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STM studies of the RT Pb–Si(111) interface structure

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Abstract. The structure of the Pb–Si(111) interface has been studied for submonolayer deposits at room temperature (RT). Two different structures are observed: triangular clusters, each located centrally on one half of a 7 × 7 unit cell and lines of atoms located along the positions of the dimers in the Si(111)–7 × 7 structure. The second type of structure observed fits the 2D close packed structure model of Grey and co-workers with an 8 × 8 overlayer of Pb atoms on top of the Si(111)–7 × 7 structure.

1. Introduction

The Si(111)–7 × 7 suface has been extensively studied using a variety of techniques including STM [2, 3, 4] and the dimer adatom stacking fault (DAS) model [5] of Takayanagi *et al* is now widely accepted. For low coverages of a variety of metals at RT this structure appears to remain reasonably intact, often with either metal atoms directly replacing Si adatoms [6] or with small clusters of metal atoms displacing or overlaying the adatoms in one half of a unit cell [7, 8, 9]. The Pb–Si(111) interface has been studied for some time [10, 11, 12, 13] and it is known that two temperature dependent $\sqrt{3} \times \sqrt{3}R$ 30° phases, known respectively as the α and β phase exist. The alpha phase may be prepared by heating the sample, either during or after deposition, to between 140 and 350 °C. Heating beyond $\sim$ 350 °C causes an irreversible phase change to the β phase [14] and desorbs Pb at increasingly higher rates as the temperature is raised. Recent work suggests that a further commensurate 7 × 7 phase exists for room temperature deposits of Pb [1, 15, 16] and that the low temperature α phase is incommensurate with the bulk, having a lattice parameter corresponding to a 2.3% compression relative to bulk Pb(111). Grey *et al* [1] suggest that the metastable RT 7 × 7 phase consists of an 8 × 8 Pb mesh in a 7 × 7 unit cell with only partial occupancy of Pb near the corners of the 7 × 7 unit cell. This structure requires a 4.0% compression of the Pb layer with respect to bulk Pb. This accounts for the ready transformation to the α phase, which requires only about half this amount of compression, on gentle heating of the sample. This work concentrates on the 7 × 7 RT interface – work on both the α and β phases is currently underway.

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2. Experimental procedure

The tunnelling microscope used here was purchased from Omicron Vakuumphysik GmbH as a bolt-on addition to an existing UHV chamber containing a combined rear-veiw 4-grid LEED optics and retarding field analyser for Auger spectroscopy. The Pb deposition source was a simple collimated beam type, cooled by liquid nitrogen during deposition and operated a rate of ~ 0.066 ML min^{-1}. The silicon substrate was cut from a 100 Ω cm resistivity *n*-type wafer and was cleaned by flashing to 1200 °C for one minute. After flashing the sample was cooled slowly (< 100 °C per min), to room temperature and its cleanliness assessed by the use of the Auger spectrometer. The flashing was repeated until no trace of carbon was found. LEED investigation of surfaces prepared in this way showed a well formed 7 × 7 pattern. Once a suitable surface was prepared Pb was then deposited with the sample at room temperature. The chamber operated at a base pressure of $< 1 \times 10^{-10}$ mbar during tunnelling and Pb deposition, rising to $< 1 \times 10^{-8}$ mbar during sample heating. Tungsten probe tips were prepared by electro-chemical etching and were cleaned *in-situ* by scanning the tip in the corner of the sample with a sample bias voltage of 10 V and a current of 40 nA.

