Structure and growth of epitaxial Pb on Si(111)

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A detailed study on the structure, growth, and morphology of epitaxial Pb layers on Si(111) is presented. Grey *et al.* already determined the structures of the Si(111)(7×7)-Pb and Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) monolayer phases with grazing-incidence x-ray diffraction. Our experimental data mainly support their models. In addition, we show that the Pb sites of the incommensurate $\sqrt{3} \times \sqrt{3}$ phase are spatially modulated by the substrate corrugation potential. At higher coverages, the Pb atoms form three-dimensional islands that are either oriented parallel to the Si lattice or slightly twisted. The twist angles are different for the 7×7 and $\sqrt{3} \times \sqrt{3}$ interfaces and can be understood on the basis of simple geometrical arguments. Also, the morphologies of the thick overlayers are different for the two types of interfaces. We argue that both phenomena can be understood if one assumes that the 7×7 and $\sqrt{3} \times \sqrt{3}$ interface structures remain preserved after depositing thick overlayers.

I. INTRODUCTION

A straightforward interpretation of the electronic properties of metal-semiconductor interfaces is often hampered by the fact that defects or chemical reactions at the interface play a dominating role. However, unreactive epitaxially grown metal-semiconductor contacts are considered ideal systems for studying coveragedependent structural and electronic properties. Only for these well-defined metal-semiconductor contacts will it be possible to relate their electronic properties directly to the crystal structure and chemical binding at the interface. The Pb/Si and Pb/Ge systems are prototypes of such unreactive, epitaxial metal-semiconductor contacts and a study of the evolution of their electronic structure during epitaxial growth may provide basic understanding in the initial stages of Schottky-barrier formation.¹

Recently, we showed that the Schottky-barrier height (SBH) of two different epitaxially grown Pb/Si(111) diodes is strongly dependent on the epitaxial orientation of the first monolayer of Pb at the interface (Fig. 1).² At a coverage of only one monolayer of Pb, the SBH's also depend on the orientation of this monolayer but their values differ from the diode measurements.^{1,3} Obviously, the Fermi-level position is dependent on the interface structure and on the thickness of the overlayer. Consequently, a detailed knowledge of the evolution of the interface structure as a function of coverage is a prerequisite for explaining the structure dependence of the SBH.

In this paper, we describe the structure, growth, and morphology of epitaxial Pb layers on Si(111). In a separate paper we will report on the electronic properties of these interfaces.⁴ First we will characterize the monolayer phases of Pb on Si(111). Some theoretical analysis is included to explain their diffraction patterns. Next, we will characterize the thicker overlayers. We will show that the Pb atoms agglomerate into islands which are either oriented parallel to the substrate lattice or twisted. The twist angles are different for the $\sqrt{3} \times \sqrt{3}$ and 7×7



FIG. 1. Schematic surface structure of a Pb monolayer on Si(111): (a) the Si(111)(7×7)-Pb structure; (b) the incommensurate Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) structure. The 1×1 unit cell of the unreconstructed Si(111) surface is shown for reference.

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interfaces. In order to understand this phenomenon, we introduce a generalized row-matching principle (Sec. IV). We conclude that the epitaxial orientations of the Pb islands reflect the structural differences at the deeply buried interfaces. This conclusion is very important for understanding the different SBH's at these interfaces.

II. EXPERIMENT

The surface characterization was performed in a molecular-beam-epitaxy system (base pressure of 10^{-10} mbar), equipped with reflection high-energy electron diffraction (RHEED; 15 kV), a reverse-view low-energy electron diffraction (LEED) apparatus, and an Auger electron spectrometer (AES), consisting of a double-pass cylindrical mirror analyzer with interior electron gun (3 kV). Pb (5N purity) was evaporated at a rate of 1 ML per 8.2 sec. The exact coverage can be determined quite easily, because the plot of the Auger intensity versus coverage shows a clear kink when the first monolayer is completed.⁵

During the deposition experiments, RHEED patterns were recorded from a fluorescent screen using a CCD camera. They were subsequently digitized by a computer. Scans were taken along circular arcs on the screen, allowing all the RHEED spots of one particular Laue zone to be recorded at the same time. Typical scanning times are 100 msec. Measurement intervals are about 1 sec.

