압축 응력 하에서의 금 나노 와이어 안정성에 관한 연구

임영태†(KAIST) · 엄윤용(KAIST)

A study on stability of Au nanowires under compression

Y.T. Im and Y.Y. Earmme

Key Words: stability(안정성), molecular simulation(원자모사), deformation twin(변형쌍정)

Abstract : The structure and properties of nano scale materials can be different from those of bulk materials due to the effects of surface. In this paper, using the molecular statics simulation with the embedded-atom method potential, the stability of Au nanowires under uniaxial compression was investigated. Au nanowires with a square cross-section and surface orientations of [100], [010] and [001] were created with initial atomic positions corresponding to the bulk face-centered-cubic crystal structure. The length and the cross-section area of the nanowires were varied. The atoms in the wire were then relaxed to a minimum energy state at 0 K. The simulation results show three kinds of instabilities : buckling, twinning and phase transformation. Comparing the simulation results with the theoretical ones of the critical buckling load proposed by Euler, it is found that the buckling occurs at a much higher load than the Euler buckling load. A new model predicting the instability for the buckling as well as the twinning and the phase transformation is now under study.

분자동역학기법을 이용한 폴리머의 표면흡착에 관한 전산모사

우영석†(서울대 원) · 이우일*(서울대)

Numerical Simulation of Polymer Adhesion on Surface using Molecular Dynamics

Y. S. Woo, and W. I. Lee

Key Words: Polymer(고분자), Surface(표면), Adhesion(흡착), Spreading(퍼짐), Coordination Number(배위수), Molecular Dynamics Simulation(분자동역학 모사).

Abstract : In this study, molecular dynamic simulations have been carried out to investigate adhesion or spreading characteristics of polymer molecules on the solid surface. The potential functions of polyethylene cluster and solid surface molecules were considered using the bond, the angle, and the Lennard-Jones(L-J) potentials. Behavior of polyethylene cluster molecules is simulated for various conditions(different chain arrays, temperatures, attractive forces, molecular weights, densities, etc...). By evaluating radial-direction spreading and atom's coordination numbers, the adhesion characteristics were examined in order to understand the adhesion phenomena according to the various conditions.