

Lawrence Berkeley National Laboratory

Recent Work

Title

THE CHEMISORPTION OF CO, CO₂, C₂H₂, C₂H₄, H₂ AND NH₃ ON THE CLEAN Fe(100) AND (111) CRYSTAL SURFACES

Permalink

<https://escholarship.org/uc/item/3kj0m6hq>

Author

Yoshida, K.

Publication Date

1978

0 0 0 4 0 0 3 1 4

Submitted to Surface Science

UC-4
LBL-6689
Preprint c-1

RECEIVED
LAWRENCE
BERKELEY LABORATORY

MAR 8 1978

LIBRARY AND
DOCUMENTS SECTION

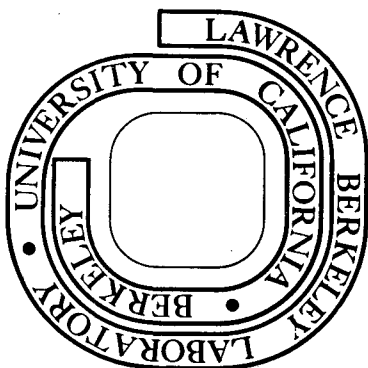
THE CHEMISORPTION OF CO, CO₂, C₂H₂, C₂H₄, H₂ AND
NH₃ ON THE CLEAN Fe(100) AND (111) CRYSTAL SURFACES

K. Yoshida and G. A. Somorjai

January 4, 1978

Prepared for the U. S. Department of Energy
under Contract W-7405-ENG-48

For Reference
Not to be taken from this room



LBL-6689
c-1

LEGAL NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

THE CHEMISORPTION OF CO, CO₂, C₂H₂, C₂H₄, H₂ AND NH₃
ON THE CLEAN Fe(100) AND (111) CRYSTAL SURFACES

by

K. Yoshida* and G. A. Somorjai

Materials and Molecular Research Division, Lawrence Berkeley Laboratory,
and Department of Chemistry, University of California,
Berkeley, California 94720

Abstract

The chemisorption of small molecules (CO, CO₂, C₂H₂, C₂H₄, H₂ and NH₃) has been studied on the clean Fe(100) and (111) crystal faces by low-energy electron diffraction (LEED) and thermal desorption. C₂H₄ and C₂H₂ yield the same sequence of surface structures that change with temperature and crystal orientation. CO and CO₂ chemisorption similarly results in the formation of the same types of surface structures that change with surface temperature and crystal orientation. Ammonia forms several ordered surface structures on both iron crystal faces. All of the molecules decompose as a function of temperature on the iron surfaces as indicated by the Auger and thermal desorption spectra.

* Present address: Institute for Catalysis, Hokkaido University,
Sapporo, Japan.

Introduction

Iron is one of the most reactive metals with complex and useful surface chemistry in both reducing and oxidizing conditions. Iron is an excellent catalyst for the synthesis of ammonia and for the synthesis of hydrocarbons from carbon monoxide and hydrogen. Because it chemically reacts readily with ambient gases, the properties of its clean surfaces can be studied only with the greatest difficulty. Nevertheless, in order to explore the elementary steps of its surface reactions, starting with chemisorption, it is essential that we learn to prepare clean single crystal surfaces of this material. Recent studies^{1,2,3} have shown that single crystal surfaces of iron can be prepared with sufficient purity to permit chemisorption studies to be carried out reproducibly. We have also succeeded in developing a cleaning procedure to obtain iron crystal surfaces with low impurity concentrations.

In this paper we report on the cleaning procedure we have employed to prepare high purity iron single crystal surfaces and on studies of the chemisorption of acetylene, ethylene, carbon monoxide, carbon dioxide, ammonia and hydrogen on two low Miller Index crystal surfaces, the Fe(110) and the Fe(111) crystal planes. These studies were carried out in the reactant pressure range of 10^{-9} to 10^{-6} torr and at surface temperatures of 300 to 900 K.

Experimental

A. Sample preparation and cleaning outside the vacuum chamber

The iron (110) or (111) single crystals were oriented using Laue back reflection X-ray analysis and were cut by spark erosion from a high

purity single crystal rod obtained from Materials Research Corporation. The samples were mechanically polished to produce surfaces parallel to (110) or (111) orientations. They were then fine polished using 0.25 micrometer diamond paste but were not electropolished to avoid pit formation.

Preliminary studies in the ultrahigh vacuum chamber using Auger electron spectroscopy have revealed that sulfur is a major contaminant in the single crystal samples. In order to reduce the sulfur bulk concentration prior to the surface studies, the iron single crystal samples were cleaned in one atmosphere of flowing hydrogen in a furnace for a period of three weeks. The single crystal samples were placed in a silica boat in the hot zone of the furnace (1100 K) using a gas flow rate of 1 liter/sec. The circulating gas passed through a cold trap where the H_2S that formed by the reaction of hydrogen with sulfur diffusing from the bulk of the sample to the surface was trapped and removed from the gas flux. Part of the difficulty in cleaning iron crystals is due to the transformation at 1183 K from bcc to fcc structure which shatters the single crystal samples. Thus all cleaning procedures have to be carried out below these transformation temperatures. At the low temperatures the rate limiting step in the cleaning appears to be the diffusion of sulfur from the bulk to the surface where it is subsequently removed by a rather rapid surface reaction with hydrogen. The bulk diffusion rates of sulfur in iron has been determined⁴ and simple calculations indicate that extended periods (weeks) are necessary to move the sulfur from the samples (1 mm thick discs of $\sim 1 \text{ cm}^2$ surface area) used in our investigation.

B. Sample cleaning inside the diffraction chamber

After treatment of the iron single crystal samples in the hydrogen

furnace, they were mounted on the manipulator on similarly cleaned iron support plates and moved into the ultrahigh vacuum chamber. This was a typical uhv LEED-Auger system equipped with ion bombardment attachment, a liquid nitrogen cooled titanium sublimation pump and a UTI quadrupole mass spectrometer. After the system was evacuated and baked out for 24 to 48 hours, the background residual gas pressure was $\sim 10^{-10}$ torr. On flashing to 900 K, H_2 , CO, H_2O and CO_2 are the main desorption products. By repeating flashing to 900 K the concentrations of these gases decreased and H_2O , CO_2 are eliminated. The liquid nitrogen cooled titanium sublimation pump was found to be effective in maintaining the iron crystal surfaces relatively free of contamination by the residual gases in the vacuum chamber (mostly H_2 and CO). The main impurities on the iron surface were carbon, oxygen and chlorine as detected by Auger electron spectroscopy (AES). By heating the sample to 900 K, sulfur and phosphorous diffused out of the bulk onto the surface. Repeated argon ion bombardment with 500 eV ions at 10^{-5} torr pressure for one hour, while keeping the sample at 700 K, and annealing at 900 K in vacuum produced a clean, well-ordered iron (110) or (111) surface but traces of carbon were still detectable. A typical Auger spectrum and LEED patterns from the clean iron crystal surfaces are shown in Fig. 1. The (110) and (111) clean surface appear to be unreconstructed: they exhibit the (1x1) surface structures expected by the termination of the bulk X-ray unit cell as detected by LEED.

In Table I we list the surface structures that were obtained on adsorption of C_2H_2 , C_2H_4 , CO, CO_2 , NH_3 and H_2 and the experimental conditions that were used to obtain them. These observations were reproducible on two different crystal faces of samples that were cut from different rods. Let us first discuss the adsorption of C_2H_2 and C_2H_4 on the (110) crystal face of iron.