3. Results and discussion

Figure 1 shows an 800 × 800 Å STM topograph of the Pb–Si(111) surface, for a coverage of $\sim$ 0.6 ML taken with +1.5 V sample bias and 0.1 nA tunnelling current. Cursory examination of this surface reveals the presence of two distinct surface regions and three different surface structures. The region in the upper left hand corner of the image appears at first glance to be rather disordered. However a closer inspection reveals a set of common repeated features. These features consist of short bright parallel ridges. Only three alignments of these ridges are found with 60° between any two of the three possible directions. This suggests a substructure with 60° rotational symmetry. The other two structures co-exist in the region located in the lower right hand corner of the image. The first of these structures consists of what appear to be interlocked hexagonal rings, each composed of six fairly well-resolved large protrusions. In the centre of each ring is a dark hole similar to those seen on the Si(111)–7 × 7 reconstructed surface. The other structure consists of long criss-crossed lines with discernable structure. As in the upper left hand region of the image, the lines only have three possible orientations with 60° between any two. This would suggest a similar substructure in both regions, or perhaps a slightly disordered version of the same substructure in the upper region, accounting for the visibly worse ordering found there. The hexagonal ring and criss-crossed line structures will be referred to as structures A and B respectively for the rest of this article. The unit cell for structure A can easily be identified as a parallelogram and one of these is outlined in the image found in figure 1. Careful measurement of the size of the unit cell shows that it is the same as that of the Si(111)–7×7 reconstruction. Thus one can conclude that the visible structure is formed as an overlayer on top of the existing 7 × 7 substrate structure in the form of clusters of one or more atoms, with two clusters per Si(111)–7 × 7 unit cell. However from this image it is not possible to obtain the registry of the overlayer with respect to the bulk. Figure 2 shows a different scale, higher resolution image of the Pb–Si(111) surface for a lower coverage of Pb. This image shows the same structure

