

Electron Stimulated Disordering of C(2x2) CO adlayer on Pt(01) Surface

H.-S. Bae¹, Jikeun Seo², S.H. Kim³, H.G. Min¹, L.-S. Kim⁴, K.H. Chung², and C.Y. Park³

1. Department of Physics, Hong-Ik University
2. Korea Research Institute of Standard and Sciences
3. Department of Physics, Sungkyunkwan University
4. Department of Physics, Sook-Myung Women's University

1. Introduction

CO gas adsorbed on Pt(001) surface at room temperature shows weakly ordered C(2x2) phase with low dosage of CO gas less than 100L. But this ordered phase is so easily destroyed by annealing just more than 130 C or by the illumination of low energy electron beam. In the current work, the microscopic origin for the lifting of C(2x2) LEED pattern formed by CO on Pt(001) under the illumination of low energy electron beam is elucidated by investigating the local bonding site, the molecular (or atomic) species and the molecular density of the remanant disorderly adsorbed ones on Pt(001) surface. The structural and the chemical information on the disordered adlayer was extracted from the I-V characteristics of the diffraction spots, not from the LEED background intensity as in the case of diffuse LEED analysis[1] via average t-matrix approximation (ATA)[2].

2. Average t-matrix approximation (ATA)

The scattering amplitude for a single scatterer, f , and t-matrix are defined as

$$\begin{aligned} f(\mathbf{k}) &= 2\pi/k \sum_l (2l+1) \sin(\delta_l) \exp(i\delta_l) P_l(\cos\theta) \\ &= 2\pi \sum_l (2l+1) t_l P_l(\cos\theta) \end{aligned}$$

$$t_l = 1/k \sin(\delta_l) \exp(i\delta_l).$$

Diffraction pattern is formed by summing all the scattering amplitude from the crystal lattice. For disordered binary alloys, for example, we cannot simply sum the scattering amplitude. In ATA, the disordered binary alloy (element A and element B) is approximated as a homogeneous crystal formed by *pseudo-atoms* whose scattering property is represented by average t-matrix such as

$$t_{\text{pseudo}} = (t_A + t_B) / 2.$$

The validity of this approximation for binary alloys with large disparity in t-matrices of alloying elements is well established experimentally[2] and theoretically[3].

For the present problem, the disordered CO atoms or possibly their derivatives on the Pt(001) were modeled as two dimensional, substitutional binary alloy of CO atoms or their derivatives and vacancies with $t_{\text{vacancy}} = 0$.

3. Experiment

Clean Pt(001) sample was prepared by alternating sputtering and annealing (1100K) procedures. Sometimes, oxygen titration while annealing the sample was needed to remove residual carbon or hydro-carbons. With 3 to 7 L(Langmuir) of CO dosage, Pt(001) surface is deconstructed into (1x1) structure with dim C(2x2) superstructure formed by CO atoms. With the electron gun on for 12 minutes, the dim C(2x2) superstructure disappears leaving P(1x1) deconstructed surface. This may results from electron stimulated migration and/or electron stimulated desorption. To clarify this point, LEED I/V for this surface with 3L of CO dosed, was taken and analyzed by tensor LEED program in ATA, where both the atomic structure and the concentration of CO or CO derivatives were varied.

4. Discussion

The best fit was obtained by the model , 9% of CO disorderly left on 4 fold hollow site with reliability factor, $R_{CO4} = 0.2735$, as in the table and figure. In the present modeling, single site occupation by CO was assumed. Well known bridge or on-top site occupation by CO gave high R-factor above 0.35, from which the possibility of the mixture of two domains of different local CO sites like bridge site or on-top site is supposed not to be high. The model where oxygen is desorbed by electron beam and carbon atoms are left behind on four fold hollow site, also gave rise to good R-factor, $R_{C4} = 0.2941$ although it is still higher than the former, R_{CO4} . So the microscopic origin of the disordering of C(2x2) CO adlayer by electron beam from LEED optics, cannot still be pin down as electron stimulated migration of CO disorderly on four fold site or by electron stimulated oxygen desorption followed by carbon migration onto the four fold hollow site or the mixture of both. To clarify the mechanism, accompanying study like thermal desorption spectroscopy would be very helpful.

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