Results

A. Acetylene (C_2H_2) and Ethylene (C_2H_4) adsorption on the Fe(110) crystal surface

Adsorption of C_2H_2 in the 270 - 320 K temperature range produces a poorly ordered (2x2) surface structure at an exposure of 6×10^{-7} torr \cdot sec (Fig. 2a). The LEED pattern does not change on increased exposure (max $\sim 4 \times 10^{-6}$ torr \cdot sec). Adsorption at ~ 400 K surface temperature produces a streaky (1x3) surface structure (Fig. 2c). Above 1×10^{-7} torr \cdot sec exposure, a poorly ordered (1x1) surface structure appears. Upon adsorption of C_2H_2 at >450 K, ^{the} (1x1) surface structure becomes poorly defined. On flashing the surface to 400 K after exposure to acetylene at ~ 270 K, the integral order and half order diffraction beams all become low in intensity. On flashing to 500 K a new LEED pattern begins to develop and upon flashing to 600 K a sharp coincidence pattern that is shown in Fig. 2d appears. On flashing to 700 K this surface structure converts to a $\begin{vmatrix} 4 & 0 \\ -1 & 3 \end{vmatrix}$ surface structure that is shown in Fig. 2e. This surface structure is the same as that reported by Buckley, et al.^{1,5,6} and is attributed to the presence of carbon. On flashing to even higher temperatures, such as 1050 K, the carbon pattern remains on the surface, it does not appear to diffuse into the bulk or be removed in any other way that is experienced after the adsorption of carbon monoxide as will be described in the next section.

Acetylene when adsorbed on a carbon contaminated iron (110) surface produces a (2x2) or (1x3) surface structure. When the molecule was chemi-

sorbed on an oxygen contaminated surface on flashing, it removed the chemisorbed oxygen as indicated by AES. The same result was obtained for the (111) crystal surface. Brucker et al.⁷ reported the same effect on the (100) surface from photoelectron spectroscopy. The flash desorption spectrum of C_2H_2 is shown in Fig. 2f. A C_2H_2 desorption peak appears at ~ 320 K and H_2 desorption peaks appear at ~ 400 K and ~ 470 K.

C_2H_4 adsorption produces the same LEED patterns as adsorbed C_2H_2 . Perhaps the only difference is that the (1x3) surface structure does not convert to the low intensity (1x1) surface structure as easily, by increasing the C_2H_4 exposure, as with C_2H_2 . The flash desorption spectra of acetylene and hydrogen after C_2H_4 adsorption are also similar to those obtained after C_2H_2 adsorption. The desorption of molecular C_2H_4 could not be ascertained from the experimental data.

B. Chemisorption of CO and CO_2 on the clean Fe(110) crystal face

Adsorption of CO at ~ 270 K produces fractional order spots in the (001) direction and near the half order positions at an exposure of $\sim 1 \times 10^{-6}$ torr·sec as shown in Fig. 3a. The LEED pattern does not change with increasing exposure (max exposure $\sim 5 \times 10^{-6}$ torr·sec). This pattern also exhibits weak streaks in the (001) direction.

CO adsorption at ~ 340 K produces the LEED patterns shown in Figs. 3a, b and d. At first diffuse half order spots form (diffuse C(2x2) surface structure) and then a streaky pattern where lines become visible in the (001) direction between the diffraction beams characteristic of the clean iron surface. With increased exposure, from 2×10^{-5} torr·sec to 4×10^{-5} torr·sec, half order spots develop with fractional order spots around them in the (001) direction. This surface structure seems to be the super-

position of the split C(2x2) (Fig. 3a) and C(2x2) structures. At an exposure of 2×10^{-4} torr*sec, all fractional order spots except the half order spots disappear and only the C(2x2) surface structure is visible. The C(2x2) structure, on increased exposure (2.5×10^{-4} torr*sec) converts to a (1x4) surface structure (Fig. 3e). These surface structures seem to be the products of CO decomposition. The flash desorption spectrum of CO from Fe(110) is shown in Fig. 3f. There are flash desorption peaks of ~ 320 K, ~ 400 K and ~ 700 K.

After CO adsorption, on flashing to high temperature, LEED shows surface structure changes. A weak $\begin{vmatrix} 4 & 0 \\ -1 & 3 \end{vmatrix}$ surface structure begins to develop at ~ 500 K. On flashing to 800 K, the $\begin{vmatrix} 4 & 0 \\ -1 & 3 \end{vmatrix}$ structure disappears and (1x1)-C, 0 or (2x2)-C, 0 surface structures appear. When flashing the surface to even higher temperatures, the carbon and oxygen recombine and desorb as molecular CO. Thus, the ordered patterns disappear on flashing to higher temperatures.

CO₂ adsorption at 270 K produced surface structures that are identical to those obtained after CO adsorption at ~ 340 K. The flash desorption peaks after CO₂ adsorption are also very similar to those obtained after CO adsorption. Thus, it appears that both CO and CO₂ form the same surface species on the Fe(110) crystal face.

C. NH₃ adsorption on the Fe(110) crystal surface

Adsorption of NH₃ at ~ 280 K produces a weak (2x2) surface structure with exposure of $> 1 \times 10^{-6}$ torr*sec. (Fig. 4a). The half order spots are destroyed by the incident electron beam and become diffuse. However, the weak half order spots again become sharp and high intensity on heating to ~ 310 K. On heating to 520 K, the (2x2) surface structure converts to the

$\begin{vmatrix} 4 & 0 \\ -1 & 3 \end{vmatrix}$ -N surface structure. This surface structure which has the same unit cell as the carbon surface structure (Fig. 2a), is converted, by heating to 600 K, to a (2x2) surface structure. However, after flashing to 600 K, the Auger spectrum shows the presence of a small oxygen peak along with the nitrogen peak. Thus, it is not certain that the (2x2) surface structure is due to nitrogen alone. On flashing, nitrogen begins to desorb at ~ 720 K (Fig. 4b).

D. H_2 adsorption on the Fe(110) crystal surface

Exposing the clean (110) crystal surface to hydrogen at ~ 300 K results in the appearance of a weak C(2x2) surface structure at an exposure of 8×10^{-6} torr \cdot sec. With increased exposure (2.5×10^{-5} torr \cdot sec), the weak spots due to this structure become streaked in the (110) direction. These streaks become fractional order spots in the (110) direction at an exposure of 8×10^{-5} torr \cdot sec, and a $\begin{vmatrix} 1 & -1 \\ 1 & 2 \end{vmatrix}$ -H surface structure develops (max exposure $\sim 8 \times 10^{-4}$ torr \cdot sec) (Fig. 5a). The flash desorption spectrum of H_2 is shown in Fig. 5b. H_2 desorption peaks after an exposure of $\sim 10^{-5}$ torr \cdot sec appear at ~ 340 K and ~ 400 K. The desorption peaks shift to lower temperature by increased H_2 exposure.

E. Chemisorption of CO, CO₂, C₂H₂, C₂H₄, H₂ and NH₃ on the Fe(111) crystal face.

The chemisorption of CO, CO₂, C₂H₂ and C₂H₄ have produced the same sequence of surface structures as a function of surface temperature. Thus it appears that all of these adsorbates readily decompose on this iron surface and the surface structures are due to the fragments, mostly to carbon. First we shall describe the surface structures that form with increasing surface temperatures and then the small differences in the ordering

characteristics obtained when using different adsorbates will be discussed.