We used *n*-type Si(111) wafers with epitaxial layers having a thickness of 6 μ m and a resistivity of 2.1 Ω cm (donor concentration $N_D \approx 2 \times 10^{15}$ /cm³). Squares of 7×7 mm² are cut from the wafers and cleaned by the Shiraki method.⁶ In ultrahigh vacuum, the thin oxide layer was removed by heating the sample to about 850 °C with an electron beam. This procedure always produced sharp 7×7 diffraction patterns. This annealing temperature is low enough to avoid spurious changes in the doping profile. The annealing procedure is also kept as short as possible to avoid carbon contamination (≈ 30 sec). The presence of SiC crystallites can easily be detected with RHEED and, therefore, we generally used the RHEED pattern as a quality check.

In order to study the island distribution on top of the first adlayers, we made *ex situ* scanning electron microscopy (SEM) photographs of different samples at coverages far beyond 1 ML.

III. CHARACTERIZATION

A. Monolayer regime

During Pb deposition onto the clean Si(111) (7×7) surface at room temperature, we recorded several RHEED patterns (Fig. 2). The $\frac{1}{7}$ fractional-order spots gradually disappear. After a deposition time of about 8 sec, only the integer order and the $\frac{1}{7}$, $\frac{6}{7}$, and $\frac{8}{7}$ fractional-order spots are left. Auger measurements, which will be discussed in detail later, show that the first monolayer is completed at this point. At very low energy (31.8 eV), the LEED pattern at 1 ML also exhibits other $\frac{1}{7}$ -order



FIG. 2. Recorded intensity of the RHEED spots lying on the zeroth Laue zone during evaporation of Pb onto the clean reconstructed Si(111)(7×7) surface. The scanning time for each spectrum is 100 msec. The numbers at the right side of each spectrum are deposition times in seconds. (a) The silicon (1,1) and ($\overline{1},\overline{1}$) reflections are indicated at the uppermost spectrum; (b) the Pb (1,0) and ($\overline{1},0$) reflections are indicated in the lowest spectrum.

spots along the hexagonal axes of the reciprocal lattice (Fig. 3). So the first monolayer still exhibits a 7×7 symmetry. This result is in agreement with the LEED patterns of Estrup and Morrison⁷ and of Saitoh et al.⁸ However, these authors attributed these fractional-order spots to multiple scattering. With grazing-incidence xray diffraction, Grey and co-workers found quite a number of fractional-order spots belonging to a 7×7 superstructure.⁹ Because multiple scattering is negligible for x rays, the appearance of these fractional-order spots is not due to multiple scattering. Based on a Patterson analysis of their diffraction data, Grey et al. proposed that the first monolayer is composed of a two-dimensional adlayer of Pb atoms occupying a lattice of 8×8 sites per 7×7 unit cell. A consequence of this structural model is that the average in-plane interatomic Pb-Pb distance is $\frac{7}{8}$ times the interatomic Si-Si distance in the (111) plane, i.e., 3.35 Å, which means that the Pb lattice is strongly compressed (the bulk Pb-Pb distance is 3.50 Å). Because 7×7 superspots are still present at monolayer coverage, it is very likely that the stacking fault of the clean reconstructed surface is still present below the Pb layer.

The background intensity in the LEED and RHEED patterns is high, which means that random disorder must be present. From their fit, Grey *et al.* deduced an occupancy disorder near the corners of the unit cell yielding an average coverage of 1.22 ML which is less than the ideal coverage of $\frac{64}{49}$ ML. The reason for this disorder is probably that it reduces the stress within the compressed Pb layer.



FIG. 3. LEED pattern of the Si(111)(7×7)-Pb surface at a beam energy of 31.8 eV. Fractional-order spots are visible around each integer order spot and along the hexagonal axes of the reciprocal lattice.

The intensity of the joint Si($L_{2,3}VV$)-Pb($N_{6,7}O_{4,5}O_{4,5}$) Auger lines versus evaporation time is displayed in Fig. 4. The kink at 8.2 sec reflects the completion of the first adlayer. Subsequent growth proceeds in islands, as will be discussed later. The RHEED patterns also indicate clustering at higher coverage. A close inspection of Fig. 2 reveals that at about 180 sec (22 ML), extra RHEED spots appear at the (1.09, 0) position, which is between the (1,0) and ($\frac{8}{7}$,0) spots. They originate from Pb islands, which are oriented parallel to the substrate, i.e., $[1\overline{10}]_{Pb} ||[1\overline{10}]_{Si}$.

