분할 적분 기법을 적용한 N-sigma-T 분자동역학 시뮬레이션

박시동†(서울대) · 조맹효*(서울대)

The splitting time integrator for fully flexible cell molecular dynamics

Shidong Park , Maenghyo Cho

Key Words: 『splitting time integrator(분할적분기법)』 『symplectic integration(심플렉틱 적분)』 『molecular dynamics(분자동역학)』 『flexible cell(변형가능 셀)』

Abstract : Fully flexible cell preserves Hamiltonian in structure, so the symplectic time integrator is applied to the equations of motion. Primarily, generalized leapfrog time integration(GLF) is applicable, but the equations of motion by GLF has some of implicit formulas. In this paper, The time integration formula are obtained for the fully flexible cell molecular dynamics simulation by using the splitting time integration. It separates flexible cell Hamiltonian into terms corresponding to each of Hamiltonian term, so the simple and completely explicit recursion formula was obtained. we compared the resulting splitting time integration with the implicit generalized leapfrog time integration.

반도체표면에 생성되는 금나노입자 증착법

임현의† · 노정현 · 김재윤 · 김완두(KIMM)

A Novel Electroless Gold Nanoparticle Deposition on Semiconductor

Hyuneui Lim, Jung-Hyun Noh, Jae-Yun Kim, and Wan-Doo Kim

Key Words: Metallization(금속화), Nanoparticle(금나노입자), Electroless Deposition(무전해도금)

Abstract : Metallization and metal nanostructures on semiconductors play a key role in the production process of MEMS/NEMS and arrayed nanosensors. We demonstrate a novel gold nanoparticle deposition as a result of the immersion of semiconductor substrates into dilute aqueous solution of $AuCl^{4-}$. Deposition proceeded via galvanic displacement in the absence of pH adjusters and external reducing agents. The deposition rate, surface morphology and nanoparticle shape depend on the plating parameters as well as underlying semiconductor substrate. Deposited gold nanoparticles exhibit excellent adhesion to GaAs and InSb surfaces but not to InP and Si, independent of the plating time. This manner of deposition serves as a cost-effective, high-throughput method with potential applications such as high resolution patterning, interconnects, and metallization of MEMS/NEMS and nanodevice.