A Strain Map Tensor Rotation and Strain Field Mapping Script for Digital Micrograph

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We present scripts developed to facilitate further analyses of results derived from Gatan Inc.’s STEMx™ strain mapping capability. Gatan’s software (based on work from Ozdol et al., [1]) measures changes in small (~ 1 mrad) convergence angle diffraction spot positions across a “4D-STEM” data cube and generates, by comparison to an unstrained reference region, relative strain maps $E_{xx}$, $E_{yy}$, and $E_{xy}$. Using Gatan’s software, care must be taken to relate the orientation of the STEM image with that of the diffraction patterns collected into the 4D data cube, which are rarely equivalent.

Initially, Gatan’s software defines strain directions $E_{xx}$, $E_{yy}$, simply as the $x$ and $y$ directions of the diffraction patterns, but STEM scanning directions are often rotated for alignment with features of the sample. This can lead to strain maps where the calculated strain tensor does not correlate with the image scan direction. The scripts we describe below, which are executed within Gatan’s Digital Micrograph software [2], were developed to first allow easy rotation of the strain tensor to accommodate operator choice of scanning direction. By imaging the sample within the condenser defocused 000 diffraction spot, the relative orientation between the sample and the diffraction pattern may be measured and our script rotates strain maps appropriately.

Figure 1 shows an example of a tensor rotation performed on data gathered from a cross-sectional sample of an epitaxial AlGaN-GaN interface. The upper images show the as-collected strain maps, in which $E_{xx}$ and $E_{yy}$ orientations are not matched to the $x$ and $y$ orientation of the STEM image. The lower Fig. 1 images show the data rotated correctly. As expected for an epitaxial layer with slightly smaller lattice constant than the substrate, the strain is dominated by compression in the $y$ direction.

Further, our script generates a stack of strain maps for a series of strain tensor rotations through 180 degrees in 1 degree increments (not shown). From the rotation stack, the script then finds the direction and magnitude of maximum strain at each pixel and generates maps of maximum strain value and angle. An example of a map of maximum strain value is shown in Figure 2(a), where color indicates strain sign (blue for positive, red for negative strain) and color intensity indicates magnitude. The script then uses this data to produce a vector field map, as shown in Figure 2(b), where a line at each pixel is aligned along the direction of maximum strain, colored according to the strain value map in Fig. 2(a). The vector field map may be useful for analyzing correlated regions with significant strain in directions away from the $x$ and $y$ directions such as those found along the threading dislocation that rises vertically through the data set shown, or strain resulting from smaller sample defects.

References:
Figure 1. (upper row) As-collected strain maps with \( x \) and \( y \) directions in the basis of the diffraction pattern, which do not correlate with STEM scanning direction, (b) rotated strain maps with \( x \) and \( y \) directions parallel and perpendicular to the AlGaN-GaN interface, respectively, with strain in the AlGaN layer primarily in the \( y \) direction. The contrast scale on the right applies to all images and the scale bar is 50 nm.

Figure 2. (a) Maximum strain in the Fig. 1 device for each pixel is mapped with red for compressive and blue for tensile strains. (b) In this strain field map, lines are drawn at each pixel along the direction of maximum strain and lines are colored following the strain value map in (a) to indicate sign and magnitude of strain. The contrast scale on the right applies to both images and the scale bar is 50 nm.