

MULTISCALE BOUNDARY CONDITIONS IN CRYSTALLINE SOLIDS

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The rapid advances in nanotechnology, nanomaterials and nanomechanics offer huge potentials in national defense, homeland security, and private industry. An emphasis on nanoscale entities will make our manufacturing technologies and infrastructure more sustainable in terms of reduced energy usage and environmental pollution. Recent advances in this area have stimulated ever-broader research activities in science and engineering devoted to their development and their applications.

Similar to other contemporary fields of research, nanomaterials are rapidly advancing due to a combined effort between engineering and science. In some cases, arenas of research that were stagnating under the exclusive domain of one discipline have been imbued with new discoveries the adjoint disciplines. In computational nano mechanics and materials, we are particularly concerned about the technological engineering interest by combining engineering technology and basic sciences through modeling and simulations.

In most applications, nanoscale materials will be used in conjunction with other components that are larger, and have different response times, thus operating at different time and length scales. Single scale methods such as “ab initio” quantum mechanical methods or molecular dynamics (MD) will have difficulty in analyzing such hybrid structures due to the limitations in terms of the time and length scales that each method is confined to. Apparently, there is a need in the so-called “multiscale approaches” for this class of problems.

Computer simulations of micro and nano scale phenomena in solids are often aimed at the study of an atomistic process in a localized region, the fine grain, while the effect and behavior of the surrounding bulk material, the coarse grain, are of interest only in an averaged or cumulative sense. As a result, the bulk material modeling usually involves a continuum formulation; therefore the issue of an adequate coupling of the classical molecular mechanics and continuum simulations arises. The topic of this presentation is a systematic approach to treating the fine/coarse grain interface, based on Fourier analysis of regular lattices structures. The approach allows elimination of the unnecessary atomic degrees of freedom over the coarse grain, without involving an explicit continuum model for the latter. At the same time, this approach can serve as a constitutive part of more general algorithms, such as the multiple field decomposition for overlapped MD/continuum domains. The mathematical formulation involves compact convolution operators that relate displacements of the interface atoms and the adjacent atoms on the coarse grain. These operators are defined by the basic geometry of the lattice structure, rather than the scaling parameters of interatomic potentials.

Applications and performance are illustrated on quasistatic nanoindentation simulations with a crystalline gold substrate, crack propagation along the $\{111\}$ plane in fcc crystals, as well as various aspects of mechanical behavior of carbon nanostructures. For the nanoindentation problem, complete atomistic resolution on the coarse grain is alternatively employed in this problem to give the benchmark solutions. The results are found to match well for the multiscale and the full atomistic simulations.