Algorithm for Parent Phase Reconstruction (PPR) from EBSD Dataset

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Orientation relationship (OR) between two crystals is obeyed during transformation from parent phase to daughter phases in many materials systems. Such OR provides clue to reconstruct crystallography of parent phase from the final crystallography of daughter phase. For example, austenite-to-martensite transformation follows approximately the Kurdjumov-Sack (K-S) or the Nishiyama-Wassermann (N-W) ORs in steels. To obtain the orientation of austenite, reconstruction can be processed by the equation: $D_iC_mM_i^{bcc}= VC_nM_j^{fcc}$, where M_i^{bcc} is the orientation matrix of daughter phase, M_i^{fcc} is the orientation matrix of parent phase, D_i is the deviation matrix, C_m and C_n are 24 symmetry rotation matrices, and V is the orientation relationship (OR) matrix between two phase. The approach was reported by Miyamoto et al., and the orientation of austenite, M_j^{fcc}, can be obtained by minimizing the value of the deviation, D_i. Hence, real and irrational OR between two crystals can also be obtained by this method. Different approaches for reconstruction were reported by Cayron et al., Abbasi et al. However, some problems remained unsolved: (1) mis-index at twinning parent phase and (2) abnormal morphology of parent phase.
In this work, a new protocol especially implanted with (1) M-Voting and (2) M-Merge, to improve the reconstruction accuracy and speed. M-Voting is a process to find the most possible M_j^{fcc} by counting votes. M-merge is a process to merge the grains who has similar "Voted M^{fcc}". The resulting reconstructed parent grains morphology are reasonable with low mis-index rate. This PPR algorithm is fully automatic, and it is expected to be embedded into the commercial EBSD software in the future.