To get the stable Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) phase, it is first necessary to prepare an intermediate hightemperature phase either by heating the metastable (7×7) phase to about 300 °C or by depositing Pb onto a hot substrate (300 °C).^{5,9} This intermediate high-temperature phase has a 1×1 LEED pattern and might be similar to the high-temperature phase of the Pb/Ge(111) system.¹⁰



FIG. 4. Evolution of the intensity of the joint $Si(L_{2,3}VV)$ -Pb $(N_{6,7}O_{4,5}O_{4,5})$ Auger lines, during room-temperature deposition of Pb onto the $Si(111)(7 \times 7)$ surface. The spectra are recorded as derivatives and the intensity is obtained by numeric integration. The solid lines are obtained by a linear leastsquares-fit analysis (see also Table I).

Their nature is controversial. According to Le Lay et al., the 1×1 phases of Pb on Si or Ge are ordered surface structures with a saturation coverage of 1 ML.^{5,11} On the other hand, Ichikawa observed diffuse streaks in the RHEED patterns of the Ge(111)(1×1)-Pb phase.¹² The position of these streaks does not depend on the azimuthal orientation of the crystal and Ichikawa concluded that this phase is a two-dimensional (2D) liquid. Recently Grey et al. reinvestigated the $Ge(111)(1 \times 1)$ -Pb phase with x-ray diffraction.¹⁰ They found a ring of scattered intensity at $|\mathbf{q}| = 2.05 \pm 0.02$ Å⁻¹ with a full width at half maximum of 0.30 ± 0.05 Å⁻¹. This ring is a cut through a diffuse cylinder in reciprocal space. Grey et al. reported that the scattered intensity is not isotropic and concluded that this phase is an anisotropic twodimensional liquid. In the LEED pattern of the $Si(111)(1 \times 1)$ -Pb phase, we could not detect diffuse rings, which is in agreement with the observation of Le Lay et al.,⁵ but we do find diffuse streaks in the RHEED pattern (Fig. 5). These diffuse streaks appear at $|\mathbf{q}| = 2.07 \pm 0.05$ Å which is close to the length of the q vector found by Grey et al. for the $Ge(111)(1 \times 1)$ -Pb phase. Their position is independent of the azimuthal orientation, suggesting that the $Si(111)(1 \times 1)$ -Pb phase is also a 2D liquid.

Cooling down to room temperature results in the Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) surface structure. Α RHEED pattern of this phase is shown in Fig. 6. For convenience, we also show the real and reciprocal lattices of this surface (Fig. 7). Both the $\frac{1}{2}$ - and $\frac{2}{3}$ -order spots are clearly visible, the latter being much more intense. Both Grey et al. and Le Lay et al. do not observe the oddfractional-order spots with grazing incidence x-ray diffraction⁹ and LEED, ⁵ respectively. However Yaguchi, Baba, and Kinbara also observed the $\frac{1}{3}$ -order streaks with RHEED.¹³ The presence of the odd-fractional-order spots means that the diffraction pattern is not simply a superposition of reflections of an unperturbed substrate and adsorbate lattice. We will come to this point later. A closer inspection reveals that the fractional-order spots are not precisely located at the $\frac{1}{3}$ -order positions. The



FIG. 5. RHEED pattern (15 kV) of the high-temperature 1×1 phase. Near the center, very faint diffuse streaks can be observed, which remain at the same position after rotation around the surface normal. The incident electron beam is along an intermediate azimuth.



FIG. 6. RHEED pattern (15 kV) of the Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) phase. The incident beam is parallel to the [112] azimuth of the Si lattice. The fat streaks near the center correspond to the (0,0) and incommensurate (0.65, 0.65) reflections.

maxima of their diffraction profiles along the Si(1,1) direction in reciprocal space are located at the $(0.35\pm0.01, 0.35\pm0.01)$ and $(0.65\pm0.01, 0.65\pm0.01)$ positions (Fig. 8). The latter is in excellent agreement with the (0.6515, 0.6515) position determined by Grey *et al.* This reflection can be indexed as the Pb(1,0) reflection and would appear at the $(\frac{2}{3}, \frac{2}{3})$ position if the overlayer were perfectly commensurate. A commensurate adlayer would demand 5% compression of the Pb layer with



FIG. 7. (a) The unit cell of the Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) surface and (b) the corresponding reciprocal lattice. In this drawing, the structure is commensurate.



