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MULTILAYER RELAXATION AND ELECTRONIC PROPERTIES OF Rh(111) SURFACE, YOUNG SOO KWON, T.H. RHO, CHAEE KANG LEE, G.B. CHA, and SOON C. HONG (Dept. of Physics, University of Ulsan, Ulsan,680-749, Republic of Korea), J.I. LEE (Dept. of Physics, Inha University, Inchon 402-751, Republic of Korea)

Determination of structural and electronic properties is one of the basic questions of surface science. Surface relaxation, surface and surface resonance states, and surface core level shift, surface energy are interesting subjects due to variety surface processes like catalysis. Computation was carried out for a ten-layer slab Rh(111) by employing a self-consistent semirelativistic version of full potential linearized augmented plane wave (FLAPW) method. We optimized 2D lattice constant with total energy calculation for the Rh bulk and then performed multilayer geometry optimization by calculating total energy and atomic force. The 2D lattice constant was calculated to be 5.05 a.u. Multilayer relaxation from surface layer to inner layer were -1.63, -0.22, 0.51 and -0.10%. We found newly an unoccupied surface resonance state in ΓM symmetry axis and reconfirmed surface and surface resonance states. Recently, a new surface state was reported experimently ΓM symmetry line with binding energy 3.5 eV. We will explain this state. Detailed analysis surface for electronic state are presented and better criterion for surface state in band calculation is proposed. The work function, core level shift, surface energy were calculated to be 5.61 eV, 0.46 eV, 1.00 eV and we will compare to those of other calculations and experiments.

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The Interfacial Reaction of Co/Si(100)

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The interfacial reaction of Co on Si(100) was studied by using MEIS(Medium Energy Ion Scattering Spectroscopy) and XPS(X-ray Photoelectron Spectroscopy). MEIS results obtained from Co/Si(100) as a function of overlayer thickness shows that the reaction layer having Co_2Si phase exists at room temperature. It is consistent with XPS results from a submonolayer of Co on Si(100). The temperature dependency of interfacial reaction was investigated on the thick over layer(13-19ML) and thin overlayer(3-5ML). For the thick overlayer, the CoSi phase was observed between 350℃ and 450℃ and the $CoSi_2$ phase was observed above 550℃. For the thin overlayer, the CoSi phase comes up at 350℃, and disappears at 450℃ and then $CoSi_2$ phase is at the interface. The results showed that the interfacial reaction of Co on Si(100) depends on the thickness of overlayer.

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STRUCTURAL PHASE TRANSFORMATION IN A LATTICE-MISMATCHED INTERFACE. Sun M. Paik, H. Song, Eung. S. Lee, Sung M. Yoo (Dept. of Physics Kangwon National University, Chunchon 200-701, Korea), Jin M. Choi, and Chung N. Whang (Dept. of Physics, Yonsei University, Seoul 120-749, Korea)

We have developed a phenomenological theory to calculate free energy of a large sized lattice mismatched interface with a Embedded Atomic Method (EAM) many body potential. This theory, along with Molecular Dynamics simulation, is applied to structural phase transitions of Au(001) and Pt(001) reconstructed surfaces. We find orientation phase transitions on both surfaces with rotation angles around $\theta \approx 0.72$, 0.86, 1.14° at temperatures below the bulk melting temperature. The type of transition is found to be a first order transition. The exact transition temperature depends on the shape and size of the surface-cluster. We predict that the orientational phase transitions should be accompanied by a pattern transformation from (5 x m) to (5 x m') where m and m' are integer between 18 and 30. The layer distance decreases as the temperature increases but a sudden increase is found at the transition temperature which is another indication of first order phase transition. These findings are in good agreement with experiments.

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LEED STUDIES OF THE ADSORPTIONS OF Mg AND Ba ON THE SINGLE DOMAIN Si(001)2×1 SURFACE J. S. KIM, K. W. IHM, C. C. HWANG, H. S. KIM, Y. K. KIM and C. Y. PARK
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The adsorptions of Mg and Ba on the single domain (SD) Si(001)2×1 surface are studied by using low energy electron diffraction (LEED). The adsorptions of Mg and Ba on the SD Si(001)2×1 surface at high temperatures are shown the similarity and difference: in case of Mg, the adsorption at 280℃ are shown the SD 2×3- and 2×2-Mg phases as a function of deposition times and in case of Ba, the adsorption at 870℃ are shown the double domain (DD) 2×3-Ba, (2×3)'-Ba, mixed and 2×1-Ba phases as a function of deposition times. The 2×3 phase is common one, but other is not. We will discuss the atomic structures of the observed phases considering the atomic size effect for the adsorption sites[1].

Reference ;
[1] K. Kobayashi, Y. Morikawa, K. Terakura and S. Bügel, Phys. Rev. B45, 3469(1992).

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