[V-22]

# Energetics of adsorptions on fcc(111) and binary system; An application of the modified embedded atom method

Yh. Shin[1], J. Seo[2] and J.-S. Kim[1]
[1]Department of Physics, Sook-Myung Women's University.
[2]Division of General Education, Cho-Dang University.

The embedded atom method (EAM) of Daw and Baskes[1, 2, 3] as a semiempirical method, has been successfully applied to the fcc or nearly filled d-band transition metals due to its computational feasibility and its methodological simplicity. Then Baskes[4] modified the EAM (MEAM) to include directional bonding and applied it to metals, semiconductors, and diatomic gases, all of which have different types of bondings. Here, we present a detailed study of the energetics of adsorption on the fcc(111) surfaces and binary system within the framework of MEAM. In adsorption on fcc(111) surface, there are two energetically favored sites, so called, fcc site and hcp site, which may trigger stacking fault in the growth of films and might switch growth mode between 3D growth and layer by layer growth. We scrutinized the role of the hcp sites, which would offer dynamic growth pathways although the dynamics are not yet clear within the limited experimental resolution. Featuring these transient motions in the atomic level should contribute to the understanding the growth mechanisms on fcc(111) surface. And we also applied MEAM for initial stage energetics at the Cr coverage of sub- monolayer on W(110). We hope that recently observed extraordinary growth behavior at the Cr coverage of 0.7 monolayer, self- organized nano-scale lines[5], can be resolved in this MEAM binary system calculation.

[References]

1. M. I. Baskes, J. S. Nelson and A. F. Wright, Phys. Rev. B **40**, 6085 (1989).
2. M. S. Daw and M. I. Baskes, Phys. Rev. Lett. **50**, 1285 (1983).
3. M. S. Daw and M. I. Baskes, Phys. Rev. B. **29**, 6443 (1984).
4. M. I. Baskes, Phys. Rev. B. **46**, 2727 (1992).
5. Center for Sciences in Nanometer Scale and Department of Physics, Seoul National University, unpublished