LATTICE GREEN'S FUNCTION APPROACH FOR MULTI-SCALE ATOMISTIC SIMULATIONS OF NANOSTRUCTURES

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Lattice Green's function methods for lattice statics calculations have been known for quite a long time (see, e.g., [1],[2]). In general, these methods allowed for significant reduction of the computational domains. However, they were typically designed for infinite lattice structures or structures with periodic boundary conditions. Furthermore, these methods were often specifically tailored for the treatment of lattices with particular point defects. A general multi-scale theory using lattice Green's function approach for finite domains is still in quest.

In this presentation, a multi-scale method for static analyses of finite periodic lattice structures will be presented. The method uses a lattice Green's function approach to model the response of the exterior coarse scale region through imposing the so-called Multi-Scale Boundary Conditions (MSBCs) at the boundaries of the reduced atomistic domain (fine scale region). The main distinctive feature of the current method, as compared to other methods utilizing the lattice Green's function concept, is that it has an intrinsic multi-scale character. It is designed for modeling large, though finite, domains, where two different length scales are involved. The method accounts for both local and peripheral effects. For instance, displacements at the outer boundary of the coarse scale domain can be prescribed. This was not the case in the earlier studies, where the Green's functions were usually found for infinite structures or those with periodic boundary conditions. The current method is concerned with the accurate modeling of finite domains of a given size that can be efficiently divided into coarse and fine scale regions. The size of the coarse scale region is characterized by the special domain reduction parameter, which is a key feature of the current method.

The method is tested and validated on the three-dimensional simulations of nano-indentation of multi-layered graphite. Then, the method is applied to study the atomic-scale stick-slip friction between the tip of the Atomic Force Microscope and the graphite substrate.

References

[1] V.K. Tewary, "Green-function method for lattice statics," *Advances in Physics*, 22(6), 757–810, 1973.
[2] R. Thomson, S.J. Zhou, A.E. Carlsson, V.K. Tewary, "Lattice imperfection studied by use of lattice Green's functions," *Physical Review B* **46**, 10613–10622, 1992.

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