Ammonia and hydrogen adsorb readily at $\sim 300^\circ\text{K}$. Ammonia has the same unit cell as the carbon surface structure obtained by decomposition of hydrocarbons, CO or CO_2 . The differences in the ordering characteristics between nitrogen and carbon will also be discussed.

Adsorption of acetylene at $\sim 270\text{ K}$ makes the diffraction pattern due to the iron/^{substrate} weak at an exposure of $\sim 1 \times 10^{-6}$ torr $^\circ$ sec. The diffraction spot intensities become successively weaker on heating to $\leq 600\text{ K}$. On heating to 600 K , the (1x1) structure becomes well defined again and a new streak pattern appears. On flashing to 750 K , this streak pattern converts to a diffuse (3x3) surface structure. On heating to 850 K , a (1x1) surface structure again forms, but the Auger spectrum indicates that the surface contains much carbon. Flash desorption spectra of adsorbed C_2H_2 produces an acetylene peak at 370 K and a broad H_2 peak at 400 K (Fig. 6a).

Adsorption of ethylene produces surface structures and flash desorption peaks that are identical to that obtained after C_2H_2 adsorption.

Adsorption of CO at $\sim 300\text{ K}$ results in broadening of the iron integral order spots. Thus it appears that adsorbed CO forms small domains of (1x1) structure. On heating to 400 K , the broadening disappears and a streaked pattern appears. This pattern changes by heating to 720 K where a poorly ordered (3x3) surface structure appears. Heating to 800 K produces a (1x1) structure again. However, the Auger spectrum indicates the presence of carbon and oxygen under these conditions.

The flash desorption of adsorbed CO produces three CO peaks at ~ 370 , 420 and 700 K . CO_2 adsorption at 270 K produces surface structures and flash desorption peaks that are identical to those obtained after CO adsorption. During CO, CO_2 , C_2H_2 and C_2H_4 chemisorption, a (5x5) surface

structure also appears after repeated adsorption and flashing. Continued heating to higher temperatures converts the (5x5) structure to a (3x3) surface structure.

Adsorption of NH_3 at ~ 270 K results in the formation of a streaky pattern. With increased NH_3 exposure the LEED pattern does not improve. This streaky pattern begins to change on heating to 420 K and convert to a (5x5) surface structure with streaks (Fig. 7a) and then to a $(\sqrt{2}\times\sqrt{2})$ $R10.9^\circ$ surface structure at 750 K (Fig. 7b). This surface structure begins to convert to a (3x3) surface structure on flashing to higher temperature and finally a sharp (3x3) surface structure is produced on heating to ~ 850 K. The flash desorption spectrum of H_2 after NH_3 adsorption at ~ 270 K is as broad as on the Fe(110) crystal surface. Nitrogen begins to desorb at ~ 750 K.

Adsorption of H_2 at 270 K does not produce new surface structure. H_2 desorption peaks shift to lower temperature by increased H_2 exposure as on the Fe(110) crystal surface. H_2 desorption peaks at exposure of 3×10^{-6} torr*sec appear at ~ 340 K and 400 K.

Discussion

Iron forms strong carbon, oxygen, hydrogen and nitrogen bonds. On adsorption of CO , CO_2 , C_2H_2 , C_2H_4 , H_2 and NH_3 , it is expected that thermodynamic equilibria will yield the decomposition products. This appears clearly to be the case on the Fe(111) as the carbon containing molecules all produce the same series of carbonaceous surface structures with increasing surface temperature. The adsorbates form disordered overlayers even at 270 K, indicating that partial decomposition may have

occurred. Textor et. al.⁸ have reported that both molecular and dissociated CO are present on the Fe(111) surface at 300 K as detected by photoelectron spectroscopy. Our results agree with this conclusion since the flash desorption spectra exhibits multiple peaks and the adsorbate monolayer is disordered. Brucker⁷ and Mason⁹ also conclude that carbon-carbon bond scission has occurred for both acetylene and ethylene at 300 K on the Fe(100) and Fe(111). We find that molecular C_2H_2 desorbs from both (110) and (111) iron surfaces upon heating. Our result would indicate that at least some of the adsorbates remain undissociated. However, C_2H_2 and H_2 are the dominant gaseous products during thermal desorption after the adsorption of C_2H_4 . This indicates C-H bond breaking in the adsorbed layer. On the Fe(110) surface, there is evidence for the presence of ordered molecular CO and C_2H_2 upon adsorption at 270 K from the flash desorption spectra and from the changes of the LEED patterns. There are desorption peaks at ~ 320 K and 400 K, and ~ 320 K for molecular CO and C_2H_2 respectively. Only upon heating to above these temperatures does complete decomposition occur and a series of carbonaceous surface structures are produced. CO_2 and C_2H_4 behave as CO and C_2H_2 , respectively. Therefore, there is little doubt that these molecules are already dissociated at 270 K. The flash desorption spectrum of CO also indicates that a certain fraction of the dissociated molecules recombine and desorb. The hydrocarbon fragments (except acetylene) however do not seem to desorb the only gaseous product that is detectable is hydrogen. This observation is in agreement with the finding that in the presence of hydrocarbons that form during methanation or Fischer-Tropsch reaction of CO and H_2 , the iron surface is covered with a carbonaceous deposit that is carbidic in some cases.

Hydrogen forms a $C(2 \times 2)$ and the $\begin{vmatrix} 1 & -1 \\ 1 & 2 \end{vmatrix}$ ordered surface structures on the Fe(110) crystal face. Although the presence of hydrogen on the surface cannot be detected by Auger electron spectroscopy, the absence of other species and the flash desorption spectra indicates that these structures are the property of adsorbed hydrogen. Ammonia forms several ordered surface structures on both iron crystal faces as seen from inspection of Table I. The Auger spectrum clearly shows the presence of nitrogen on the iron surface. The surface structures obtained after heating the ammonia covered surface to higher temperature have unit cell sizes that are multiples of the iron surface unit cell (3×3) , $\begin{vmatrix} 4 & 0 \\ -1 & 3 \end{vmatrix}$ etc. This indicates that the chemisorbed nitrogen fits into the iron lattice and that iron nitride (that would have different lattice parameters) did not form. Iron does not remain an inert substrate during the adsorption of these reactive gases but chemically interacts with the molecules to form surface compounds. Further exploration of the chemistry of the adsorbate (CO , CO_2 , C_2H_2 , C_2H_4 , H_2 , NH_3)-iron system thus require the use of higher exposure and temperatures that permit the solid state reactions to approach equilibrium. In this circumstance, the rich surface-solid state chemistry of iron can be fully explored.

Acknowledgment

This work was performed under the auspices of the U. S. Energy Research and Development Administration.

