and the scratches stand out as a consistent low point of reference on the fit and CI maps of
481 each dataset regardless of DA processing. Thus, we find that the DA is only improving EBSP
482 features that are present, within regions where electron diffraction would be expected and
483 observed. Regions of pure noise, such as those within the mounting compound, are not being
484 falsely improved nor is non-existent data is being generated by the model as we do not see an
485 indexing solution in these areas. Indeed, examining Figure 6 we find that denoising leads to
486 improvement in CI within grains that were mapped with low confidence, rather than defects
487 mapped with zero, and we observe that the DA results in an increase in frequency of high
488 confidence points only within the melt pool boundary.

489 The noise limitations of the Hough transformation indexing procedure can be addressed by
490 denoising the EBSPs prior to the transform as a form of image pre-processing, and a higher
491 degree of angular fit, CI, IQ achieved while still using the conventional Hough indexing method.
492 Because this denoising occurs post-collection, no additional processing time or latency is
493 introduced at the point of data collection while still utilizing faster and more conventional Hough
494 indexing once the EBSPs have been denoised, enabling more noise tolerant collection at the
495 detector without additional time penalties induced by frame averaging or conventional image
496 processing. The indexing uncertainties of the Hough-transform that arise from noisy images can
497 be alleviated, and the autoencoder method of denoising we demonstrate shows greater robustness
498 to pattern noise than convolutional neural network based indexing methods. [38] The DA method
499 demonstrated offers improvements over the Hough-transform augmented with various forms of
500 image post-processing, without the losses in resolution associated with NPAR. [24] The latency
501 of the DA, running only on the CPU on a modest workstation (Intel i9-9900, 64GB RAM), is
502 ~10.4 patterns/second and is comparable to that of the dictionary method at ~11.6
503 patterns/second. [27] The total calculation time from denoising to indexed solution is less, taking
504 approximately 4 hours to denoise and reindex a dataset of 124658 EBSPs, compared to
505 approximately 110 hours to index a dataset of 333227 EBSPs using the DI method; but is slower
506 than the SHT methods discussed in the introduction. [25] We also note that the denoising method
507 demonstrated here is agnostic towards its material crystal system, it simply denoises EBSPs,
508 while the DI method becomes increasingly computationally complex with increasing crystal
509 symmetry due to increasing dictionary size. [51], [52]

510 As denoising was run on the CPU only, computational overhead could be reduced by processing
511 images on the GPU by enabling CUDA support. The DA could also be translated to hardware, at
512 the detector level, in FPGA form for a more energy and computationally efficient
513 implementation. [53], [54] We also must stress that the model was trained with a specific EBSP
514 resolution and detector binning (2x2) in mind, and thus alterations to the model architecture may
515 be necessary for compatibility with patterns collected at higher or lower resolutions. Although
516 EBSP denoising does add computation time following data collection, it does not do so at the
517 point-of-collection or point-of-indexing, and thus could easily be integrated into existing high
518 speed EBSD workflows. When used as EBSD data post-processing, this DA method can enable
519 faster data collection speeds at the detector by allowing collection of noisier EBSPs at lower
520 exposure times. This can help further enable the capture of larger microstructural areas with
521 greater spatial resolution while utilizing conventional Hough-transformation indexing methods.

522 *5.2) Implications of DA post-processing towards HR-EBSD Strain Measurement*

523 As discussed in the introduction, quantifying absolute strain from HR-EBSD pattern cross
524 correlation relies on good convergence between a simulated, zero strain, EBSP and the
525 experimental EBSP. This can be achieved by way of enabling higher accuracy measurement of
526 orientation with DA-processed EBSPs, and with ~36% of the data showing sub-1° of fit, a higher
527 accuracy Hough procedure enables more accurate pattern simulation and absolute strain cross
528 correlation. The improvements to the fit parameter, CI, and orientation indexing observed in
529 Figure 5 translates to a more accurate generation of simulated EBSPs for cross correlation due to

530 increased accuracy of the measured Euler angles, and when combined the enhanced band
531 contrast and edge definition of the DA-processed EBSPs, produces a cross-correlation result with
532 less error and requires less computational iteration to arrive at a solution. This is because
533 uncertainty and error in the Hough indexing procedure carry into the EBSP pattern generation
534 and strain cross correlation procedure, and a poorly indexed experimental point will generate a
535 poorly fit simulated EBSP. Thus, if orientation measurement error can be minimized so to can
536 absolute strain measurement error. [1] As Figure 8 would indicate, increasing the orientation fit
537 accuracy with refined Euler angles does increase correspondence between the simulated zero-
538 strain EBSP and the experimental pattern used to calculate the deformation gradient tensor, while
539 Figure 7.A and B show it is not merely the improved Euler angle fit but that EBSP image quality
540 improvements themselves also drive improvements as well. A combination of the more
541 accurately fit simulated pattern and the DA-improved EBSP image quality is the source of the
542 increased mutual information seen across the datasets in Figure 5.A and this results in reduced
543 ‘phantom’ or erroneously calculated strains across the entirety of the dataset. As the zero-strain
544 point of cross correlation is more accurately fit, the contributions of phantom strains calculated
545 from erroneous ROI shifts as shown in Figure 8, is reduced, leading to an overall lower average
546 strain. Hence when comparing the strain maps in Figure 7.B and C to D we see more areas of
547 contiguous strain being resolved with less high strain points randomly distributed, as point-to-
548 point misorientation noise is reduced and the patterns have less noise between them. This is why
549 there is significantly higher phantom strains manifested in Figure 7.B, as we are comparing a
550 more accurately simulated pattern to a poorer quality, as-collected image, which results in even
551 greater shift magnitudes between ROIs and a larger perceived deformation gradient. As the strain
552 cross-correlation process is sensitive to high degrees of misorientation between the reference and
553 experimental pattern, a more accurate and correctly fit input orientation map from Hough-
554 indexing results in a better fit zero-strain pattern simulation, and thus reduced ROI shifts and
555 strain magnitude. [1] The reduced number of iterations, and thus time, required to arrive at a
556 cross-correlated strain solution when utilizing the DA-processed patterns and indexing solution
557 could serve to increase the speed of this method, which is the subject of future research.

