On frequencies of occurrence of symmetric and improperly quasi-symmetric grain boundaries

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To understand the contribution of grain boundary networks to properties of polycrystalline materials, characterizations of boundary structures at both atomic and macroscopic levels are needed. Studies at the atomic scale - within current experimental capabilities - are limited, but since experimental techniques designed for three-dimensional microstructure imaging have advanced considerably, it is possible to collect geometric (so-called ”macroscopic”) parameters for significant numbers of boundaries. This allows for carrying out some statistical studies of boundary networks. Macroscopic geometry of a boundary can be described by a misorientation between adjacent grains and boundary plane indices. It is unlikely that the influence of different boundaries is identical. Based on the geometry, boundaries can be classified into various groups, e.g., tilt, twist, symmetric, properly and improperly quasi-symmetric boundaries are distinguishable. Symmetric and improperly quasi-symmetric boundaries have very special geometric features, and therefore, they may have special physical properties. To verify whether a given boundary can be qualified to any of the aforementioned groups, a distance between two boundaries defined in the five-dimensional space of boundary parameters is used. For instance, if the distance from a boundary to the nearest symmetric boundary is below a specified limit then the boundary is identified as symmetric. Probability density functions (PDFs) for the distances may serve as characteristics of microstructures. We provide PDFs for the distances to the nearest symmetric and improperly quasi-symmetric boundaries for both "random" boundaries (the reference isotropic case) and a data set collected from Ni-based alloy.