Table I

Surface Structures of Chemisorbed Molecules on (110) and (111) Surfaces of Fe Obtained at Various Surface Temperatures

Crystal Face	C ₂ H ₂	T°(K)	C ₂ H ₄	T°(K)	CO	T°(K)	CO ₂	T°(K)	H ₂	T°(K)	NH ₃	T°(K)
Fe(110)	(2x2)	300	(2x2)	300	split C(2x2) ^b pattern	300	split C(2x2) + C(2x2) (1x4)	300	C(2x2)	300	(2x2)	300
	(1x3)	400	(1x3)	400	split C(2x2) ^c pattern + C(2x2)		$\begin{vmatrix} 1 & -1 \\ 1 & 2 \end{vmatrix}$		$\begin{vmatrix} 4 & 0 \\ -1 & 3 \end{vmatrix}$		500	
	coincidence structure ^a	500	coincidence structure ^a	500	(1x4)	340	$\begin{vmatrix} 4 & 0 \\ -1 & 3 \end{vmatrix}$	500				
	$\begin{vmatrix} 4 & 0 \\ -1 & 3 \end{vmatrix}$	700	$\begin{vmatrix} 4 & 0 \\ -1 & 3 \end{vmatrix}$	700	$\begin{vmatrix} 4 & 0 \\ -1 & 3 \end{vmatrix}$	>500						
Fe(111)	(1x1)	300	(1x1)	300	(1x1)	300	(1x1)	300	(1x1)	300	disordered	300
	(5x5)	700	(5x5)	700	(5x5)	600	(5x5)	600				
	(3x3)	750	(3x3)	750	(3x3)	700	(3x3)	700			(5x5) ($\sqrt{2}T \times \sqrt{2}T$) R10.9	750
											(3x3)	850

- a) The diffraction pattern for this structure is shown in Figure 2d.
 b) The diffraction pattern from this structure is shown in Figure 3a.
 c) The diffraction pattern from this structure is shown in Figure 3c.

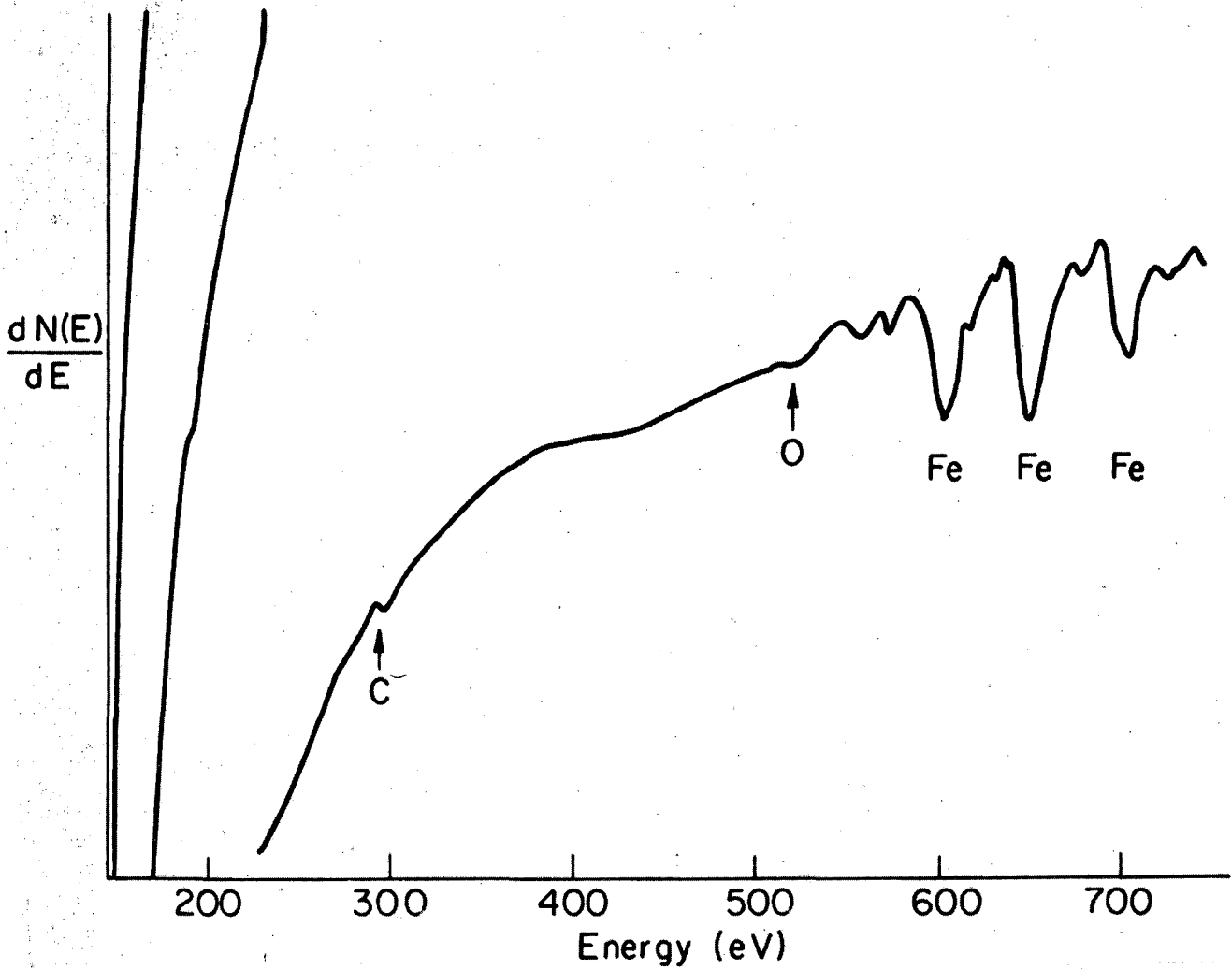
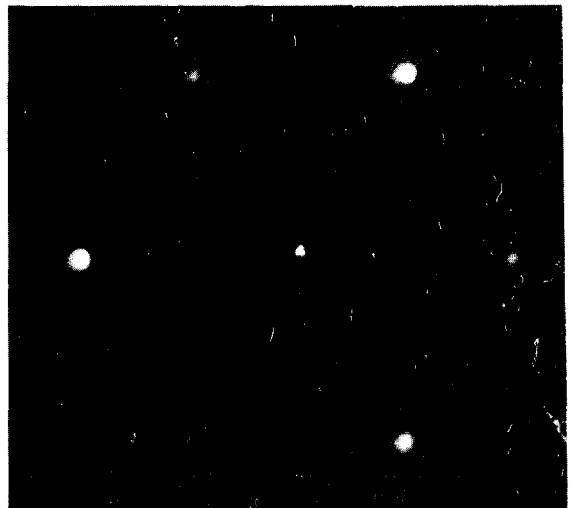
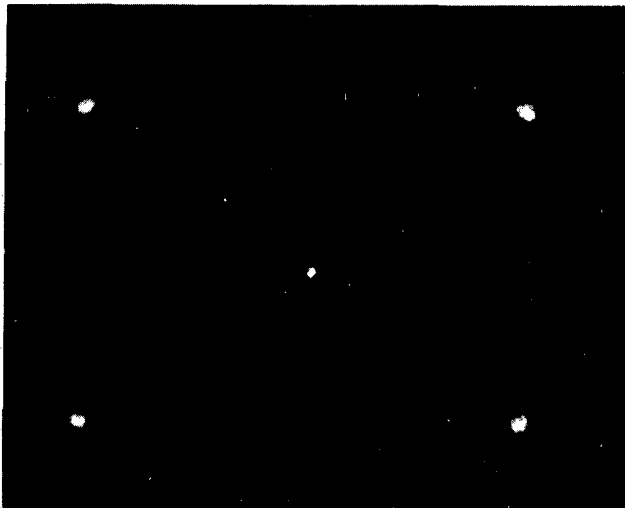
Figure Captions