FIG. 8. The digitized RHEED pattern of Fig. 6. The FWHM of the incommensurate reflections [(b) and (c)] is twice as large as the FWHM of the integer order spots [(a)].

respect to the bulk Pb-Pb distance. Thus, the Pb(1,0) reflection is slightly moved from the commensurate position toward the origin of reciprocal space, which means that compression of the Pb layer is somewhat relieved (2.9%). Because the (0.35, 0.35) reflection is not observed in the x-ray diffraction pattern of Grey *et al.*, it is tempting to ascribe the presence of the (0.35, 0.35) reflection in the RHEED pattern to double diffraction, where the diffracted waves from the substrate are scattered again by the incommensurate overlayer with $\mathbf{q} = (0.65, 0.65)$. However, the presence of the odd-fractional-order spots can also be explained from a kinematical approach if there is a finite interaction between the substrate lattice and the Pb lattice. We will explore this possibility in more detail below.

If both sublattices are considered to be independent, then the reciprocal lattice will be a superposition of the reciprocal lattices of the substrate surface and the Pb layer. Therefore, all reflections can be indexed with respect to a basis of four vectors.¹⁴ Expressing the basis vectors of the reciprocal Pb lattice $(\mathbf{g}_{a,1}, \mathbf{g}_{a,2})$ in terms of the reciprocal lattice vectors of the substrate $(\mathbf{g}_{s,1}, \mathbf{g}_{s,2})$, we have

$$g_{a,1} = 0.65g_{s,1} + 0.65g_{s,2},$$

$$g_{a,2} = 1.30g_{s,1} - 0.65g_{s,2},$$
(1)

with $|\mathbf{g}_{a,1}| = |\mathbf{g}_{a,2}|$. Then the entire reciprocal lattice is described by four indices:

$$\mathbf{H} = h \, \mathbf{g}_{s,1} + k \, \mathbf{g}_{s,2} + m \, \mathbf{g}_{a,1} + n \, \mathbf{g}_{a,2} \,. \tag{2}$$

Substrate reflections are obtained if (hkmn)=(hk00)with h and k integers. Adsorbate reflections are obtained if (hkmn)=(00mn) with m and n integers. Now we introduce a finite interaction between the two sublattices and assume that the atomic positions of each sublattice will be modulated with the periodicity of the other sublattice. In that case, we expect satellite reflections.¹⁵ It is likely that the substrate is far more rigid than the overlayer, so we will only discuss the substrate-induced spatial modulation of the overlayer. The substrate potential will induce a shift of the overlayer atoms from their mean atomic positions. If the position of the *j*th adatom is given by \mathbf{R}_j when substrate adsorbate interaction is absent, then the substrate potential will induce a small deviation \mathbf{u}_j from this position and its final position becomes $\mathbf{R}_j + \mathbf{u}_j$. The substrate potential can be expanded in plane waves having the periodicity of the substrate.

$$V(\mathbf{r}) = \sum_{G} V_{G} \exp[i\mathbf{G} \cdot \mathbf{r}] .$$
(3)

If the adatoms respond linearly to the applied potential, then the shift of the *j*th adatom becomes¹⁶

$$\mathbf{u}_j = \sum_G \mathbf{u}_G \exp[i \mathbf{G} \cdot \mathbf{R}_j] , \qquad (4)$$

where the sum is over all possible reciprocal lattice vectors **G** of the substrate surface. The modulation amplitude $|\mathbf{u}_G|$ is determined by the lattice mismatch and the substrate-adsorbate and the adsorbate-adsorbate interactions. The scattering amplitude $A(\mathbf{q})$ of the incommensurately modulated overlayer at scattering vector \mathbf{q} is

$$A(\mathbf{q}) = F(\mathbf{q}) \sum_{j} \exp[-i\mathbf{q} \cdot (\mathbf{R}_{j} + \mathbf{u}_{j})], \qquad (5)$$

where $F(\mathbf{q})$ is the atomic scattering factor. If the modulation \mathbf{u}_j is small, substitution of Eq. (4) into Eq. (5) yields¹⁶

$$A(\mathbf{q}) = NF(\mathbf{q}) \left[\sum_{g_a} \delta(\mathbf{q}_{\parallel} - \mathbf{g}_a) - i \sum_{g_a} \sum_{G} \mathbf{q} \cdot \mathbf{u}_G \delta[\mathbf{q}_{\parallel} - (\mathbf{G} - \mathbf{g}_a)] \right],$$
(6)

where N is the number of adatoms which contribute to the diffracted intensity, δ denotes the delta function and \mathbf{q}_{\parallel} the component of the scattering vector \mathbf{q} parallel to the surface. The reciprocal lattice vector of the unmodulated overlayer is \mathbf{g}_a . The first term yields the main spots of the incommensurate adlayer. The second term represents the satellite spots which appear at $\mathbf{q}_{\parallel} = \mathbf{G} - \mathbf{g}_{a}$. G is a reciprocal-lattice vector of the substrate surface; \mathbf{g}_a is a reciprocal-lattice vector of the average overlayer lattice. Note that the adsorbate reflections now interfere with substrate reflections at $q_{\parallel} = G$. So the entire diffraction pattern can be constructed with the aid of Eq. (2) using the same set of basis vectors. However, satellite spots appear having indices (h, k, m, n) with either m or n or both unequal to zero. Therefore, the symmetry of the substrate-overlayer complex is not properly described by a two-dimensional space group but should be described by a (2+2)-dimensional space group.¹⁴

