

## Using the elastic far-field for efficient crystal defect computations

Julian Braun

The elastic field around a defect in a crystalline material is known to be described by continuum linearised elasticity in leading order away from the defect core for dislocation or crack openings. And it is known to be described by a defect-dipole tensor for point defects. If both approaches are combined and generalised, one can derive higher order asymptotic expansions of the elastic far-field. These can be used as high accuracy boundary conditions for atomistic defect computations. I will showcase an outline of the theory and specific resulting numerical methods for point defects, dislocations, and a Mode III crack. In the latter case, our results show the incompleteness of the classical ansatz for flexible boundary conditions by Sinclair.