

## Crystal Interface Lab. Seminar Series

## On the decomposition formula of symmetrical tilt grain boundaries

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Grain boundary geometry has been intensively studied after the successful formulation of the coincidence-site-lattice theory. Symmetrical and asymmetrical tilt grain boundaries have been investigated both experimentally and theoretically since more than three decades ago and it is widely accepted that the structures of grain boundaries can be realised by the periodic(or quasi-periodic) arrangements of certain structural units with a small index.

We report the application of the O-lattice theory to systematically analyse the structures of symmetrical tilt grain boundaries and demonstrate a theoretical interpretation of the experimentally observed structures in terms of the structural-units model and the periodicity of the O-points on the boundary. We further derive generalized decomposition formulae which are closely related to the distribution of irreducible rational numbers. The established theoretical formulae will help to elucidate the fundamental structural relationship in grain boundaries and provide a basis for probing structures of random grain boundaries.

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