Emergence of rigid polycrystals from atomistic systems

We investigate the emergence of rigid polycrystalline structures from atomistic particle systems. The atomic interaction is governed by a suitably normalized pair interaction energy, where the `sticky disk' interaction potential models the atoms as hard spheres that interact when they are tangential. The discrete energy is frame invariant and no underlying reference lattice on the atomistic configurations is assumed. By means of Gamma-convergence, we characterize the asymptotic behavior of configurations with finite surface energy scaling in the infinite particle limit. The effective continuum theory is described in terms of a piecewise constant field delineating the local orientation and micro-translation of the configuration. The limiting energy is local and concentrated on the grain boundaries, i.e., on the boundaries of the zones where the underlying microscopic configuration has constant parameters. The corresponding surface energy density depends on the relative orientation of the two grains, their microscopic translation misfit, and the normal to the interface. Joint work with Leonard Kreutz (Münster) and Bernd Schmidt (Augsburg).