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Pb thin films on Si(111): Local density of states and defects

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Abstract
Local density of states and atomic structure of the stripped incommensurate phase, the √3 x√7 phase and the 1 x 1 phase of a monolayer of Pb on Si(111) are characterized by scanning tunneling microscopy and spectroscopy. The dI/dV-images reveal congruent local density of states structures for the stripped incommensurate and the √3 x√ phase but suggest a hexagonal lattice of the local density of states for the 1x1 phase while the atomic structure consists of one more atom in the center of each hexagon. Vacancy defects and impurities show a depletion of local density of states for the stripped incommensurate and √3 x√7 phase. Vacancies and impurities show an increase and no clear depletion in local density of states for the 1 x 1 phase, respectively.

Keywords
states, local, 111, si, films, thin, density, pb, defects

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Pb Thin Films on Si(111): Local Density of States and Defects

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***Abstract*—Local density of states and atomic structure of the stripped incommensurate phase, the √3×√7 phase and the 1 × 1 phase of a monolayer of Pb on Si(111) are characterized by scanning tunneling microscopy and spectroscopy. The *d*I/*d*V-images reveal congruent local density of states structures for the stripped incommensurate and the √3×√7 phase but suggest a hexagonal lattice of the local density of states for the 1×1 phase while the atomic structure consists of one more atom in the center of each hexagon. Vacancy defects and impurities show a depletion of local density of states for the stripped incommensurate and √3×√7 phase. Vacancies and impurities show an increase and no clear depletion in local density of states for the 1 × 1 phase, respectively.**

Keywords*— lead thin films, stm, sts, dI/dV-mappings, local density of states

I. INTRODUCTION

Surfaces and thin films can exhibit various reconstructions different from bulk materials. A silicon surface for example has been studied intensively because of the 7 × 7 reconstruction of its (111) surface until scanning tunneling microscopy (STM) measurements revealed its atomic structure [1]. Thin metal films, *e.g.* lead (Pb), were grown on silicon (Si(111)–7 × 7) and studied extensively because of their surface and nanosize induced quantum effects different from those of bulk materials [2-4]. Thin films of Pb are produced by MBE [5]. For Pb thin films of about one monolayer coverage which can be regarded as two-dimensional (2D) materials a striped incommensurate (SIC) phase can be obtained [6]. For slightly higher coverage a √3 × √7 phase can be found. A 1 × 1 phase of the Pb film is revealed in a mixed phase together with √3 × √7. The electronic properties of 2D materials are sensitive to the structural defects that may appear during growth or processing. It is possible to tailor the local properties of Pb thin films and to achieve new functionalities by the effects induced by the defects. In this work, STM as well as scanning tunneling spectroscopy (STS) is applied to get insight into the different structural phases of monolayer Pb thin films and make them comparable. The atomic structure of the phases visible in STM images is discussed regarding the appearance of defects. Subsequently the influence of structure and defects on the local density of states revealed by dI/dV-images is analyzed.

II. EXPERIMENTAL SECTION

Growth and all characterizations were carried out *in-situ* in an ultra-high vacuum low-temperature STM system equipped with a molecular beam epitaxy (MBE) preparation chamber (UHV LT STM, UNISOKU USM-1500). A clean and reconstructed Si(111)-7 × 7 surface was prepared by heating up (flashing) a n-type Si wafer to 1250 ℃ at least 10 times after degassing for 8 h at 500 ℃.. Ultra-thin films of Pb were grown on the Si(111)-7 × 7 surface applying MBE. Pb deposition rate at room temperature was about 0.1 ML/min. STM images and *d*I/*d*V-images were taken simultaneously at 77 K. Measurements were performed at similar positive sample voltages which corresponds to probing the unoccupied states of the conduction bands of the Pb thin film samples. A modulation voltage of 50mV at imaging voltages between 1.2 V and 1.6 V and a frequency of 924Hz were applied at the Lock-in amplifier for *d*I/*d*V-imaging.

III. RESULTS AND DISSCUSSION

A. SIC and √3 x √7 phases of Pb

Deposition of Pb with a coverage of about one monolayer atomic density results in a single-atom-layer Pb film in the SIC phase along with a pronounced Moiré superstructure. A STM image revealing the atomic structure of the thin film in the SIC phase and the √3 × √7 phase is shown in Fig. 2a and b. Quad-mer and tri-mer atomic structures are suggested to be fused to one light spot in the STM image [6]. Atomic models illustrating lattice and oligomer structures are shown in Fig. 1c and 2c for the SIC and the √3 × √7 phase, respectively. The dI/dV-images measured in parallel to the STM images enable the comparison of local density of states (LDOS) and atomic structure. As a result, each structure atomic structures and LDOS including Moiré superstructures appear largely identical (congruent) for the SIC and the √3 × √7 phase, respectively. Impurities (I) owing to adatoms as well as vacancies (V) are visible for the SIC phase in Fig. 1a. These adatoms appear as decrease of *d*I/*d*V-image intensity which is proportional to the LDOS. This decrease is visible in Fig. 1b. The Kondo-effect was found to be responsible for variations of LDOS for energies near the Fermi-level but does not suggest variations at higher electron energies studied here [7]. STM-image contrast and *d*I/*d*V-image contrast change at the two impurities which could be explained by *e.g.* oxidized Pb atoms (quad-mers). A

