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THE ATOMIC STRUCTURE OF SILICON AND METAL SURFACES

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Abstract.—Using FIM, we have studied the atomic structure of thermally equilibrated surfaces of silicon and metals. The (1x2) reconstruction of Pt and Ir (110), the (1x5) reconstruction of Ir (001) and the reconstruction of Pt (001) can be directly observed with a pulsed-laser-heating technique. Images of atomically resolved and well ordered silicon surfaces are obtained for the first time with FIM. Most surfaces are reconstructed. Two distinctly different structures are found for the Si (023) and some other surfaces.

I. INTRODUCTION

In field ion microscopy, an atomically well developed clean emitter surface is almost always developed by low temperature field evaporation process. For metals, the field penetration depth is only about 0.5 Å. This is much smaller than the step height of most surfaces. Thus atoms field evaporate from edges of lattice steps. The surface so formed almost always has the (1x1) structure. For silicon, the effective field penetration depth at a field of a few V/Å is several Å, which is much larger than the lattice step height of most surfaces. Thus atoms have almost equal probability of being field evaporated from plane edges as from the inside of a plane. Surfaces prepared by field evaporation should be disordered. In fact silicon surfaces prepared by field evaporation in vacuum are disordered. This difficulty can be alleviated by reactive gas induced field etching method such as using hydrogen as the image gas.1/ Hydrogen tends to react with silicon atoms at lattice steps and field desorbs as silicon hydride ions at a much reduced field. The surface so formed is slightly better with ring structures clearly visible, but no atomically resolved, well ordered images have been obtained despite considerable efforts of many investigators. In any case, surfaces prepared by low temperature field evaporation are not thermally equilibrated surfaces as surface atoms cannot diffuse at such temperature to form a structure of lowest free surface energy. Of course a surface can be prepared by high temperature field evaporation. But then the structure reflects only a surface of lowest free energy state in the applied field. Most surface structure sensitive phenomena occur in the absence of an applied high electric field, and almost all surface structure studies are done in the absence of a high electric field. This explains why many FIM studies of surface atomic reconstructions do not agree with other studies. Although the structures observed in FIM studies are of interest in their own right, one should also recognize the fundamental differences of surfaces prepared by field evaporation and those prepared by thermal annealing.

We report here an FIM study of surface reconstruction of metals and silicon in the absence of an applied field. Two different techniques have been used. They are a resistivity heating method and a pulsed laser heating method. The latter method

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needs a little clarification. A structure is considered 'thermally equilibrated' if further heating does not produce a change in the atomic structure of the surface. During heating, no field is applied. FIM observations are done below 60 K. Under this temperature, no structure changes are observed by application of the imaging field. For silicon surfaces, all the structures are observed without field evaporation after the annealing. For metal surfaces, temperature field evaporation is found not to change the thermally equilibrated atomic structures of the surfaces.

II. RECONSTRUCTION OF SILICON SURFACES

Atomically resolved and well ordered FIM images of silicon surfaces can be obtained by annealing a field evaporated surface of a very carefully cleaned silicon emitter to 700-850° C for one minute to a few hours at UHV.121 Fig. 1 shows the difference between a field evaporated surface and an annealed surface. As explained in the last section, the field evaporated surface shows only lattice layer ring structures, whereas the annealed surface shows atomically resolved and well ordered image structures. We find that most of the surfaces on this annealed emitter surface do not agree with the (1x1) surface of silicon, thus they are mostly reconstructed. The (111) surface shows no structure features of the (7x7) structure, possibly because the surface so formed is too large. Reducing the plane size by field evaporation can only destroy the well ordered atomic structure of the surface. At this moment, we really cannot understand why the (7x7) structure cannot be seen in the field ion image.

