

Special Grain Boundaries between Crystals with Large Unit Cells: From Coincidence Sites to Coincidence Motifs

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Low energy boundaries can be expected if there is a good structural fit at the interface between two crystals of the same phase but differing in orientation. For disorientations at which there is a coincidence site lattice (CSL), there is the possibility that some atoms at the boundary are located on sites that fit both crystals. Disorientations that give rise to a three-dimensional CSL with a large fraction of fitting atoms have long been used as part of the defining criteria for special low-energy grain boundaries in metallic body- and face-centered cubic crystals.

We have observed grain boundaries in large unit cell metallic crystals in which entire motifs fit into both crystals. We suggest a more general “coincidence motif” criterion applicable to all crystals: Special grain boundaries can occur for rotations that are part of the pseudo-symmetry of the motifs but are not in the symmetry group of the crystal. Because an individual atom has the pseudo-symmetry of the infinite rotation group, the CSL criterion is included in the coincidence motif criterion.

