MULTIPLE SCALE MODELING OF MATERIALS

Peter W. Chung
U.S. Army Research Laboratory
Aberdeen Proving Ground, Maryland USA

The accurate modeling of local mechanical deformation in crystallites has important implications for constitutive theories for solids. This is particularly true for materials that have dual-use applications such as load-bearing sensor materials or materials with tailored failure properties, where the distortions of atoms around defects due to deformation effects macroscopic electronic and extremal material properties. The development of multiscale modeling methods is one among other basic research programs that comprise the multiscale modeling portfolio at the Army Research Laboratory. After a brief overview of multiscale modeling research at ARL, the talk will present the development of a multiscale asymptotic homogenization method suited for studying local mechanical deformation around lattice imperfections.

The objective of this work is to devise a numerical method through which mechanical stress-strain relationships of lattice defects can be determined through accelerated energy minimizations over a reduced solution space of the crystal. The method is based on a mathematical derivation of asymptotic homogenization whose material integral is determined from an atomistic energy. The derivation leads to an instantaneous tangent stiffness equation whose solution indicates the direction towards an approximate minimum energy state. By a normalization scheme, the solution vector is scaled by a single parameter. Through numerical experiments, the subsequent scaled solution for which a minimum energy is found is shown to be thermodynamically admissible. Conjugate gradient minimizations of the full atomistic problem are used to verify the quantitative results. Validations with experiments from the literature also show good agreement.