

**[NP-15]**

## Chemical Mechanical Polishing 공정에 관한 원자단위 반응 모델링

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This paper shows the results of atomistic modeling for the interaction between spherical nano abrasive and substrate in chemical mechanical polishing processes. Atomistic modeling was achieved from 2-dimensional molecular dynamics simulations using the Lennard-Jones 12-6 potentials. The abrasive dynamics was modeled by three cases, such as slipping, rolling, and rotating. Simulation results showed that the different dynamics of the abrasive results the different features of surfaces. We proposed and investigated three mechanical models, such as (1) Constant Force Model, (2) Constant Depth Model, and (3) Variable Force Model, and three chemical models, such as (1) Chemically Reactive Surface Model, (2) Chemically Passivating Surface Model, and (3) Chemically Passivating-Reactive Surface Model. From the results obtained from classical molecular dynamics simulations for these models, we concluded that atomistic chemical mechanical polishing model based on both Variable Force Model and Chemically Passivating-Reactive Surface Model was the most suitable. The proposed model can be extended to investigate the 3-dimensional chemical mechanical polishing processes in the atomic scale.

[감사의 글]

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