

The spectroscopic study of the interaction of CO and W(111) surface

S.Y.Lee, Y.D.Kim, S.B.Lee, T.S.Yang*, C.Y.Park**

Department of Chemistry, Sungkyunkwan University, Suwon 440-746

*Department of Vacuum Science and Technology,

Sungkyunkwan University, Suwon 440-746

**Department of Physics, Sungkyunkwan University, Suwon 440-746

The adsorption of CO on W(111) surface in the range of adsorption temperature between 300K and 1000K has been studied using AES, LEED, TDS, XPS and UPS in UHV system. After saturated adsorption of CO at 300K four desorption states are observed at about 400K, 850K, 1000K and 1150K in thermal desorption spectra, called as α , β_1 , β_2 , and β_3 respectively. These similar states are also observed in the case of CO adsorption on W(110) and W(100). On the basis of the simulation of thermal desorption spectra and the fundamental arguments of desorption process, the β_3 -state is interpreted as to be attributed to the desorption of a molecular surface species of CO in the contrast to the previous results, in which its similar state observed on the surface of W(110), and W(100) appeared from the recombination of the dissociated C and O species on surface. And β_3 -state reveals attractive lateral interactions resulted in a peak shift to higher temperatures as the initial coverage is increased. The lateral interaction energy calculated by simulated thermal desorption spectra according to lattice gas model by Zhdanov is -2.0Kcal/mol. Also the observed three domains of quasi-(3x1) structures corresponding to the β_3 -state could be interpreted in relation to the CO adsorption structures. Finally spectra obtained using XPS and UPS would be discussed.

chemical evolution of the formed TiN was also monitored by XPS at several annealing steps to 900 °C.

III. Results and Discussions

It has been clearly proved that the co-deposition process at 40 K can produce TiN without annealing as follows: (1) When NH₃ exposure was large enough to embed evaporated Ti ($P_{NH_3} = 1.0 \times 10^{-7}$ mbar, $Ti_{rate} = 2$ A/min), the surface was covered mostly with non-dissociated NH₃. Annealing at 300 °C for a few seconds, most of non-dissociated NH₃ desorbed and TiN and TiNH_x were exposed. For annealing to 900 °C, TiN still remain on the surface with small portion of hydrogen-related defects. (2) When NH₃ exposure was relatively small ($P_{NH_3} = 5.0 \times 10^{-8}$ mbar, $Ti_{rate} = 2$ A/min), TiN and TiNH_x were detected even without annealing process. On the other hand the excessive Ti starts to be clustered with annealing. (3) Instead of simultaneous exposure of NH₃ and Ti, if Ti is sequentially evaporated onto the previously adsorbed NH₃ overlayer, TiN is not formed on the surface.

These results imply that, for Ti atom to react with NH₃ overlayer, at least one of H should be removed from NH₃. But, in the previously formed NH₃ overlayer, NH₃ molecules bond strongly with each other through multiple hydrogen bondings and the post-evaporated Ti can not easily dissociate any H from NH₃. Therefore, in order for Ti atoms to react with N in NH₃, Ti atoms should meet NH₃ before NH₃ molecules form an inert NH₃ overlayer. This deduction justifies our TiN formation through simultaneous NH₃ exposure and Ti evaporation.

IV. Conclusion

Forming condition of TiN at 40 K is quite different from that of Ti oxide. When Ti is evaporated onto previously condensed O₂ layer, Ti oxide can be readily formed. In the case of N₂O condensation followed by Cr evaporation, Cr reacts selectively with O species and the dissociated N₂ just desorbs without forming any nitride. These results imply that in order to form a nitride by these techniques, i.e. gas condensation and metal evaporation, it should be satisfied that the single N source like NH₃ should meet reactive metal atoms prior to forming the non-reactive NH₃ overlayer with multiple hydrogen bondings.

The present studies were supported by the Basic Science Research Institute program, Ministry of Education, 1995, project No. BSRI-95-2433.