- Fig. 1 a) LEED pattern of the clean Fe(110) surface at 67 eV; b) LEED pattern of the clean Fe(111) surface at 32 eV; c) Auger spectrum of the clean Fe(110) surface.
- Fig. 2 a) LEED pattern of the (2x2) surface structure obtained after chemisorption of C_2H_2 on Fe(110) at 270 K; b) Diagram of the LEED pattern where o are diffraction spots from the iron lattice; c) Schematic diagram of the LEED pattern of the (1x3) surface structure obtained after chemisorption of C_2H_2 on Fe(110) at ~ 400 K (118 eV); d) LEED pattern after heating to 600 K (86.5 eV); e) LEED pattern of the $\begin{vmatrix} 4 & 0 \\ -1 & 3 \end{vmatrix}$ surface structure after heating to ~ 700 K (83 eV); f) Flash desorption spectra of acetylene and hydrogen from C_2H_2 adsorbed on Fe(110) at 270 K.
- Fig. 3 a) LEED pattern of the split C(2x2) structure obtained after CO adsorption on Fe(110) at 270 K (93 eV); b) LEED pattern due to the superposition of the split C(2x2) and C(2x2) structures obtained after CO adsorption on Fe(110) at 340 K and at exposure 2×10^{-5} torr \cdot sec (106 eV); c) Diagram of the LEED pattern where \bullet are diffraction spots from the iron lattice, \circ are diffraction spots from the split C(2x2) structure, x are diffraction spots from C(2x2) structure; d) LEED pattern of the C(2x2) structure obtained after CO adsorption on Fe(110) at 330 K and at 2×10^{-4} torr \cdot sec (101 eV); e) LEED pattern of the (1x4) surface structure obtained after adsorption of CO on Fe(110) at 330 K and at an exposure of 2.5×10^{-4} torr \cdot sec (103 eV); f) Flash desorption spectra from CO adsorbed on Fe(110) CO adsorption at 280 K (2) adsorption at 340 K.

- Fig. 4 a) LEED pattern of the (2x2) surface structure obtained after adsorption of NH_3 on Fe(110) at 280 K (48 eV); b) Flash desorption spectra of hydrogen and nitrogen from NH_3 adsorbed on Fe(110).
- Fig. 5 a) Schematic diagram of the LEED pattern of the $\begin{pmatrix} 1 & -1 \\ 1 & 2 \end{pmatrix}$ surface structure obtained after adsorption of H_2 on Fe(110) at 300 K; b) Flash desorption spectra from H_2 adsorbed on Fe(110).
- Fig. 6 Flash desorption spectra of acetylene and hydrogen from C_2H_2 adsorbed on Fe(111).
- Fig. 7 a) Schematic diagram of the LEED pattern of the (5x5) surface structure obtained after heating the ammonia covered surface to 750 K (35 eV); b) Schematic diagram of the LEED pattern of the $(\sqrt{2T} \times \sqrt{2T}) R10.9$ surface structure obtained after heating the ammonia covered surface to 750 K (36 eV).

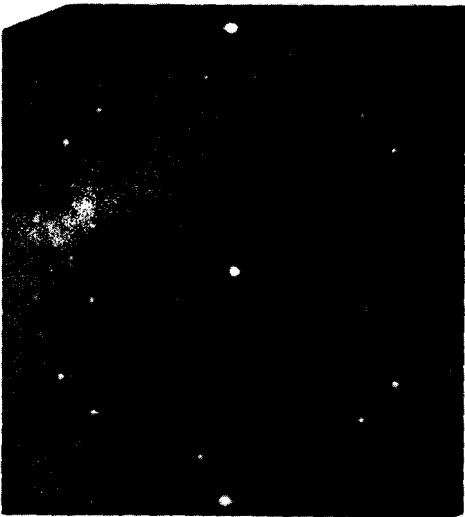
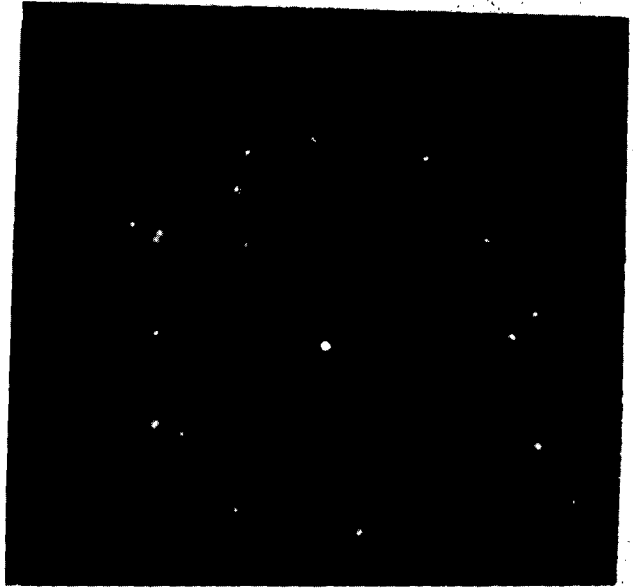
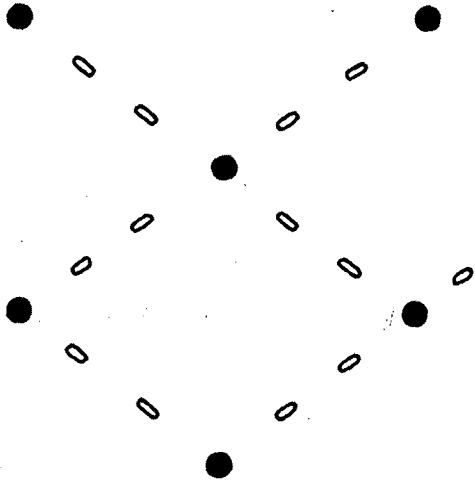
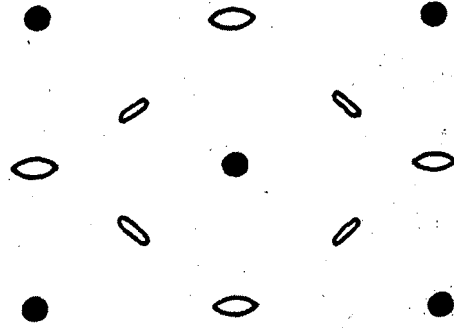
References

1. D. H. Buckley, *Wear.* 20, 89 (1972).
2. G. Ertl, M. Grunze and M. Weiss, *J. Vac. Sci. Technol.* 13, 314 (1976).
3. C. F. Bruckner and T. N. Rhodin, *Surface Sci.* 57, 523 (1976).
4. N. G. Ainslie and A. E. Seybolt, *J. Iron. St. Inst.* 194, 341 (1966).
5. C. Leygraf and S. Elselund, *Surface Sci.* 40, 609 (1973).
6. G. Gafner and R. Feder, *Surface Sci.* 57, 37 (1976).
7. C. Bruckner and T. N. Rhodin, to be published.
8. H. M. Textor, I. D. Gay and R. Mason, to be published.
9. R. Mason and M. Textor, to be published.