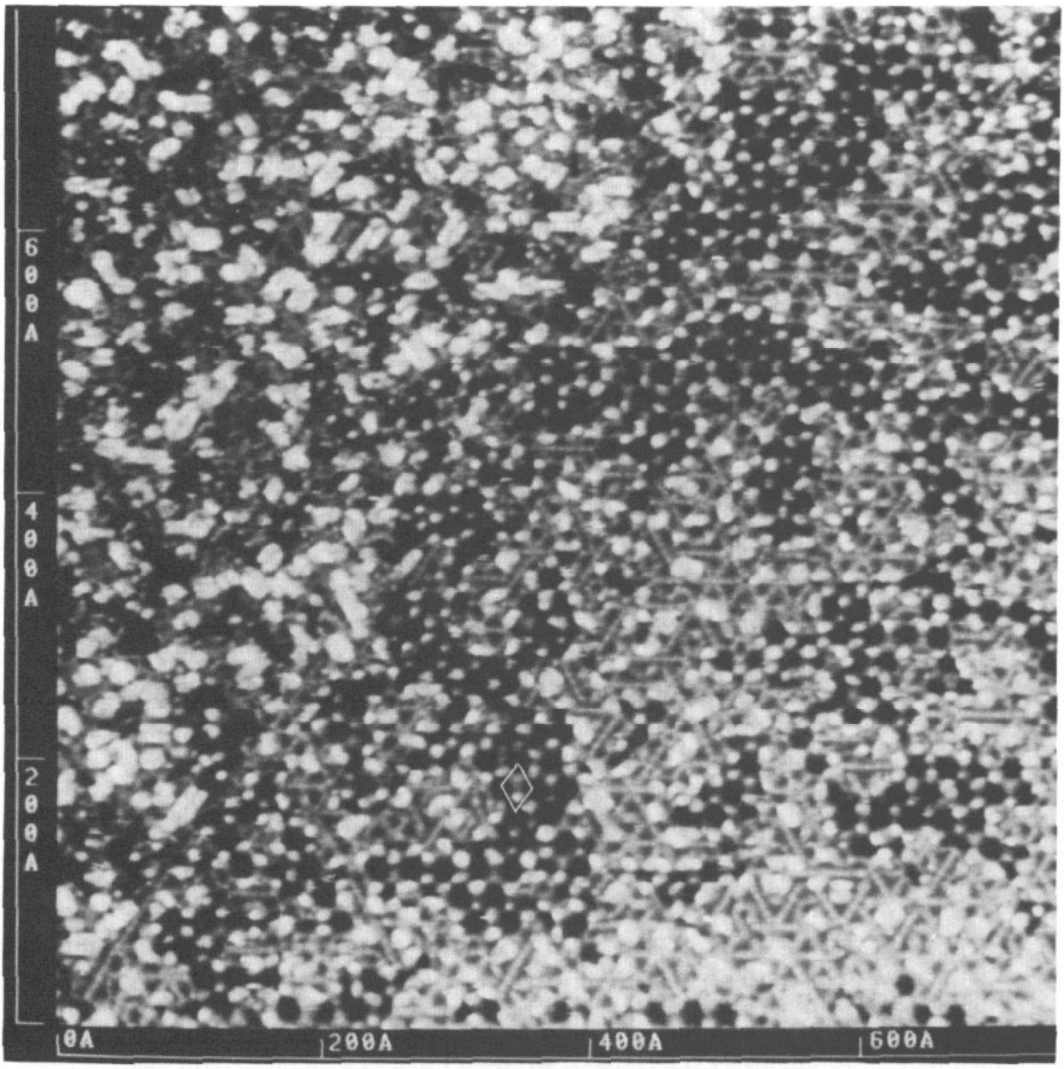

Figure 1. STM topograph of Pb–Si(111) taken at +1.5 V, 0.1 nA. One unit cell is outlined. Black to white represents a height change of ~ 3.5 Å.

as seen in the lower right hand region of figure 1, but with worse ordering and only structure A present. Additionally one can also see some remnants of the substrate Si(111)–7 × 7 structure. Particularly noteworthy is the presence of visible Si(111)–7 × 7 adatoms, especially around the deep corner holes in the lower right hand side of the image. One full unit cell is outlined in the centre of the image in which the adatoms on the upper half are clearly visible. This shows that the Pb clusters are each positioned centrally on one half of a 7 × 7 unit cell. A recent study of the same surface by Ganz *et al* [17] found regions containing features similar to those described above for structure A. They propose a model for this structure which is entirely consistent with our observations. This consists of a triangle of Pb atoms located above and between Si(111)–7 × 7 adatoms, with occasional occupancy of the central site. They do not find any evidence for structure B. However this may be due to the lower coverages of Pb used in their work. We were unable to determine accurate values for coverage.

However from a rough calibration using LEED measurements, we believe that it was of the order of 0.2 ML for the image in figure 1 and 0.1 ML for the image in figure 2. From the proposed model of structure A it can be shown geometrically that the lines of structure B run mainly between half unit cells along the positions of the dimers in the Si(111)–7 × 7 structure. The positions of the atoms in these lines compare well with those predicted from the Patterson function of Grey *et al* [1] with every other edge site, starting at the corner hole, occupied. The actual positions most often observed are above the three dimer bonds on each 7 × 7 unit cell edge. We therefore propose that we are observing the initial stage of the 8 × 8 overlayer structure proposed in [1].

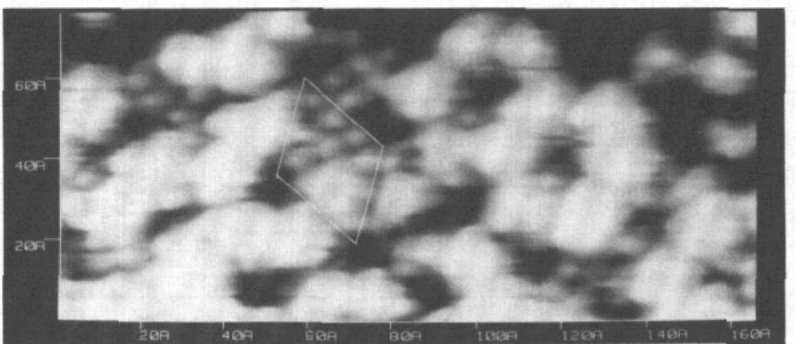

Figure 2. STM topograph of Pb–Si(111) taken at −2.5 V, 2 nA. One unit cell is outlined. Black to white represents a height change of ~ 3.5 Å.

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