

THE EFFECT OF ADSORBATES ON THE ANGULAR
PATTERNS OF ION-INDUCED RH ATOM EJECTION
FROM RH(111): SURFACE STRUCTURE DETERMINATIONS

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Surface structure can be determined through various ion beam techniques. Recently our research group has made detailed measurements of target particle ejection (sputtering) from single-crystal surfaces by incident low energy heavy ions. The energy and angular distributions of desorbed ionic and neutral species reflect details of surface structure¹ and adsorbate location² and orientation.³ If desorption mechanisms are adequately understood, surface structure can therefore in principle be obtained from careful measurements of the desorption phenomenon.¹

Material desorbed from ion-bombarded metals is dominantly uncharged. Neutral atoms are easier to characterize than ionic species⁴ due to the presence of fewer matrix effects.⁵ Therefore, a high efficiency multiphoton resonance ionization (MPRI) detector was recently built to simultaneously measure kinetic energy- and angle-resolved neutral (EARN) desorbed atom distributions.⁶ This detector provides a detailed view of the desorption process and is an invaluable aid to understanding how these processes relate to surface structure.

We have examined bombardment of clean,⁷ oxygen-⁸ and ethylene-dosed Rh(111). The clean Rh(111) surface was prepared by standard techniques.⁹ A p(2x2) overlayer of atomic oxygen was created by exposing the clean Rh(111) surface to molecular oxygen. Exposing the surface to ethylene led to a c(4x2) overlayer of ethylidyne, C₂H₃.¹⁰ Oxygen atoms occupy three-fold hollows over third layer Rh atoms;¹¹ and under low temperature conditions ethylidyne is bonded vertically (one carbon on top of the other) in three-fold hollows over second layer atoms.¹⁰ It is not known what site ethylidyne occupies at room temperature, which is the temperature at which our studies are performed.

We briefly review the features of Rh ejection from clean Rh(111).⁷ The relevant crystallographic directions are defined in Fig. 1, as are the possible adsorbate sites discussed below. Some examples of clean Rh(111) EARN data are shown by the solid curves in Figs. 2 and 3. First, ejection in the "open" directions $\phi = \pm 30^\circ$ is favored. This is due to channeling of a moving surface Rh atom by pairs of adjacent Rh atoms on the surface. Second, for low kinetic energy (KE), ejection in the $\phi = -30^\circ$ direction is favored

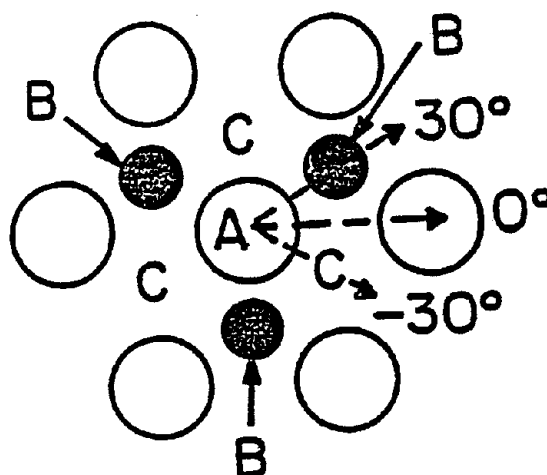


Fig. 1 Surface geometry of Rh(111). Open circles represent first layer atoms, closed circles represent second layer atoms. The three azimuthal directions $\phi = \pm 30^\circ$ and 0° are indicated, as are the three important adsorbate sites A, B, and C.

over the $\phi = +30^\circ$ direction; however for high Rh KE this favoritism is only weakly expressed. The reasons for this trend are as follows. At high KE, a Rh atom leaves the surface early in the collision cascade and is therefore sensitive mainly to the first layer, yielding approximately six-fold symmetric ejection patterns. Low KE particles leave later on after the second layer atoms start interacting with the surface. Therefore three-fold symmetry characteristic of the first two layers results in the ejection patterns. Second layer atoms efficiently push first layer atoms in the $\phi = -30^\circ$ direction, resulting in enhanced ejection in that direction. Third and last, normal ejection is characterized by relatively higher KE than is off-normal ejection. Simulations¹² reveal that this is due to second layer atoms being channeled straight up by triples of surface atoms after being hit from below by incident ions which channel three or four layers into the solid, and then undergo a hard collision of about 180° .

With the above mechanisms in mind, we now treat the adsorbate cases. EARN patterns from $p(2 \times 2)$ O/Rh(111) were previously obtained.⁹ Recently obtained data is shown in Fig. 2. The distinguishing feature of this data is that ejection off-normal in the $\phi = -30^\circ$ direction is attenuated relative to off-normal ejection in the $\phi = +30^\circ$ direction. This immediately suggests that oxygen atoms occupy the C-site, where they more easily block ejection in the $\phi = -30^\circ$ direction.