XBB 770-12655

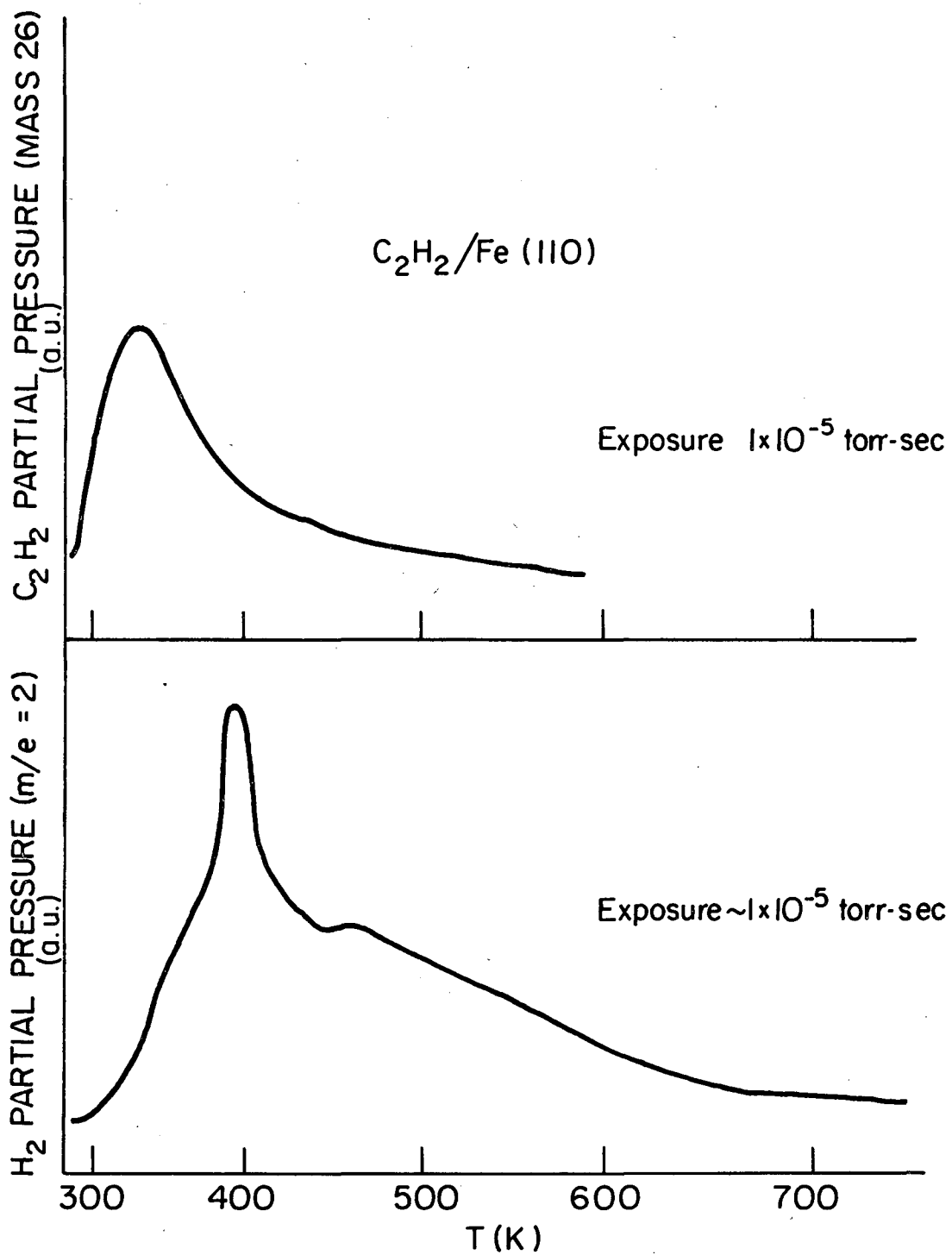
Fig 1



XBB 770-12656

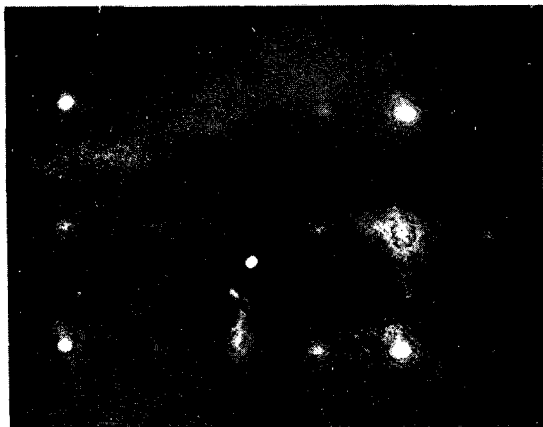
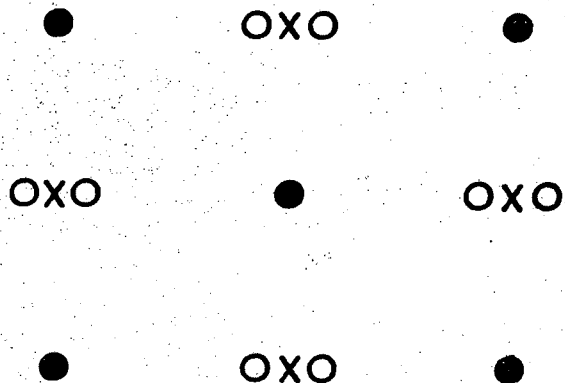
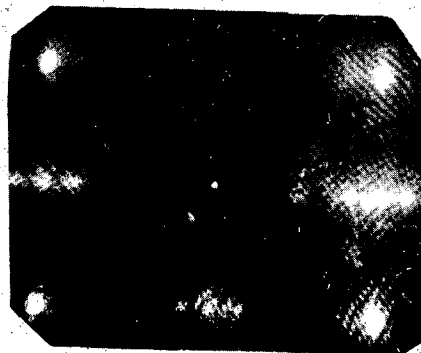
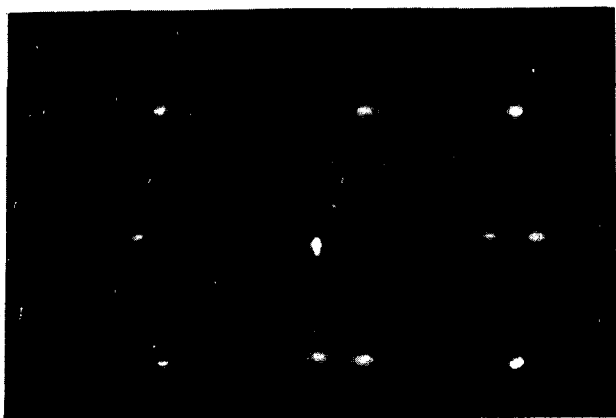
Fig 2

