Compact representation of texture for the prediction of macroscopic yield surfaces using machine learning methods

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Abstract

Among microstructural features, crystallographic texture has one of the largest influences on the macroscopic yield behavior of polycrystalline materials. It is thus advantageous to include representations of texture in novel surrogate models as trained by machine learning algorithms, which themselves become data-hungry as a function of increases in input (i.e., microstructural and texture descriptions) and architecture (i.e., number of hidden units, layers) complexity. Consequently, it is desirable to reduce the complexity of material description. Discrete spherical harmonics (DSH) expansions have been widely utilized to provide a reduced-order description of the orientation distribution function (ODF). Adept in reproducing general ODF distributions, DSH, however, often requires 64 or more harmonic modes to reproduce ODFs with an acceptable amount of error, often too complex for realistic use in ML training. We propose an approach to represent ODFs as a linear combination of "N" basic texture modes (e.g., cube, brass, copper, goss), characterized fully by the weight of the component and its spread, thus requiring "2N" descriptors. We show that this method offers the possibility to represent ODFs of known processing routes with comparable error to DSH while requiring an order of magnitude fewer descriptors. This approach is applied to both idealized ODFs and existing ODFs measured from Electron Backscatter Diffraction (EBSD). To assess the efficiency of this method compared to well-established ones, we provide a comparison with DSH. Implementation in a workflow for an established ML framework for the prediction of macroscopic yield surfaces is then discussed, and results are discussed.

Keywords: Texture representation, Discrete spherical harmonics, Yield Surfaces, Machine Learning

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