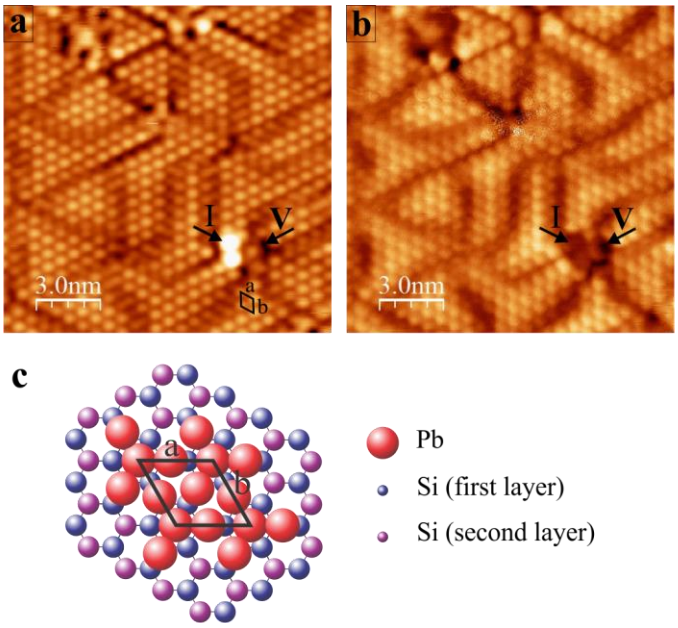

Fig.1. (a) STM height image, (b) *d*I/*d*V-image, and (c) structure model of the stripped incommensurate (SIC) phase of a Pb thin film. Defects are indicated by “I” for impurity and “V” for vacancy. The unit cell corresponding to the atomic lattice is indicated in (a) and (c). (V = 1.2 V, I = 0.1 nA)

(quad-mer) vacancy (V) visible in Fig. 1a next to the two impurities (I) appears as vacancy (depletion of LDOS) in the *dI/dV*-image in Fig. 1b as well. Similar behavior is revealed for the √3 × √7 phase for the defects and (tri-mer) vacancies visible in Fig. 2a and 2b. The Impurity (I) in the STM image appears as LDOS depletion in the *dI/dV*-image. The vacancy (V) causes a subduction of density of states.

B. 1x1 phase of Pb

Some remarkable features appear comparing the LDOS and the atomic structure of the 1 × 1 phase of the Pb thin film. Pb thin films in the 1 × 1 phase are obtained for slightly higher coverage of a monolayer appearing mixed with the √3 × √7 phase. The atomic structure of the 1 × 1 phase of the Pb thin film is revealed by the STM image in Fig. 3a. The STM image shows a slightly different image contrast for atoms in hexagons and atoms in the center of these hexagons. To guide the eye one hexagon (including a defect) in Fig. 3a and 3b is marked by a white hexagon. The LDOS of the 1 × 1 phase revealed by Fig. 3b exhibits a hexagonal (honeycomb) lattice. Surprisingly, the Pb atoms in the center of the hexagons do not contribute to the LDOS. This can only be explained by different interaction with the silicon substrate since no lateral difference in structure relative to the surrounding atoms is found. A different interaction to the substrate should cause a shift of the energy level and therefore result in different local density of states when imaged. Farther, the simple structure model using a buckled Si(111) surface including a first and a second layer of silicon atoms is shown in Fig. 3c does not consider possible remaining reconstructions originating from the Si(111)-7 × 7 reconstruction. This possible remaining reconstruction might also have a large influence on the Pb thin film and its LDOS.