Applying the above to the incommensurate $Si(111)(\sqrt{3} \times \sqrt{3})R 30^{\circ}$ -Pb(β) surface, its diffraction pattern may be constructed from Eqs. (1) and (2) (Fig. 9). We only consider reflections which are close to the commensurate $(\frac{1}{3}, \frac{1}{3})$ and $(\frac{2}{3}, \frac{2}{3})$ positions. From Fig. 9, it is clear that we obtain a triangular cluster of diffraction spots around the $\frac{1}{3}$ -order positions. The satellite spots represent the so-called modulation superlattice, which is close to the 22×22 superlattice, as already pointed out by Grey et al.⁹ These authors did not find the satellite spots near the $\frac{1}{3}$ -order position but they observed satellite spots close to the $\frac{2}{3}$ -order position. They suggested that these satellites resulted from a misfit dislocation superstructure. They pointed out that if the Pb layer is not a fully relaxed incommensurate overlayer, its interaction with the substrate potential will result in regularly spaced misfit dislocations in the overlayer. These superstructure domains give rise to similar satellite reflections near the commensurate position. However, from our arguments, the presence of all satellite spots can be fully explained by Eqs. (1) and (2) so that from the diffraction data alone, one cannot draw conclusions about the presence of such dislocations. Of course, in both cases the satellite spots are due to the substrate-adsorbate interaction. To distinguish between the two possibilities, a quantitative analysis is necessary. Such an analysis can only be made if a large number of satellite reflections can be measured with x-ray diffraction.

Experimentally, the triangular cluster of spots can hardly be resolved. If these spots have comparable intensity, it is expected that they would average together to give a single broad diffraction spot, having its centroid at the commensurate position. However, the RHEED experiments showed that the maxima of the diffraction profiles are located at incommensurate positions. This



FIG. 9. Reciprocal lattice of the Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) surface. The solid lines constitute the unit cells of the Si reciprocal lattice. The fat dots form the reciprocal lattice of the adsorbate. Dashed arrows are reciprocal lattice vectors of the average overlayer structure. The misfit between the substrate and adsorbate layer is exaggerated. The positions of the satellite reflections are indicated by small dots. The satellites are due to the spatial modulation of the position of the Pb atoms by the substrate potential.

simply means that the (0.35, 0.35) and (0.65, 0.65) reflections dominate in this scattering geometry.

B. Beyond monolayer coverage

1. Auger observations

Auger electron spectroscopy can be used to study the growth mechanism of Pb on Si(111). Unfortunately the main $Pb(N_{6,7}O_{4,5}O_{4,5})$ and $Si(L_{2,3}VV)$ Auger lines coincide, so it is only possible to measure their joint intensity. Although this complicates the analysis, we can still use AES to get some information about the growth mechanism.

The spectra are recorded in the derivative mode and the intensity is determined by numeric integration. The background is substracted by a linear interpolation between the peak end points. Measurement of the peak-topeak height will produce erroneous results because the line shape changes as the coverage increases.

The initial linear decrease of the joint Auger intensity (Fig. 4) is characteristic for two-dimensional overlayer growth. It is known that Pb on Si(111) grows according to the Stranski-Krastonov mechanism, i.e., first one monolayer is completed and subsequent growth proceeds in islands.⁵ Therefore, the position of the first kink coincides with the completion of the first monolayer. From the behavior of the Auger intensity after the monolayer break, we can obtain some information about the evolution of the island morphology. For this purpose, we will derive some expressions for the joint Auger intensity *I*.