![Fig. 1](image-url)

An interesting observation is that many high index planes form large facets, thus they are crystal planes of very low surface energy. From the point of view of surface energies, they should be the most stable and important surfaces of silicon. Another interesting observation is that two distinctly different atomic structures are seen for a few equivalent surfaces, but they never coexist on the same plane. An example is the {023} surfaces as shown in Fig. 2(a) and (b). These two structures do not agree with the (1x1) structure of the surface which is shown in Fig. 3. One of the image structures, Fig. 2(a), can be formed by dimerization induced displacements of surface atoms as shown in Fig. 3. The other structure can be formed by a set of displacement vector of surface atoms as is also shown in the figure, but at the present no understanding of why these displacements should occur. Building atomic models from field ion images alone is most difficult and uncertain. We must therefore await information from other studies before some of these structures can be clarified. In Fig. 4, we show FIM images of some other silicon surfaces and a
tentative identification of crystal planes. As the entire silicon emitter surface seems to be completely reconstructed, identification of high index surfaces and figuring out how these surfaces are reconstructed are quite difficult. Currently we are using computer simulation and computer assisted structure analysis to overcome these difficulties.

Fig. 2

Fig. 3

III. SURFACE RECONSTRUCTION OF Pt AND Ir SURFACES

The (1x2) reconstruction of Pt and Ir (110) surface has been observed in the FIM. Not only the structure can be clearly seen, but the atomic steps leading to this reconstruction can be studied. Here we will not discuss this plane as reports have already appeared in print. Instead we will discuss the reconstruction of Pt and Ir (001) surfaces.

Ir (001) is known to be reconstructed to the (1x5) structure above about 800 K. The structure proposed can be simply described by squeezing six [110] atomic rows into five [110] atomic row spacings of the underneath unreconstructed layer. As the spacing is not quite enough, these atomic rows are shifted to form a quasihexagonal structure. In addition they are buckled with heights of 0.25 to 0.5 Å. Fig. 5 shows such a model. Field ion images of a non-reconstructed Ir (001) surface is shown in Fig. 6(a). In 6(b), a (1x5) reconstructed surface is shown. As the surface layer is too large, the structure cannot be seen clearly. By slowly field evaporating this layer away, the buckled [110] atomic rows can be seen to give rise to different image intensity. Near the edge of a reconstructed layer, the buckling may be slightly
Fig. 4
relaxed and the quasihexagonal atomic arrangement sometimes can be directly seen. This atomic arrangement can be better revealed by a gradual field evaporation of the layer, and by mapping out the positions of these atoms. Fig. 7 shows results obtained by such a mapping method. Indeed, atoms in the (1x5) reconstructed layer are arranged in a hexagonal pattern. Thus the model is confirmed with atomically resolved FI images.

Reconstruction of Pt (001) surface is much more complicated. It is believed that the reconstruction goes through a disordered phase, and eventually ends up with a quasi-hexagonal structure with the [110] atomic rows lining up with some skewed angles with respect to the [110] atomic row directions of the underneath layer; in one direction it is about 11° and in the other direction it is about 4°. In FI images,7 the structure of the reconstructed layer is quite similar to that of Ir (001), also showing buckled [110] atomic rows with different image intensity. The skewness of the [110] atomic rows in the reconstructed layer can be seen. They are indeed about 11° and 4°, respectively. Atoms in these atomic rows, however, do not arrange in a hexagonal pattern. Instead, they arrange in a "parallelogram" pattern. Thus the proposed structure model, though valid overall, is not valid in atomic details. For details of this study, Ref. 7 may be consulted.

In summary, we have emphasized the difference between surfaces prepared by field evaporation and those prepared by thermal annealing. By recognizing the basic differences, we are able to study surface reconstruction of Pt and Ir surfaces. Our result is in general in very good agreement with other techniques and proposed models. However, we are able to provide details of atomic arrangements, one of which is in variance with an existing model. We are also able to image with full atomic resolution, well ordered surfaces of silicon prepared by thermal annealing. We believe that FIM, when properly used, can be a powerful tool in the structure analysis of solid surface reconstruction.

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