558 While the results demonstrate that the DA-processed images are more similar to an idealized
559 simulated EBSP and the improved fit map results in less noise across the strain map with reduced
560 phantom strain contributions relative to the as-collected dataset and patterns, other contributions
561 to phantom strain are not accounted for in this study. The relatively low resolution of the
562 patterns, intentionally poor sample surface preparation, and lack of pattern center (PC)
563 calibration prohibits us from claiming these strain measurements as a ground truth. We recognize
564 contributions from PC error were not addressed, although we argue that achieving such a low
565 absolute strain measurement (.10%) on a heat-treated sample does indicate this contribution is
566 minimal, but without further experimentation cannot quantify this. We note that the sample
567 EBSD area shown is ~.1mm² in surface area; and deviations from the as-calibrated PC and the
568 true PC would be expected. [14] We would expect greater strain accuracy and precision utilizing
569 higher resolution EBSPs or with higher resolution EBSD scans taken over a smaller imaging area
570 where less beam shift would be expected, but this requires additional study. Furthermore, no PC
571 recalibration or recalculation occurred in post-processing, and doing so could result in further
572 reductions to phantom strain and improved precision of the local crystal orientation. [55]

573 Although the improvements to indexing demonstrated by the DA framework shown translates to
574 improved convergence between experimental and simulated patterns, they do not account or
575 correct for PC shift error.

576 **6) Conclusions**

577 The noise limitations of the Hough transformation method of EBSD indexing can be overcome
578 and noisy EBSPs datasets indexed with greater success and accuracy with the use of a denoising
579 autoencoder to process the EBSPs prior to re-indexing. The autoencoder improves indexing
580 quality by improving Kikuchi band contrast and definition, and thus improves IQ, CI, and fit; the
581 neural network learning from noise-free, high contrast, EBSPs to discern high quality image
582 features from noisy ones. Thus, without the introduction of new indexing algorithms, the Hough-
583 transformation indexing process can be improved and made more accurate by denoising the
584 source EBSP prior to indexing. Even with physical dead zones in the detector screen and a
585 poorly polished sample, by combining our DA with existing image processing methods high
586 levels of indexing confidence can be achieved. Both with and without dataset background
587 correction, the denoised EBSPs resulted in a more coherent orientation map with higher CI, IQ,
588 and fit parameters than the as-collected dataset under identical conditions. The ability to index
589 EBSD datasets with greater noise tolerance can allow for faster data collection rates at the
590 detector, enable higher spatial resolution data collection for mesoscale EBSD experiments, and
591 the higher orientation fit accuracy enabled by DA-processing serve to improve the Hough-
592 transform method as a whole.

593 The improvements made to EBSP quality and subsequent indexing metrics also had implications
594 for cross correlative absolute strain measurement, although there are challenges still present with
595 the method. When using the denoised EBSPs and the higher fit accuracy Euler angles in absolute
596 strain cross correlation, the DA-processed dataset resulted in a more accurate generation of
597 simulated EBSPs from which strain is calculated and required less computational iteration to
598 arrive at a solution. When using the DA-processed EBSPs, there was less apparent
599 misorientation between the experimental pattern and simulated one, which resulted in a reduced
600 ROI shifts necessary to correlate the two patterns and the origin of the reduced phantom strains.
601 Thus, using DA-processed and re-indexed EBSPs offers improvement of correspondence
602 between the experimental and simulated patterns being cross correlated, and much more reliable
603 absolute strain measurements are enabled via HR-EBSD, in addition to improving the
604 indexability of noisy EBSD datasets in general.

605 **Acknowledgements**

606 We would like to thank Dave Rowenhorst at the Naval Research Laboratory for their helpful
607 conversations and insight towards working with '.up2' file structures. Additionally, we would
608 like to thank Jean-Baptiste Forien for their work on the manufacture of these samples and
609 continued support. Portions of this work was performed under the auspices of the Office of
610 Naval Research under contract N00014-20-1-2788. Portions of this work was performed under
611 the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory
612 under Contract DE-AC52-07NA27344.

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