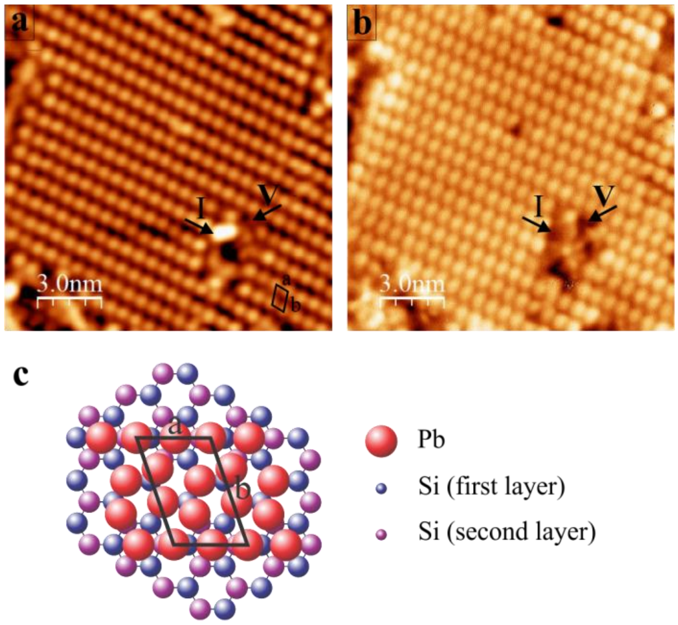

Fig.2. (a) STM height image,(b) dI/dV-image, and (c) structure model of the √3 × √7 phase of a Pb thin film. Defects are indicated by “I” for impurity and “V” for vacancy. The unit cell corresponding to the atomic lattice is indicated in (a) and (c). (V = 1.4 V, I = 0.1 nA)

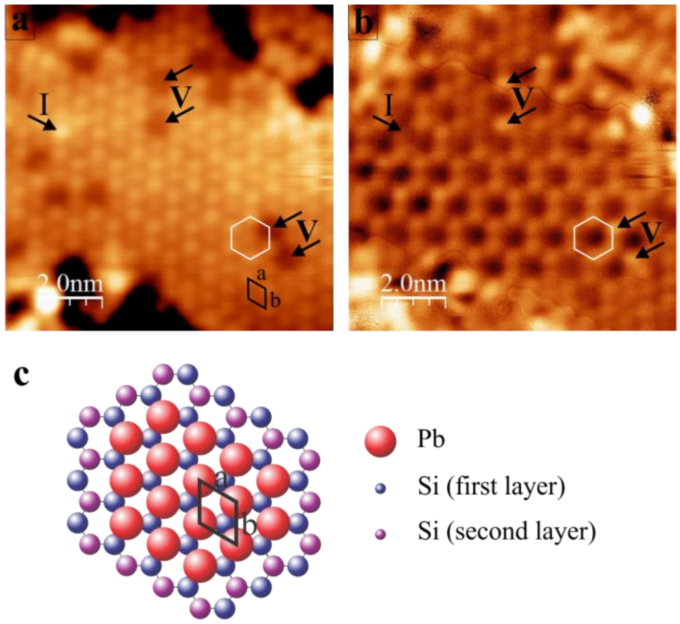

Fig.3. (a) STM height image, (b) dI/dV-image, and (c) structure model of the 1 × 1 phase of a Pb thin film. Defects are indicated by “I” for impurity and “V” for vacancy. Two double vacancies are indicated. A white hexagon indicates the hexagonal atomic structure and LDOS. The unit cell corresponding to the atomic lattice is indicated in (a) and (c). (V = 1.6 V, I = 0.1 nA)

The impurity (I) shown in in Fig. 3a is not clearly causing a corresponding depletion of LDOS (Fig. 3b) as it was found for the other phases. This is the case despite equal conditions during measurements since the 1×1 phase appears mixed with the $\sqrt{3} \times \sqrt{7}$ phase. Atomic vacancy defects (V) clearly visible in Fig. 3a appear as increase of LDOS in the corresponding dI/dV-image in Fig. 3b. This is surprising because vacancies caused LDOS depletions for the other phases. The increase might be due to the generation of additional 'surface'-states at the generated additional 'surface' represented by the surrounding six hexagon atoms and also by the local substrate surface at the given electronic energy.

IV. Conclusion

We studied the structures and the local density of states of thin layers of Pb on Si(111) for different coverage. We investigated the striped incommensurate (SIC) phase, the $\sqrt{3} \times \sqrt{7}$ phase and the 1×1 phase originating from slightly different coverage of a monolayer of Pb on Si(111). Atomic structures and local density of states appear largely identical for SIC and $\sqrt{3} \times \sqrt{7}$ phases. The lead thin film in the 1×1 phase exhibits a hexagonal lattice for the local density of states appearing different from the atomic structure. We found different characteristics of defects for the stripped incommensurate and the $\sqrt{3} \times \sqrt{7}$ phase compared to the 1×1 phase. We revealed impurities and vacancies appearing as depletions in local density of states for the stripped incommensurate and the $\sqrt{3} \times \sqrt{7}$ phase. We found impurities and vacancies resulting in increased local density of states for the 1 x 1 phase.

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