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Statistical Mechanics for Linking Length Scales in Complex Solids

YING HU, SOKRATES T. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, Nashville, TN — Linking scales is usually pursued by computational means, either by passing information from calculations at one scale to another or by constructing a composite simulation with different features treated at different length scales. Here we report on a formulation that is based on the principles of statistical mechanics, applied to a complex solid. Two new concepts, 'lattice space' and 'atom space', are introduced. The deformed state of a crystal is described in terms of deformations of the lattice space and atom space. The distribution function is decomposed in a Born-Oppenheimer-like fashion into slow and fast components. Phonons are integrated out to give a driving force to the lattice deformation. Interplay between the two spaces leads to the formation of defects and such phenomena as elastic deformation, thermal expansion, creep, and dislocation motion. New distribution functions are constructed by adapting the method of local integrals of motion from the theory of liquids. Simulations can be implemented at different mesoscopic length scales, tracking fluxes of point defects, impurities, dislocations, etc.

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