We assume that each atomic monolayer of the adsorbate will reduce the Auger flux coming out of the bulk by a factor $\exp(-t_0/\lambda)$ where t_0 is the thickness of one adsorbate monolayer (2.86 Å). The parameter λ is the effective escape depth of the Auger electrons, including a factor $\cos(42.3^\circ)$ which accounts for the acceptance angle of the analyzer. Then, up to a coverage of 1 ML, we have

$$\frac{I}{I_0} = (1-y) + y \exp(-t_0/\lambda) + y \frac{I_{\infty}}{I_0} [1 - \exp(-t_0/\lambda)], \qquad (7)$$

where y is the fraction of the surface which is covered with a monoatomic Pb layer. After the monolayer break, the Auger intensity is given by

$$\frac{I}{I_0} = x \exp[-(h+t_0)/\lambda] + (1-x)\exp(-t_0/\lambda) + \frac{I_{\infty}}{I_0} (x \{1 - \exp[-(h+t_0)/\lambda]\} + (1-x)[1 - \exp(-t_0/\lambda)]).$$
(8)

In this equation, x is the fraction of the surface covered with adsorbate islands with a mean height h. For simplicity, we neglect the difference between the attenuation factors of the close-packed (111) planes in the Pb islands and the slightly compressed 2D adlayer. I_0 is the Auger intensity of the bare substrate and I_{∞} is the saturation intensity of a thick film. In addition, it is assumed that the escape depths are the same for the Si and Pb Auger electrons. This assumption is reasonable because both Auger electrons traverse the same overlayer with the same kinetic energy. Above one monolayer, we also have

$$xh = t_0 \left[\frac{N_i}{N_a} (\Theta - 1) \right].$$
⁽⁹⁾

 N_i and N_a are the density of atoms in the interfacial Pb layer and in the (111) planes of the bulk crystallites, respectively.

On the basis of Eqs. (7), (8), and (9), we will discuss the evolution of the island morphology. We distinguish two regions.

a. $\Theta \leq 3 \, ML$. After the monolayer break, the joint Auger intensity varies linearly. This behavior is also observed by Le Lay *et al.*⁵ who measured the peak-to-peak height. Linearity after a monolayer break is reminiscent of a layer-by-layer growth mechanism. However, the very large change of the slope at the monolayer break suggests that a layer much thicker than the first monolayer is formed, i.e., islands of constant height only grow in directions parallel to the surface. From the derivative of Eq. (8), it can easily be shown that if the mean height of the islands is effectively constant, i.e., $\partial h / \partial \Theta = 0$, the joint Auger intensity will behave linearly.¹⁷ In that case we have

$$\frac{d(I/I_0)}{d\Theta} = \begin{cases} \left[1 - \frac{I_\infty}{I_0}\right] [\exp(-t_0/\lambda) - 1], \quad \Theta \le 1 \quad (10) \\ \frac{N_i}{N_a} \frac{t_0}{h} \left[1 - \frac{I_\infty}{I_0}\right] \exp(-t_0/\lambda) \\ \times [\exp(-h/\lambda) - 1], \quad \Theta > 1 \; . \end{cases} \quad (11)$$

From the ratio of these two slopes, we can calculate the mean height of the islands after the monolayer break, assuming some reasonable value for λ . The results are summarized in Table I where we also included the values of the mean height, which can be derived from the data of Le Lay *et al.*⁵ If $\lambda = 4.5$ Å, then the mean height is ten atomic layers and at a nominal coverage of 2 ML, only 10% of the surface will be covered with islands. The mean height is inversely proportional to the slope after the monolayer break so an accurate determination of this height is difficult when the slope is almost zero. The estimated uncertainty for the mean height is 30%.

If the islands grow with a constant mean height, the ratio of the mean height and width must change as a function of coverage. This means that these clusters do not adopt their three-dimensional equilibrium shape. Finally, because we do not know the ratio between the mean height and the mean width, we cannot derive the number density of islands from these Auger measurements.

b. $\Theta \ge 3$ ML. Above three monolayers, the joint Auger intensity increased (not shown).¹⁸ This behavior cannot be understood on the basis of Eq. (8), which predicts that the joint Auger intensity should be a monotonous function of coverage. Therefore, we were unable to fit the Auger data in this regime with an appropriate

TABLE I. Calculated values of the mean height of the islands for different values of λ . The ratio r of the slope before and after the monolayer break is obtained from Fig. 4 and Ref. 5 (Le Lay *et al.*).

Experiment	r	λ(Å)	h (ML)
This work	0.081	4.5	10
		5.5	13
		6.5	17
Le Lav et al.	0.106	4.5	8
(Ref. 5)		5.5	10
		6.5	13

growth model. In order to obtain more information about the growth and morphology of the overlayers, we can only rely on the SEM study which is presented next.

