(SP-18)

Molecular dynamics study on NO adsorption on Si(001)

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NO adsorption can be used in synthesizing oxynitride thin films which have potential application in nanodevices. However, it is very difficult to understand the oxynitridation process since too many factors are involved in it. In this paper, we present our first-principles molecular dynamics calculation on the NO molecule adsorption on the Si(001) surface as the initial stage of the oxynitridation process. The previous first-principles calculation[1] has argued the NO molecule is dissociated with a very small activation barrier, 0.07 eV, which acutally corresponds to 1.60 eV considering thermodynamics. This is in clear contrast to the observation that NO is dissociated at temperatures as low as 20 K. From extensive searches of NO on the Si(001) surface, we have found the new dissociation processes that have the much lower activation energies. In this paper, we present the dissociation and penetration processes with the corresponding activation energies and discuss their experimental implications.[2]

[참고문헌]

1. K. Kato, Y. Nakasaki, and T. Uda, "Atomic processes of NO adsorption on Si(100) surfaces", Phys. Rev. B 66, 075308 (2002).
2. This work was supported by Korea Research Foundation Grant (No. R05-2004-000-10728-0).