Abstract Submitted for the MAR10 Meeting of The American Physical Society

**Coupling the atomistic and continuum simulation** GUOWU REN, DIER ZHANG, XINGAO GONG, Department of Physics, Fudan University, Shanghai 200433, China — A hybrid multiscale method coupled atomistic and continuum model is present. In the continuum region, an atomic-scale finite element method (AFEM) is proposed and exhibits a perfect coupling with molecular dynamics (MD) method used for the atomistic region. In the framework of hybrid method, utilizing the concept of filter, we also design a new interfacial condition which damps out the spurious reflection of high-frequency phonons at the atomistic/continuum interface without much influence on the low-frequency ones. A series of simulation results show the advantage of our schemes.

Guowu Ren Department of Physics, Fudan University, Shanghai 200433, China

Date submitted: 12 Nov 2009

Electronic form version 1.4