2. LEED and SEM

Additional information on the growth and morphology of thick Pb layers on both types of interface structures was obtained from a combined LEED and SEM study. We also investigated the influence of growth temperature. Next, we will give a detailed account of our observations. Twist angles quoted are with respect to the orientation of the unrotated domains.

a. $\Theta = 35 \ ML$. At this coverage, the islands can be clearly resolved (Fig. 10). For both types of interfaces, the island morphology is qualitatively the same. At a coverage of 35 ML, most of the islands are elongated along a common preferential direction which is one of the high-symmetry directions of the Si substrate. The small crystallites exhibit a hexagonal shape, the edges reflecting the high-symmetry directions in the islands. The elongated islands are formed by coalescence of the small hexagonal-shaped crystallites. The contrast differences between the islands indicate different heights. The number density of islands is larger for the $(\sqrt{3} \times \sqrt{3})$ -type interface. On both interfaces slightly misorientated islands can be seen.

The LEED pattern of the $\sqrt{3} \times \sqrt{3}$ sample (Fig. 11) seems rather complicated. We observe both isolated spots and clusters with three or four spots. The isolated spots are the $\frac{2}{3}$ -order reflections from the intermediate adlayer. The clusters contain reflections from the substrate and the adsorbate. The inner spots are first-order reflections from the Si substrate. The outer spots are integer-order reflections, which originate from Pb islands. These islands are oriented parallel to the substrate, i.e., $[1\overline{10}]_{Pb} \| [1\overline{10}]_{Si}$, or slightly misoriented. Their diffraction spots clearly fall outside the main Si spots which is, of course, due to the smaller lattice constants in the (111) plane of bulk Pb. All spots have a comparable intensity, which means that large fractions of the substrate are still uncovered. The twist angle of the Pb clusters is very different for the two types of interfaces. For the $\sqrt{3} \times \sqrt{3}$ interface, the twist angle is about 3°. For the 7×7 interface, the twist angle is about 6^0 , as will be shown later (Fig. 14). In Sec. IV, we will discuss this phenomenon in more detail.

The Pb spots have hexagonal symmetry. This becomes particularly clear if the beam energy in LEED is changed. Of course, cubic-close-packed islands should have trigonal symmetry along the [111] axis. The sixfold symmetry indicates that different domains with ABCand ACB-type stacking are present in roughly equal amounts.

b. $\Theta = 210 \ ML$. The SEM photographs at 210-ML coverage show the coalescence of the Pb islands (Fig. 12). In particular, the Pb film on top of the $\sqrt{3} \times \sqrt{3}$ interface shows a beautiful network leaving empty channels or regions with sharp edges. These edges are again oriented along high-symmetry directions of the substrate. On top of the 7×7 surface coalescence is quite different from the $\sqrt{3} \times \sqrt{3}$ interface. For the 7×7 interface, small crystallites can still be observed and it is likely that even at this stage nucleation still takes place. It is clear that extraordinarily high coverages are needed to get a continuous film. This behavior is quite different from Pb on Ge(111), where the Auger signal saturates at a coverage of about 75 ML.¹¹

c. $\Theta = 840$ ML. At this coverage, the meanders merged into a continuous crystalline film for both samples leaving some pinholes behind, their number density being largest for the $\sqrt{3} \times \sqrt{3}$ interface (Fig. 13). Both films are ridgy, as can also be observed under the optical microscope. These ridges are the boundaries where the elongated islands have merged. At the boundaries of these crystallites, we might expect dislocations. The



FIG. 10. Scanning electron microscope image of epitaxial Pb films on top of (a) the Si(111)(7×7)-Pb interface, and (b) the Si(111)($\sqrt{3}$ × $\sqrt{3}$)R 30°-Pb(β) interface. The nominal coverage is 35 ML in both cases.



FIG. 11. LEED pattern of the Si(11)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) surface, covered with 35-ML Pb. For an explanation of this pattern, see text.

LEED patterns of these samples only showed adsorbate reflections from the parallel and twisted domains. A LEED pattern of the sample with the $Si(111)(7 \times 7)$ -Pb interface is displayed in Fig. 14. The twist angles do not depend on the coverage, which means that they are fully determined by the substrate-adsorbate interactions.

d. Growth temperature. Our Auger data already indicated that the Pb clusters do not attain their equilibrium shape at room temperature. Their morphology, however, is expected to be dependent on the growth temperature.



FIG. 12. Scanning electron microscope image of epitaxial Pb films on top of (a) the Si(111)(7×7)-Pb interface, and (b) the Si(111)($\sqrt{3}$ × $\sqrt{3}$)R 30°-Pb(β) interface. The nominal coverage is 210 ML in both cases.



