An Efficient Boundary Condition for Molecular Dynamics Simulations

Zhijian Yang
Wuhan University

This talk presents an absorbing boundary condition for molecular dynamics simulations of materials defects. The purpose of the boundary condition is to eliminate spurious reflections of phonons at the boundary and minimize the finite size effect. In contrast to other existing methods, our emphasis is placed on the ease of implementation. In particular, we propose a method for which the implementation can be done within existing molecular dynamics code, and it is insensitive to lattice structure, the geometry and space dimension of the computational domain. To demonstrate the effectiveness, the results from two test problems are presented.