

Nye Tensor Dislocation Density Mapping From Precession Electron Diffraction: Effects of Filtering and Angular Resolution

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The Nye Tensor describes the geometrically necessary dislocation (GND) density in terms of the number of dislocations required to accommodate a given contortion in the crystal lattice. It has been used extensively in recent years to quantify GND densities from data acquired using electron backscatter diffraction (EBSD) in a scanning electron microscope [1,2]. Thanks to the development of precession electron diffraction automated crystallographic orientation mapping (PED-ACOM) for transmission electron microscopes (TEM) [3], the same type of spatially resolved orientation data produced using EBSD can now be acquired at a much smaller length-scale. By utilizing nano-scale orientation data to calculate GND densities, the detailed dislocation structure of deformed metals can be observed and quantified.

In [4] a methodology for applying Nye tensor analysis to map GND densities from PED-ACOM data is presented. In the present work, this technique is demonstrated with a focus on the effects of angular resolution and data filtering on the dislocation density values calculated. PED-ACOM patterns were acquired and indexed using a JEOL 2100 LaB₆ TEM equipped with NanoMEGAS SPINNING STAR™ precession electron diffraction and ASTAR™ ACOM systems with approximately 0.5° angular resolution and a step size of 10.4 nm. Five out of nine Nye tensor components are calculated and used to estimate the total GND density at each point in the scan using a least-squares method to provide the most continuous curvature between the orientation of a given point and its eight nearest neighbors.

Fig. 1 shows GND density maps for a nanocrystalline Fe thin film (A,C,E,G) and a jet-thinned Cu TEM specimen (B,D,F,H). The average density values produced using this method are on the order of 10^{15} m^{-2} , higher than those reported from EBSD [1,2]. Three different methods of enhancing the dislocation maps are evaluated in order to determine what role, if any, noise due to comparatively poor angular resolution has on the values produced by this method. A low-pass Gaussian Fourier filter is used to remove high frequency noise such as that produced by from the calculated GND density values. This reduces the noise in the data visibly, causing a decrease in average density on the order of 10^{11} m^{-2} , well below the range of density values present. A Kuwahara filter is applied to the orientation data prior to the calculation of the Nye tensor. This results in substantive, qualitative changes to the maps produced and is therefore not recommended. An interpolation method [5] is used to enhance the angular resolution of the indexing software to approximately 0.3°. Improving the angular resolution in this fashion causes some change in the average density calculated for a given scan area, as would be expected when re-indexing orientation data using different parameters; it does not result in a systematic decrease in density values, however, as would be expected if noise due to lack of angular resolution were causing the GND density values to be significantly inflated.

References:

- [1] A.J. Wilkinson, D. Randman, *Philosophical Magazine*. 90 (2010) p. 1159.
 [2] T. Hardin, B.L. Adams, D.T. Fullwood, R.H. Wagoner, *Mater. Sci. Forum*. 702–703 (2011) p. 492.
 [3] E.F. Rauch and M. Veron, *Materwiss. Werksttech*. 36 (2005), p. 552.
 [4] A.C. Leff, C.R. Weinberger, and M.L. Taheri, *Ultramicroscopy* 153 (2015), p. 9.
 [5] E.F. Rauch, M. Véron, *Mater. Charact.* 98 (2014) p. 1.
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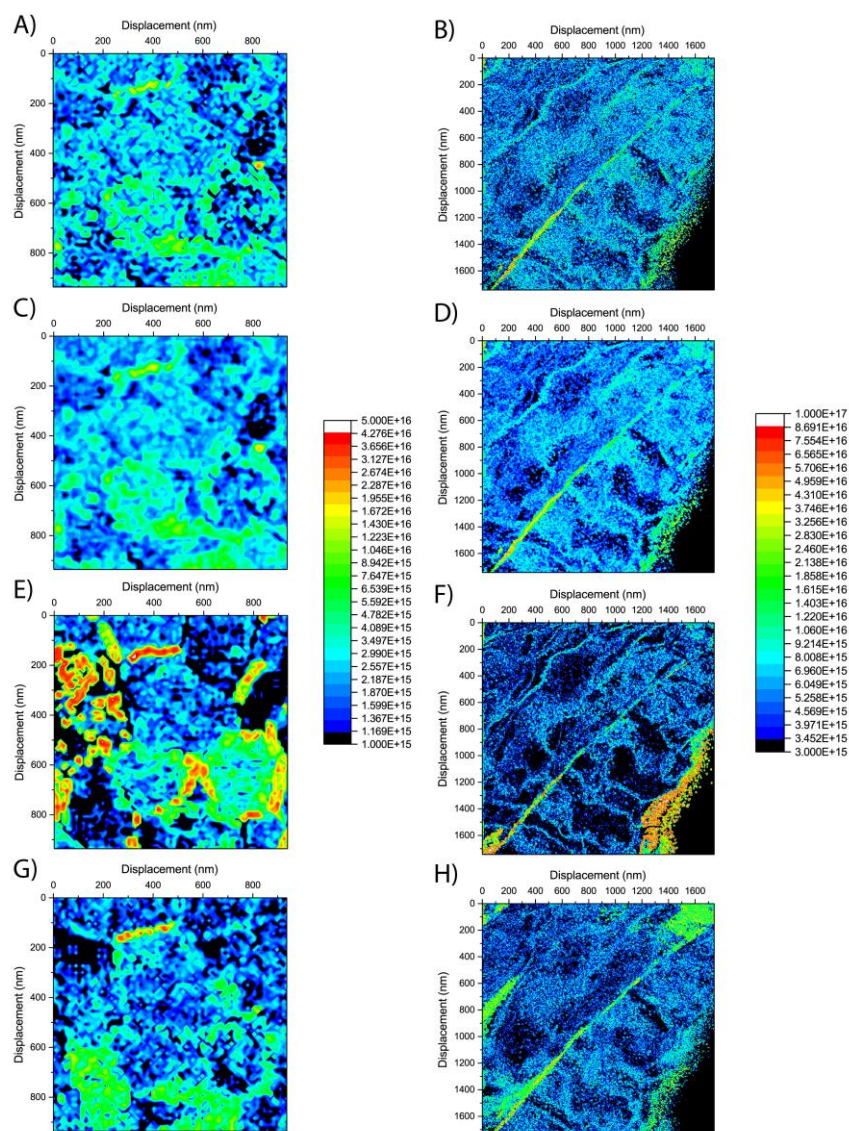


Figure 1. (A&B) GND density maps produced from raw data (no filtering). (C&D) GND density maps for the same regions as (A&B) produced from data that has been filtered using discrete Fourier transform analysis. (E&F) GND density maps produced using Kuwahara filtering. (G&H) GND density maps produced using interpolation method to refine the angular resolution. Color map units of m^{-2} .