-18a-



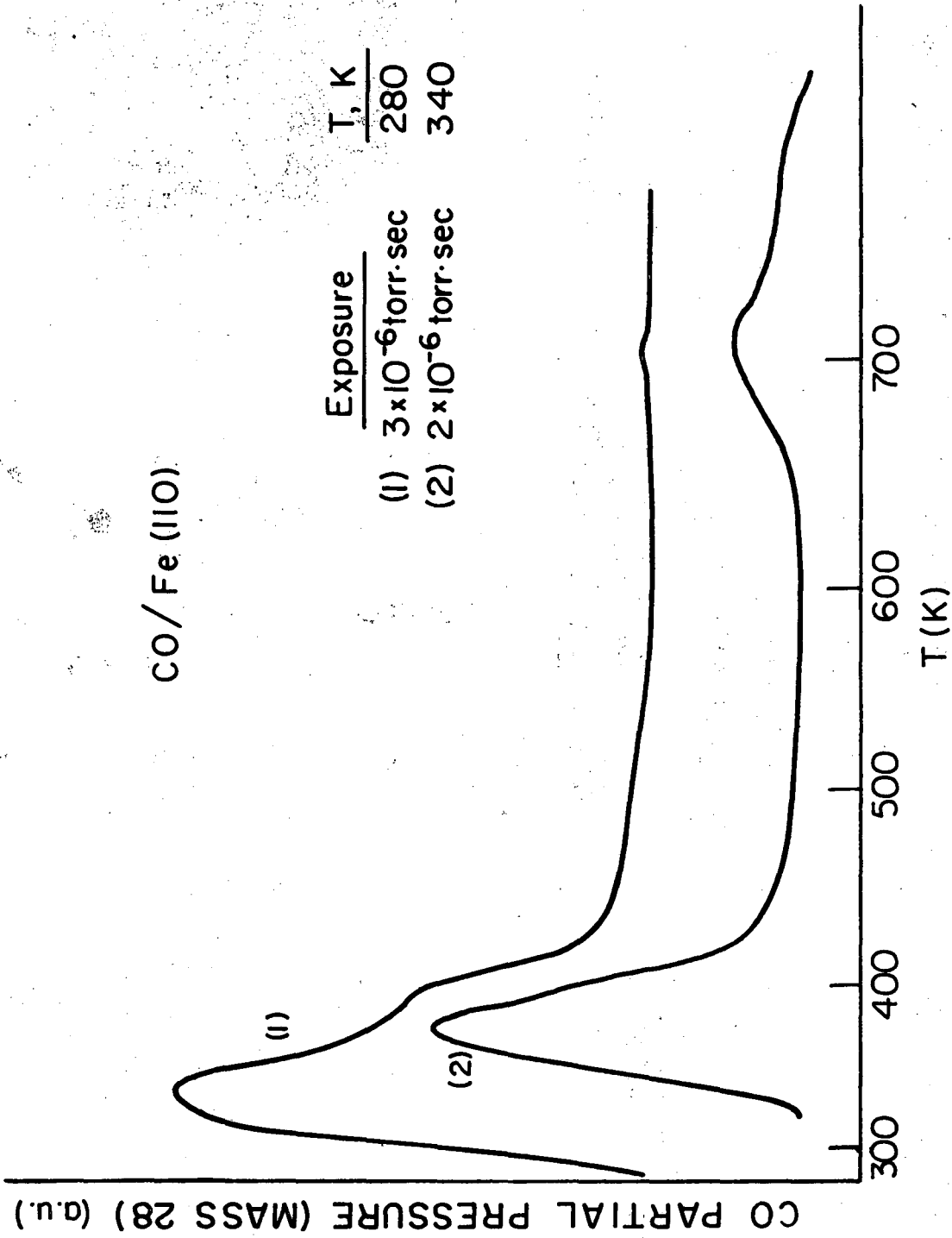
XBL7710-6319

Fig 2f



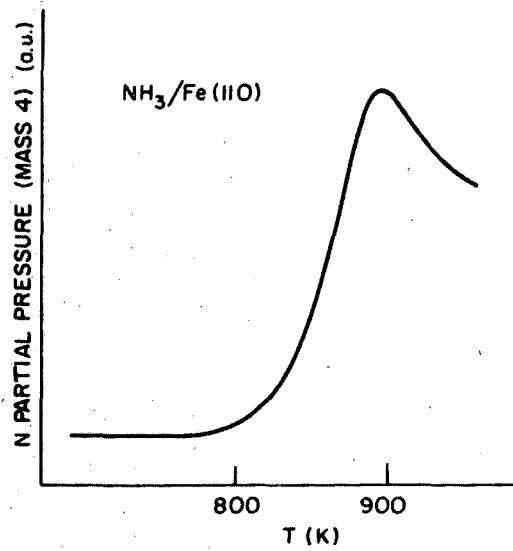
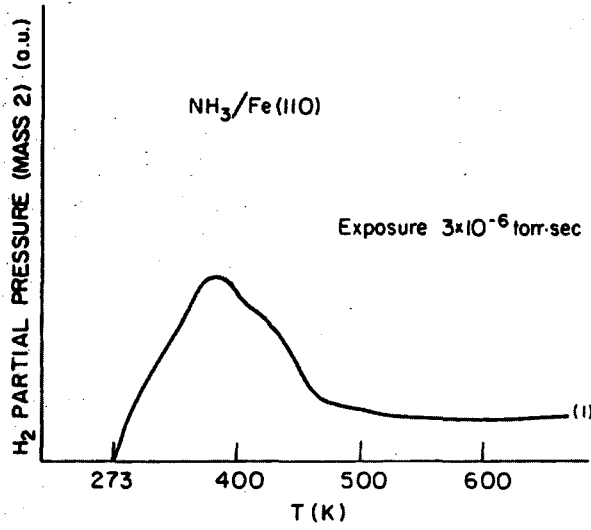
XBB 770-12657

Fig. 3



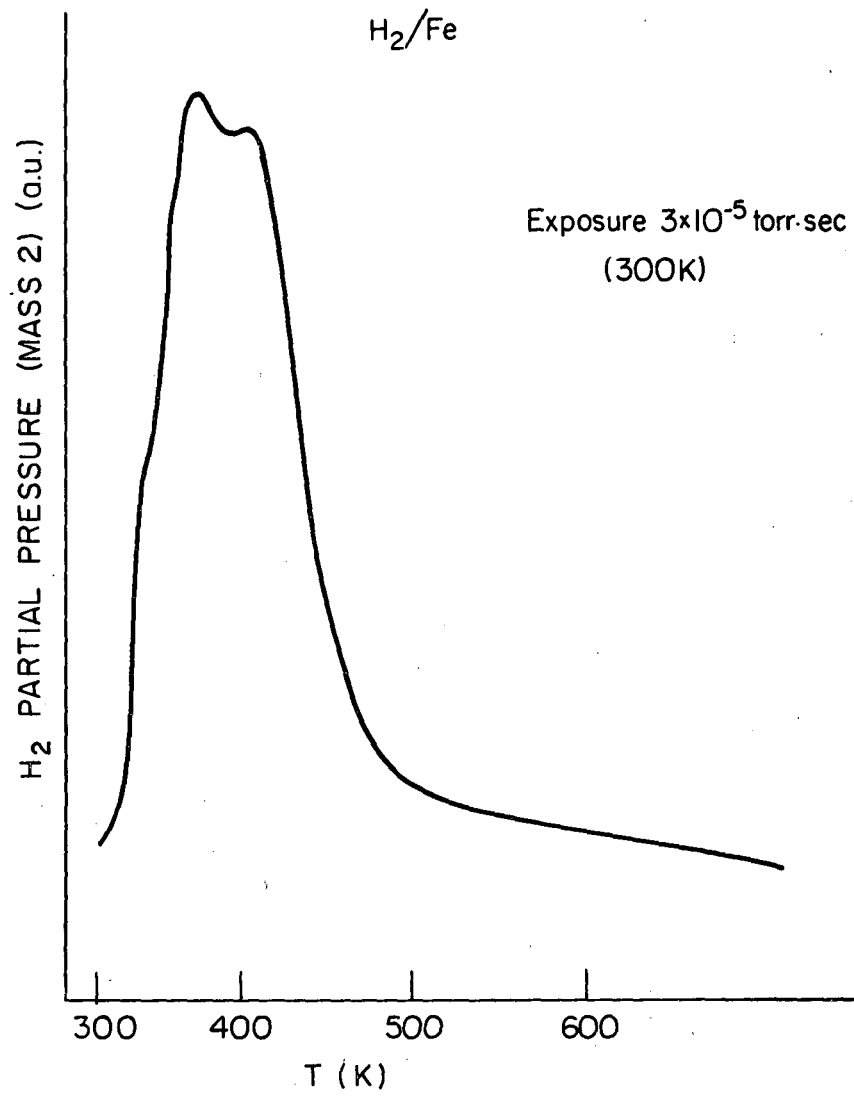
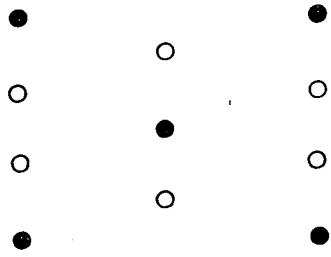
XBL 7710-6318

