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Atomic structure of ultrathin Fe films on Pd(100)

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Ultrathin Fe films on clean Pd(100) were studied by LEED I/V curve analysis. Although the large lattice mismatch between fcc Fe and fcc bulk Pd is -8.4%, LEED pattern of Fe film on Pd(100) showed p(1×1) pattern, suggesting pseudomorphic growth. After we failed TLEED analysis with the model assuming pure Fe film, we investigated the possibility of alloying and could obtain the acceptable fit in ATA.

0.5ML Fe film showed Fe atoms residing only in the first layer and the contraction of the first interlayer spacing, compared to bulk Pd. Moreover, from the results of Bader et al.[1] and Jin et al.[2] we suspect that the alloyed Fe film in the surface layer is the flat homogeneous 2D island.

For 1ML Fe film, we noticed that Fe atoms interdiffused into the subsurface layer with Pd substrate atoms. The first two interlayer spacing were contracted by 2.5% and by 10.5%, respectively, from that of bulk Pd. More tensile strain is expected in our film than in the films of Boeglin et al.[3] because our Fe content in the subsurface layer is much larger in our experiment and our contracted fct(c/a=0.93) structure different from the expanded fct(c/a=1.05) by Boeglin et al. supports the agument.

For 2ML Fe film, we found the Fe atoms migrated deeper into third layer. We suspect that the structural transition from alloyed fct to pure bct occurs for the thicker films, because of the distinct change of LEED I/V characteristics at 3ML film.

[참고문헌]

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