분과초청 7

# Surface State and Its Role in Surface Phase Transistion

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Recent development and sophistication of experimental techniques including photoemission and scanning tunneling microscope (STM) have made it possible to investigate surface states (SS's) extensively and revealed that surface states play a key role in determining physics and chemistry of metal surfaces. Therefore understanding the basic nature of a surface state is an essential ingredient in elucidating the fundamental mechanism of various surface related phenomena, for example, surface reconstruction, reaction, non-adiabatic damping of adsorbate vibratons, certain type of contrast in STM image, non-linear susceptibility of surfaces, surface magnetism of metals and layered metal systems.

As a prototypical example of a surface state-driven surface reconstruction, we will consider the reconstruction of Mo(001) surface and discuss the role of SS in revealing the basic driving mechanism of the reconstruction. We have measured temperature dependence of the two-dimensional Fermi surface contours using angle-resolved photoemission to distinguish two theoretical models, charge density wave model and local bonding model, which have been competing for almost two decades since the discovery of the reconstruction in 1977.

We find that a surface state $S_1$ just below Fermi energy ($E_F$), known as a Swanson hump state, plays a decisive role in nesting the Fermi surface contour at transition temperature $T_C$=230K. The curvature of the Fermi surface contour perpendicular to the $\bar{\Gamma}\bar{M}$ azimuth has been found to charge from convex to concave upon cooling below $T_C$, and provide a good change of forming a staight segment at exact $T_C$. The wave vector of reconstruction agrees with twice the value of the $E_F$-crossing of the $S_1$ state, thus suggesting that the reconstruction should occur essentially by Peierls-type $2k_F$ instabilities with significant matrix effects. Further physical implications will be discussed in comparision with results of a theoretical calculation of electronic energy bands of the surface states and surface resonances.