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Ad Hoc Determination of Local Misorientations and Boundary Planes between Grains in TEM by a Dedicated Software Package Developed for the Gatan DigitalMicrograph Platform

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Mechanical and electrical properties of materials are often highly dependent on the crystallographic direction by which they are measured. For properties being measured over spatially limited extents, grain boundaries (GBs) present in crystals can greatly complicate interpretation of results. It is therefore necessary to characterize GBs in terms of the rotation of a particular vector in one grain to a similar vector in another. In a similar fashion the GB between two crystal grains can have a multitude of possible GB plane configurations. These different GB plane configurations could potentially have a strong correlation with the properties of a crystal system, requiring the precise GB plane configuration to be determined for accurate interpretation of results. Understanding these geometric parameters defining the boundary between grains is essential for appropriate analysis of many problems facing a transmission electron microscope (TEM) operator. Often the method of investigation may change depending on the misorientaiton of two grains or the particular GB plane encountered by the microscopist during a microscope session. To expedite the process of TEM investigation involving individual GBs a method of determining a full geometric description of a GB during a microscopy session is desirable (ideally on-th-fly measurements). This project presents the creation of a software package for the Gatan Digital Micrograph platform that provides simple *ad hoc* determination of the misorientation and GB plane normal vector of a GB with minimal input from the microscopist.

For practical descriptions of the change in crystallographic directions and the GB plane between two grains an axis and angle of misorientation and GB plane normal are commonly used. A method for determining this axis/angle pair for describing the grain misorientaiton using only two convergent beam electron diffraction (CBED) patterns that include Kikuchi lines, proposed by Young et al. [1]. This method makes use of Euler's rotation theorem where two coordinate systems (A and B) may each be rotated onto a common coordinate frame, the rotation matrices describing each of these individual rotations may be combined into a matrix describing the rotation from A to B. The trace of this misorientation matrix provides the misorientation angle and the eigenvector with the corresponding real eigenvalue provides the axis of rotation. Determination of the GB plane normal requires further tilting of the specimen inside the TEM. A set of CBED patterns must be taken after specimen tilt, along with images of the GB before and after the tilt is performed. The CBED patterns are used to determine the physical crystal rotation inside the microscope and the GB images are used to determine the GB width before and after tilting. Performing this specimen tilt in the microscope allows the coordinates of two vectors in the GB plane to be determined, the cross product of these vectors results in the GB plane normal vector.

The software package for DigitalMicrograph was developed to determine both the misorientation axis/angle pair and the GB plane normal requires the user to take 3 CBED patterns and 2 GB images. The first two CBED patterns must be taken at the same specimen tilt conditions in an instrument with a well calibrated camera length. From these patterns the user selects the beam direction and either an indexed pole axis and a Kikuchi band incident on that axis, or two indexed Kikuchi bands on the diffraction pattern. The selection of the transmitted beam and bands or band and axis on each of the two diffraction patterns allows the computation of all the variables required to determine the misorientation axis/angle pair for the bicrystal. Similarly, with a third CBED pattern acquired after a specimen tilt the real specimen rotation axis can be calculated. The GB plane is determined by the user who selects the boundary trace and boundary width vectors on two GB images (before and after specimen tilt). Figure 1 shows a CBED pattern with a Kikuchi band and a pole axis [001] selected along with the incident beam direction. The variables needed to complete the misorientation analysis are shown on the Kikuchi pattern with D being the distance from the transmitted beam spot to the pole axis, δ being the angle from vector connecting the transmitted beam spot and pole axis to the Kikuchi band normal vector, and γ being the angle between the Kikuchi band normal vector and a reference axis x-direction. Figure 2 shows two possible [100]/45° bicrystals each with different GB normal vectors, illustrating the independence of GB plane with regards to GB misorientation.

[1] C.T. Young, J.H. Steele, JR, and J.L Lytton, *Met. Trans.* **4** (1973), 2081.
[2] The authors wish to acknowledge financial support from the NSF through grants DMR-0804528 and DMR-1040229.

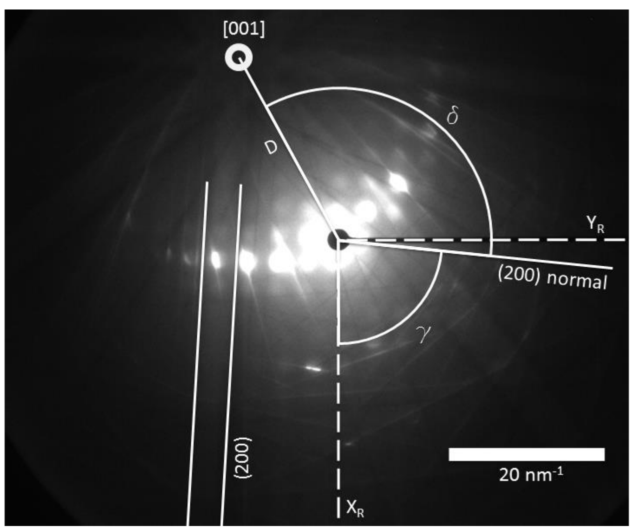

Figure 1 - A CBED pattern showing Kikuchi band and pole axis required for determining misorientaiton

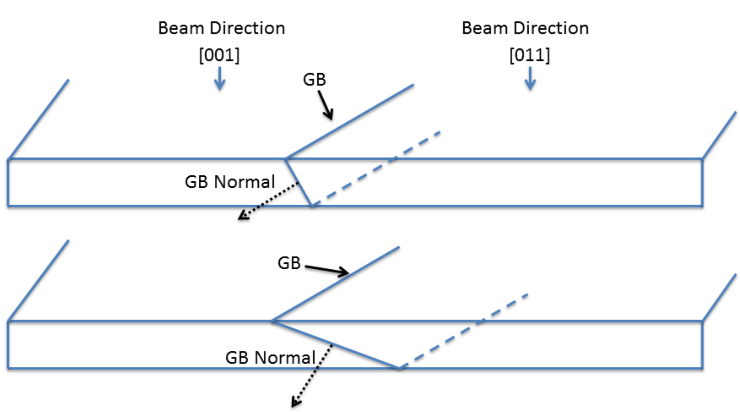

Figure 2 - Schematic diagram of two identically misoriented [100]/45° GBs with different GB planes

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