분자 동역학 해석에서 원자 수준의 응력에 대한 연구

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A Study of Atomic-level Stress Calculation in Molecular Dynamics Simulation

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Key Words: Molecular dynamics(분자동역학), stress(응력), SPH(완화입자유동법)

Abstract : To calculate atomic-level stress, we choose the stress formulation proposed by Shengpin Shen and S.N. Atluri. The formulation based on the SPH(Smoothed Particle Hydrodynamics) method does not need atomic volume. The formulation is not only robust, accurate, and easy to implement, but also appropriate for both homogeneous and inhomogeneous deformation. We illustrate various numerical examples of molecular dynamics simulation.

연속체 가정을 통한 Thema1-NIL 공정의 전산모사

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Numerical Simulation of Thermal-NIL Process Based on Continuum hypothesis

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Key Words: Surface tension(표면장력), Wall adhesion(벽면흡착), Polymer(고분자), Fixed grid(고 정격자계), Lithography(석판술)

Abstract : Nano imprint lithography(NIL) is a cost-efficient, high-throughput processing technique to transfer nano-scale patterns onto thin polymer films. Polymers used as the resist include the UV cured resin as well as thermoplastics such as polymethyl-methacrylate(PMMA). In this study, an analytic investigation was performed for the process of transferring nano-scale patterns onto polymeric films. Process optimization calls for a thorough understanding of the polymer flow during the process. We carried out two-dimensional numerical analysis of polymer flow during NIL process. The simulation incorporated a continuum-hypothesis, and the effects of surface tension were taken into account. The numerical model also employed a proper viscosity model for the polymeric liquid. For a more effective prediction of the free surface, the fixed grid scheme was used. A parametric study was performed for the process condition. Numerical results were compared with the experimental data. Agreement between two results was acceptable.