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First principles calculation for Ag diffusion on the hydrogenated and clean Si(111) surface.

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Modification of the substrate surface by introducing the hydrogen layers can alters the metal growth mode. For instance, the Ag films deposited onto Si(111), which is one of the most extensively studied system so far, the Stranski-Krastanov growth mode conventionally observed on the clean Si(111) surface, is changed to Volmer-Weber mode on the hydrogenated Si(111) surface.

The growth mode is generally determined by the mobility of the adatom deposited on the surface. In this study, using the first principles calculation, we study the Ag adatom adsorption and diffusion behaviors on the hydrogenated and clean Si(111). On the hydrogenated Si(111) surface an Ag atom has a extremely small diffusion barrier of 0.14 eV. The diffusion barriers for moving inside the half unit cell (HUC) and hops out of HUC on the clean Si(111) surface are calculated of 0.26 eV and 0.88 eV, respectively, well consistent with the value of obtained by the direct STM observation.[1]

[참고문헌]

1. P. Sobitik, P. Kocan, I. Ostadal, Surf. Sci **537**, L442 (2003)