We now switch attention to the ethylidyne overlayer. The experimental results are summarized in Fig. 3. Focusing first on the polar angular distribution, we see that $\phi = +30^\circ$ and $\phi = -30^\circ$ off-normal peaks are attenuated by about the same amount: 70% and 72% for the 5-10 eV case respectively and 80% and 74% respectively for the 20-50 eV case. Evidently, to whichever site ethylidyne is bonded, B or C, it stands tall enough to have some influence on ejection in all directions. However, the kinetic energy spectra provide an additional clue. The spectra are relatively depleted in

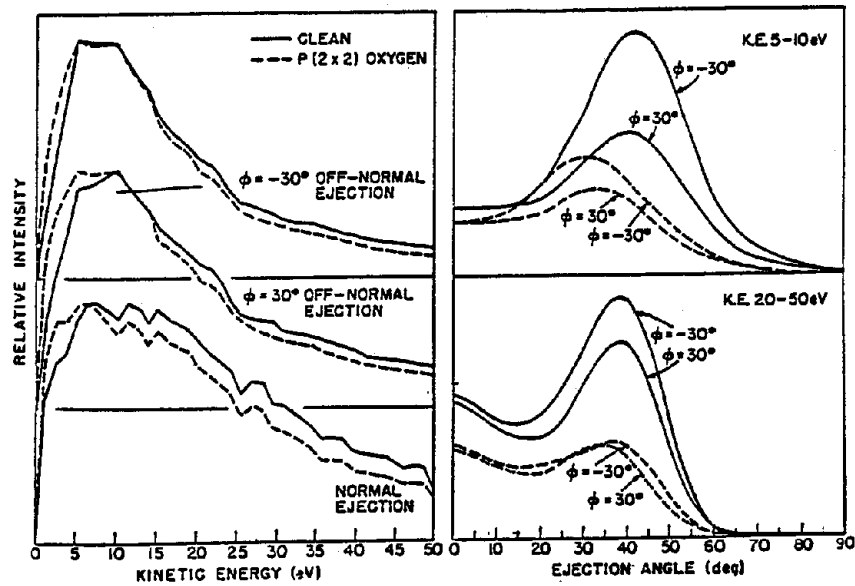


Fig. 2 Kinetic energy (KE) and polar angular distributions of Rh desorbed from clean Rh(111) and p(2x2) O/Rh(111). Angular distributions are integrated over the indicated KE ranges. The KE spectra are peak normalized. The normal KE spectra were integrated over a 6° polar angle range centered at a polar angle of zero. The off-normal KE spectra were integrated over a 6° polar angle range centered at the off-normal polar peak of the appropriate low KE angular distribution.

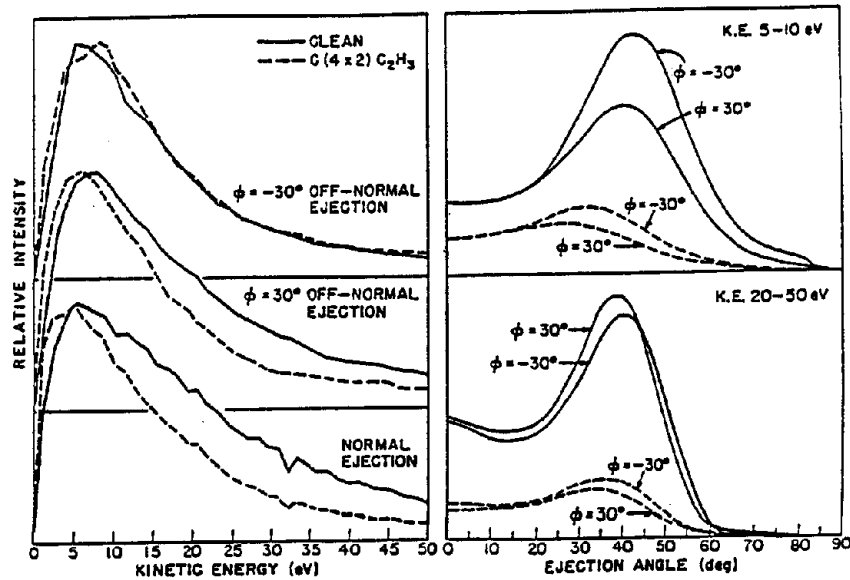


Fig. 3 Kinetic energy and polar angular distributions of Rh sputtered from clean Rh(111) and c(4x2) C₂H₃/Rh(111).

the high KE ranges only off-normal in the $\phi=+30^\circ$ direction and in the normal direction. The latter result particularly suggests that ethylidyne binds to the B-site where it can block second layer atoms ejected via the third mechanism discussed above for clean Rh(111). This is a new site determination which is the same as the one observed for low temperature ethylidyne adsorption.

The EARN technique for surface structure determination should have some continued use in other cases which are being investigated now in our laboratory. We are also beginning a program of simulation of keV ion-induced desorption in the presence of adsorbed overlayers. Such simulations may provide additional insight into the details of how adsorbates alter the desorption patterns of single crystals.

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