MIC file format

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These microstructure files (extension '*.mic*') contain the results of an orientation reconstruction run using the IceNine implementation of the forward model method.[1, 2] The file is composed primarily of a list of volume elements or voxels which are quasi-two dimensional objects giving crystallographic orientations within small measured volumes. Each voxel's characteristics are given on one line of the file. The voxels are equilateral triangles which, in most cases, fill a planar measured area which may be smaller than or larger than the actual sample cross-section.

Here is the file format with comments given below the Table:

1. Line 1: a single floating point number, B = Basis length[1]
2. Lines 2 - N: Voxel characteristics

Table 1. Voxel characteristics

Column(s)	
1 - 3	(x, y, z) coordinates in millimeters[2]
4	triangle orientation: 1 = vertex up, 2 = vertex down
5	g = triangle generation number (side length= $B/2^g$
6	crystallographic phase number[3]
7 - 9	Bunge Euler angles (degrees)
10	C = Confidence parameter[4]

[1] B is the reference length for triangle dimensions. Generation 0 ($g = 0$) triangles have this side length.

[2] x and y coordinates refer to the left-most vertex of an upward (in the xy-plane) or downward pointing equilateral triangle; by default, $z = 0$ but this can be replaced as appropriate for 3D data sets. Note also that the coordinate system is such that, at sample rotation angle $\omega = 0$, the x-ray beam propagates in the $+x$ direction.

[3] Default phase number is 1 or 0 for an accepted reconstructed orientation or lack thereof, respectively. For a MIC file merged from separate reconstructions using different crystal phases, this parameter can be used to keep track of which phase had, for example, a higher confidence parameter in each voxel.

[4] $\mathcal{C} = N_{exptl}/N_{sim}$, the fraction of simulated Bragg peaks (for the optimized lattice orientation) that match experimental diffracted beams. $\mathcal{C}$ is NOT a rigorous statistical metric as it depends on the range of Q included in the reconstruction compared to the range that is observed in the experimental data set. However, $\mathcal{C}$ can serve as a useful comparative characterization of the amount of scattering that was detected that corresponds to the optimized orientation for each voxel. $\mathcal{C}$ tends to be reduced i) for voxels near grain boundaries where diffracted beams project to the edges of observed diffraction spots, ii) for voxels that are located in regions where the material is highly deformed, and iii) when the voxel does not contain the relevant crystallographic phase (including edges, voids, second phases, etc).

References

[1] R.M. Suter, D. Hennessy, C. Xiao, U. Lienert, "Forward Modeling Method for Microstructure Reconstruction Using X-ray Diffraction Microscopy: Single Crystal Verification," Rev. Sci. Instr., **77**, 123905 1-12 (2006). (document)

[2] S.F. Li and R.M. Suter. Adaptive reconstruction method for three-dimensional orientation imaging. *J. of Appl. Cryst.*, 46(2):512–524, Apr 2013. (document)