A continuum approach to structure of twist grain boundaries

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The structure of a twist-grain boundary is a lattice of screw dislocations separating a periodic array of regions with good registry. This structure is usually explained using atomic-scale models. My talk presents recent joint work with Antti Pihlaja (Merrill Lynch) exploring a different, continuum approach. We view the pattern as arising from minimization of an "incoherence energy" $\int W(H)\, dx_1\, dx_2$ where H is the incoherency tensor of Cermelli and Gurtin. The rows of H are curl-free, so this resembles a problem of 2D elasticity. In particular, when W is not quasiconvex, minimizing sequences develop spatial patterns. Our main contributions are (a) identification of the patterns and Young measures associated with the standard picture of a twist grain boundary; and (b) identification of a specific energy density W for which this pattern is optimal. The identification of a physically plausible W – representing, perhaps, the continuum limit of an atomic-scale model – remains an open problem.