정렬 알고리즘과 격자형 셀을 이용한 분자동역학 해석방법의 근접원자 탐색방법 개발

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The development of neighbor searching method using a grid-cell and sorting algorithm

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Key Words: Molecular Dynamics(분자동역학), Neighbor List(네이버 리스트), Quick Sorting Algorithm(퀵 정렬 알고리즘), Grid-Cell(격자형 셀)

Abstract : Sorted list of atom position in each grid-cell is applied to neighbor searching method of molecular dynamics (MD) simulations. Using quick sort algorithm, atoms in the grid-cell are sorted sequentially in each x, y, and z direction. Compared with the conventional method, whose neighbor searching time is $O(n^2)$, computing time of present study increases in the scale of $n \cdot log(n)$. Also optimal grid-size of system are investigated for various models.

나노압입 전산모사에서의 서모스탯 연구

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Thermostat Study in nanoindentation simulation

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Key Words: Nanoindentation(나노압입), Molecular dynamics(분자동역학), Thermostat(서모스탯)

Abstract : Molecular dynamics simulations are performed for the study of thermostat effect on the defect generations under nanoindentation. We set target temperature with thermostat in order to keep the temperature of the system constant. Berendsen and Nose-Hoover thermostats are employed for comparison study. Nose-Hoover thermostat maintain the temperature closer to the target value than Berendsen. In the case of Berendsen thermostat we observe relatively higher temperature fluctuations at the time defect generation. In the mean time, Berendsen thermostat allows the greater time step compared with the Nose-Hoover thermostat.