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— Note —

ADSORPTION OF CO ON A STEPPED Fe(111) SURFACE

By

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Crystal surfaces with high Miller indices are of interest in relation to their atomic structure and stability under ultra-high vacuum conditions, and to gas adsorption and catalytic reaction on them.[1]

The present note reports results of thermal desorption spectroscopy (TDS) and LEED studies of the effects of the steps on CO adsorption on a stepped Fe(111) surface at 300 K. Details of the experimental equipment and sample cleaning procedure were reported previously.[2] A stepped (111) surface, 3(111)×(110), was prepared by cutting a single crystal at 5.8° from the (111) face towards the (110) plane.[3] The orientation was determined by back reflection Laue X-ray technique with an accuracy of ±1/2°. The specimen (1 mm thick disc of 1 cm^2 area) was mounted on the sample holder after cleaning in one atmosphere of flowing hydrogen in a furnace kept at 1100 K. Repeated argon ion bombardment with 500 eV at 10^{-5} Torr, while keeping the sample at 700 K, and annealing at 900 K in the vacuum chamber produced a clean stepped (111)–(1×1) surface in accordance with Fig. 1.[3]

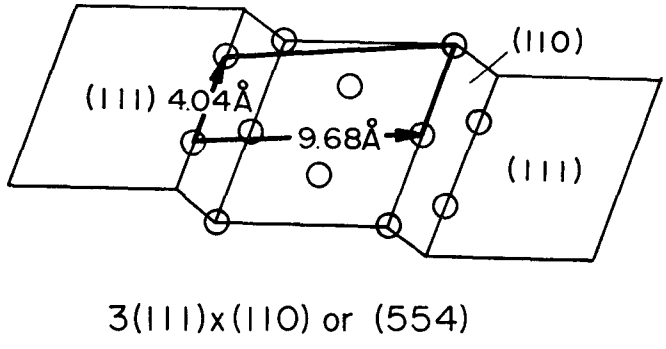

Fig. 1. Schematic diagram of the Fe-3(111)×(110) surface.

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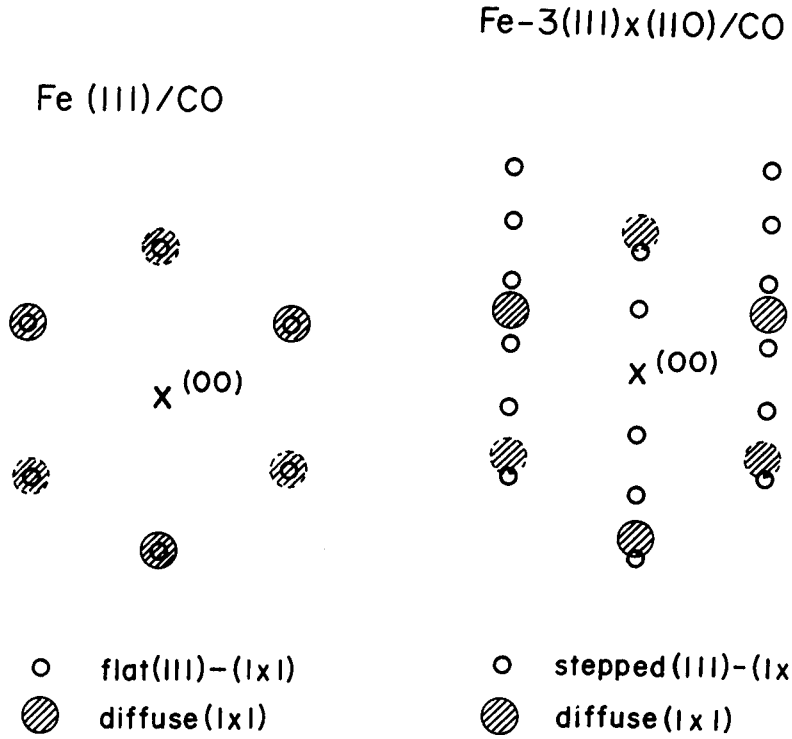

Fig. 2. Schematic diagram of the LEED pattern of the poorly ordered (1×1) surface structure obtained after adsorption of CO on the flat (111) surface around 300 K.

Fig. 3. Schematic diagram of the LEED pattern of the poorly ordered flat (111)-(1×1) surface structure obtained after adsorption of CO on the stepped Fe(111) surface around 300 K.

