**SF-003**

**Variation of the Si-induced Gap State by the N defect at the Si/SiO₂ Interface**

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Nitrided-metal gates on the high-$κ$ dielectric material are widely studied because of their use for sub-20nm semiconductor devices and the academic interest for the evanescent states at the Si/insulator interface. Issues in these systems with the Si substrate are the electron mobility degradation and the reliability problems caused from N defects that permeates between the Si and the SiO₂ buffer layer interface from the nitrided-gate during the gate deposition process. Previous studies proposed the N defect structures with the gap states at the Si band gap region. However, recent experimental data shows the possibility of the most stable structure without any N defect state between the bulk Si valence band maximum (VBM) and conduction band minimum (CBM).

In this talk, we present a new type of the N defect structure and the electronic structure of the proposed structure by using the first-principles calculation. We find that the pair structure of N atoms at the Si/SiO₂ interface has the lowest energy among the structures considered. In the electronic structure, the N pair changes the eigenvalue of the silicon-induced gap state (SIGS) that is spatially localized at the interface and energetically located just above the bulk VBM. With increase of the number of N defects, the SIGS gradually disappears in the bulk Si gap region, as a result, the system gap is increased by the N defect. We find that the SIGS shift with the N defect mainly originates from the change of the kinetic energy part of the eigenstate by the reduction of the SIGS modulation for the incorporated N defect.

**Keywords:** silicon/silica interface, N defect, first-principles

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개미산에서 수소 생산용 Pd 기반 합금 촉매의 제일원리 설계

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