Fig 3f



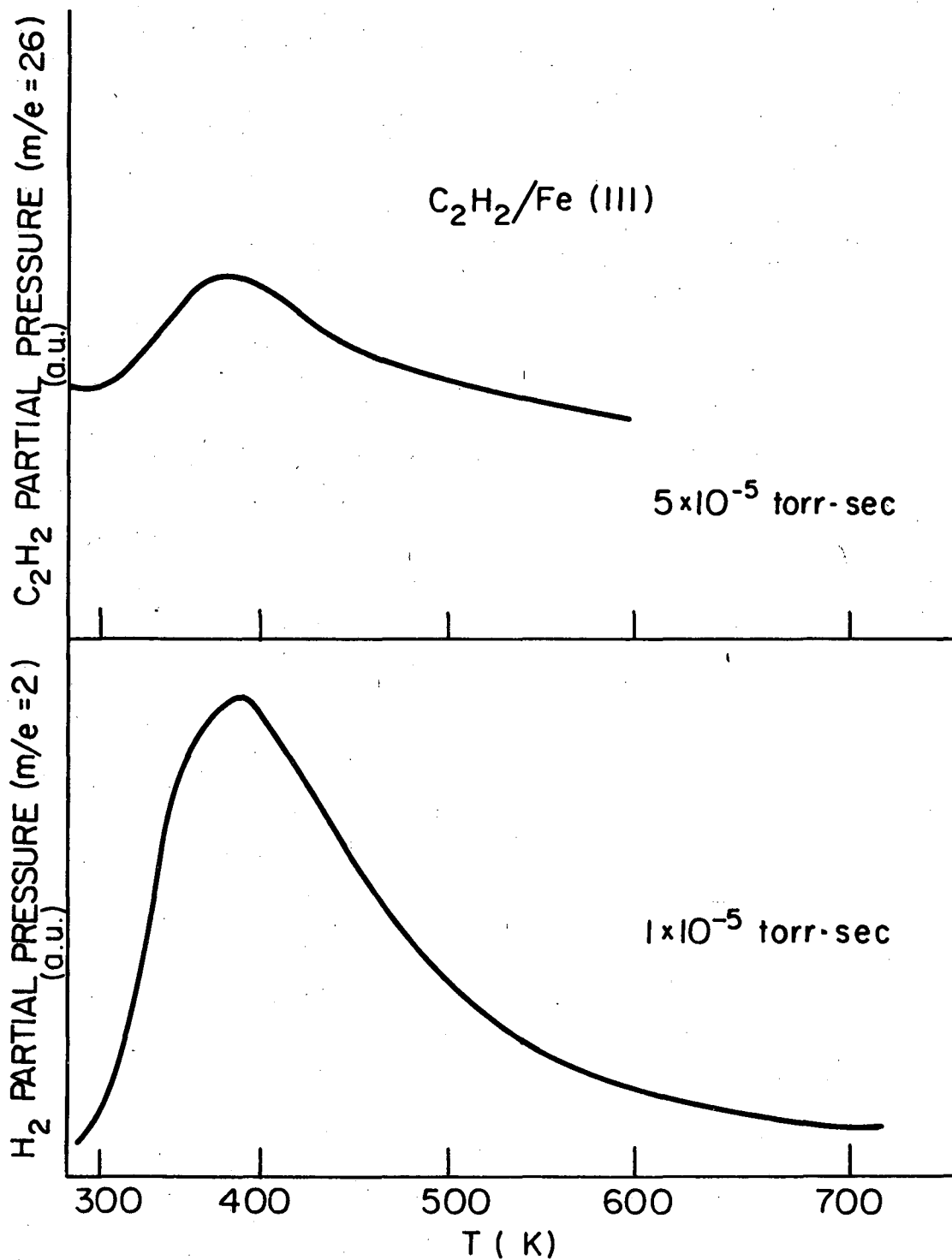
XBB 770-12658

Fig 4



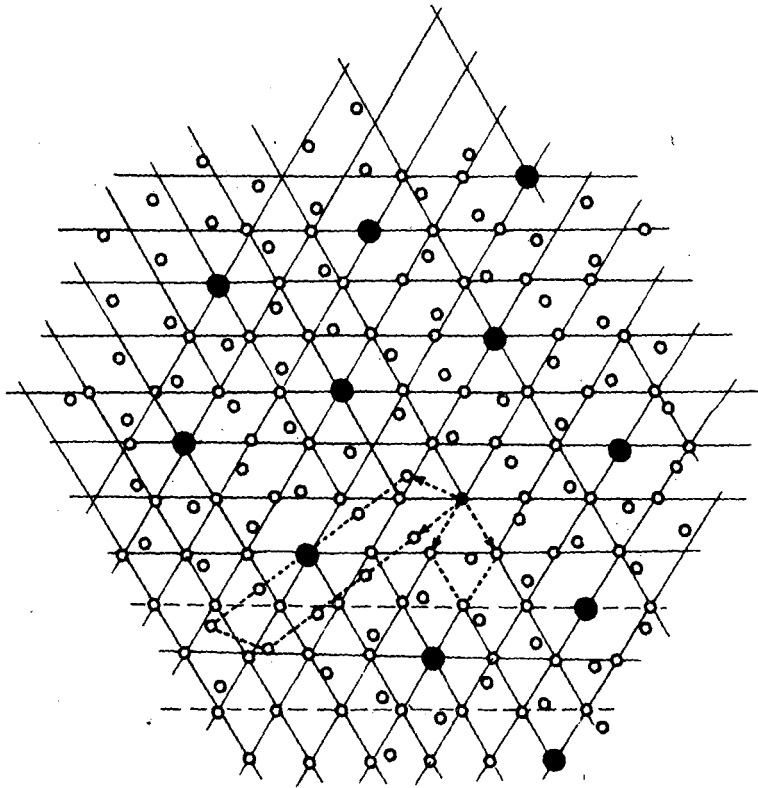
XBL 7710-63 15

Fig 5



XBL7710-6311

Fig 6



XBL 7710-6321A

$(\sqrt{21} \times \sqrt{21}) - R 10.9^\circ$

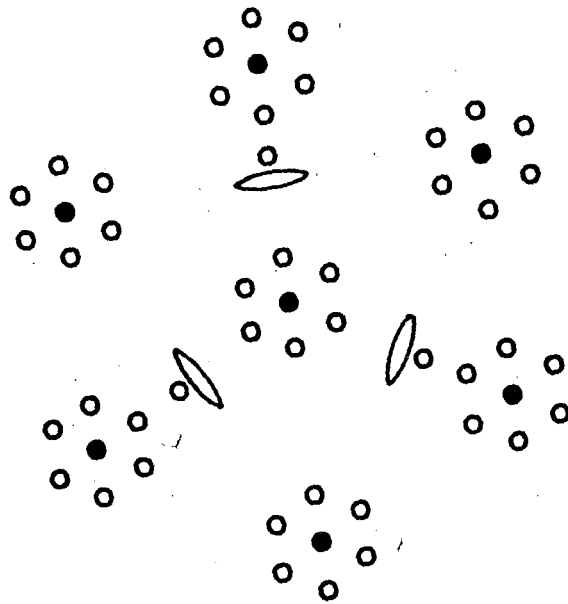


Fig 7

This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

TECHNICAL INFORMATION DEPARTMENT
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720