The adsorption of CO on the stepped (111) surface at 300 K produced much the same diffuse flat (111)-(1×1) pattern above 1.5 L (1 L=10^{-6} Torr•sec) as on the flat (111) surface. Figures 2 and 3 show the schematic diagrams of the diffuse flat (111)-(1×1) patterns from the CO adsorbed flat and stepped (111) surfaces, respectively.

Figure 4 shows CO desorption spectra from the CO adsorbed stepped (111) and flat (111) surfaces. CO desorption spectra obtained for CO adsorption on the flat (111) surface around 300 K show two peaks (α_1, α_2) at lower temperatures, ~380 K and ~435 K, and a small and broad peak (β) at higher temperature, 700 K.[3] All the peak temperatures are apparently independent of the exposure. Assuming the pre-exponential factor $\nu=10^{13}\,\mathrm{sec}^{-1}$, the activation energies for desorption of α_1-, α_2- and β-CO are estimated at 22.5, 25.8 and 43.5 kcal/mole, respectively using Redhead's formular.[4] With the CO adsorbed stepped (111)

surface the spectra exhibit a α-peak and a broad β-peak at ~380 K and ~700 K, respectively. The peak temperatures are also independent of the exposure. The desorption energies are estimated at 22.5 and 43.5 kcal/mole, respectively in a similar manner as above. On comparing the spectrum for the stepped (111) surface with that for the flat (111) surface it is readily found that in the former the α_2–CO desorption does not occur and the population of β–CO is higher.

Recent XPS and UPS studies of CO adsorption at 300 K on the flat (100),[5,6] (110)[7,8] and (111)[9] surfaces suggest that on the (100) and (111) surfaces CO is dissociatively adsorbed at low coverages while CO begins to be adsorbed molecularly at high coverages. On the (110) surface, on the other hand, CO is molecularly adsorbed even at low coverage.[7] Molecularly adsorbed CO on the (110)[7] and (100) surfaces is partly desorbed as α–CO at low temperatures and partly converts into dissociated CO. After these results, the α–CO at 380 K (α_1) and 435 K (α_2) in Fig. 4 can be ascribed to molecularly adsorbed CO, and β–CO at 700 K to dissociated CO which is produced during flashing the surfaces besides being induced at 300 K although the desorption obeys the first order kinetics. In conclusion, the feature of Fig. 4 mentioned above suggests that the stepped surface has higher catalytic activity for C–O bond breaking.

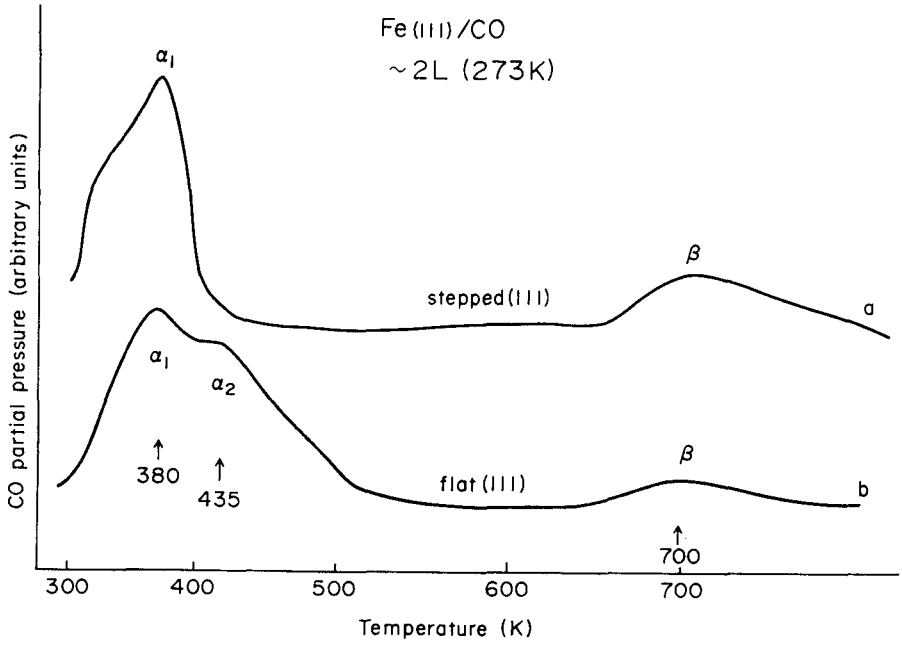

Fig. 4. Thermal desorption spectra of CO from the CO adsorbed flat Fe(111) and stepped (111) surfaces.

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