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Algorithms for generating coincidence site lattices (CSLs) and near-CSLs in arbitrary Bravais lattice systems

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The formulation of coincidence site lattices (CSLs) has played a fundamental role in the analysis of interfaces in both experiments and simulations of inorganic materials systems. For example, the prediction of habit planes during precipitation and phase transformations relies on the determination of near-CSLs between the parent and the product lattice. The distributions of internal interfaces are generally analyzed as a function of their corresponding Σ-misorientations. Therefore, the ability, to automatically generate the Σ-rotations and their corresponding CSLs will not only enable the high-throughput prediction of interface structure-property relationships but will also help understand microstructure evolution during phase transformations. Grimmer, in a series of articles, has proposed the generating functions for determining the coincidence site lattices for cubic, hexagonal, trigonal and tetragonal Bravais lattices. These generated routines increased in complexity as the underlying symmetry of the lattice is reduced. In this talk, I will present a simple algorithm that computes all the unique CSL generating rotations for any Σ, and in arbitrary Bravais lattice systems. The algorithm involves two simple steps: (i) determination of all the unique sub-lattices of volume Σ; and (ii) the computation all the unique pairs of sub-lattices that are not related by the symmetry operations of the underlying crystals. I will also present strategies for extending this algorithm for computing near-CSL rotations between any two Bravais lattice systems (i.e. both homo-phase and hetero-phase interfaces).

Biography

Srikanth Patala received his BTech in Metallurgical and Materials Engineering from the Indian Institute of Technology Madras in 2005 and did his PhD in Materials Science and Engineering from the Massachusetts Institute of Technology in 2011. Prior to joining the NC State Faculty in 2013, he was a Post-doctoral Researcher in the Department of Materials Science and Engineering at Northwestern University. His research is focused on developing computational and analytical techniques to quantify the structure-property relationships in complex heterogeneous materials.

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