FIG. 13. Scanning electron microscope image of epitaxial Pb films on top of (a) the Si(111)(7×7)-Pb interface, and (b) the Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) interface. The nominal coverage is 840 ML in both cases.

Figure 15 shows a (room-temperature) SEM image of a 35-ML deposit onto a hot substrate (300 °C). This temperature is *below* the melting point of bulk Pb. Compared to Fig. 10, the number density of islands has been significantly reduced. Because desorption is negligible at 300 °C, ^{5,8} the Pb atoms must be agglomerated and only a few big clusters are left at the surface. The triangularly shaped islands have large (111) facets and are either parallel to the Si lattice or 60° rotated. They exhibit simi-



FIG. 14. LEED pattern of the Si(111)(7×7)-Pb surface, covered with 840-ML Pb. The diffraction spots only originate from the adsorbate layer. The twisted domains are easily recognized. The twist angle is about 6°.



FIG. 15. Scanning electron microscope image after deposition of 35 ML of Pb onto a hot Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) substrate (300 °C).

lar kinetic shapes as the Pb islands on the Ge(111) surface at 250 °C.¹¹ We also observed some 30°-rotated islands. The diffraction pattern only shows reflections of the $\sqrt{3} \times \sqrt{3}$ structure. No diffraction intensity of the islands could be observed. It is clear that the high surface mobility at 300 °C is responsible for the agglomeration of the adsorbate atoms into large islands. The Pb crystallites tend to minimize their contact area with the substrate. This is probably due to the high strain contribution to the interface free-energy term, which makes wetting of the 2D Pb layer unfavorable. This also means that the surface morphology at *room-temperature* deposition is not determined by thermodynamic equilibrium, but by kinetics.

At lower substrate temperature, the kinetic barrier for adatom diffusion will become higher and thermally activated clustering of the Pb adatoms will be suppressed. In that case, we expect that the Pb atoms will form a quasi-two-dimensional overlayer. Indeed, after deposition of 35 ML of Pb onto the $\sqrt{3} \times \sqrt{3}$ and 7×7 substrates at 135 K, our SEM images showed very smooth surfaces with no traces of island formation. Jalochowski and Bauer even reported RHEED intensity oscillations for the deposition of Pb onto Si(111)7×7 at 95 K (Ref. 19) which is indicative for a quasi-layer-by-layer growth mode. Note that the quasi-layer-by-layer growth at low temperature is governed by kinetic effects, as already pointed out by Bauer and van der Merwe.²⁰

IV. ROTATIONAL EPITAXY AND INTERFACE STRUCTURE

Finally, we want to discuss the presence of twisted Pb islands on both types of interfaces showing distinctly different twist angles, i.e., 6° for the Si(111)(7×7)-Pb and 3° for the Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb substrate. Rotated domains with twist angles of 4° were also observed by Li and Tonner²¹ for Pb on the Ge(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) surface. These authors reported that the twisted domains were stable with respect to heating above 300°C. On the contrary, Grey *et al.* claim that the twisted domains are metastable and do not reappear after a heating cycle.²² We found that the corresponding LEED satellites for Pb

on Si(111) do not reappear after heating the samples, thus supporting the observations of Grey et al.

It is very likely that these rotated islands grow out of small rotated clusters which may even be stable when they are still small. Once the islands are big enough, the kinetic barrier to change to a more stable configuration may be too high at room temperature. The resulting configuration is metastable, i.e., it corresponds to a local minimum in the interface free energy as a function of rotation angle.

Epitaxial rotation occurs for a lot of different substrate overlayer complexes. Physisorbed rare gases on graphite²³ and strongly chemisorbed Na on Ru(100) (Ref. 24) are well known examples of this phenomenon. In those cases, the overlayer is incommensurate and nonrigid and a rotation may be favored because transverse strains have lower energy than parallel strains, as was shown by Novaco and McTague.²⁵ In the initial stages of growth, when small planar clusters come into being, similar arguments can be applied to the epitaxial growth of the Pb islands as well. However, if the islands attain a macroscopic size, the layers in the interface region have effectively become rigid and displacement relaxation at the interface has become much less important. For that reason, it is worthwhile trying to explain the observed rotations by applying simple geometrical principles, such as coincidence of substrate and adsorbate lattices,²⁰ row matching, or aligning of domain walls along symmetry directions.²⁶ These principles are usually justified by the notion that if an overlayer is rigid, free energy can only be gained if it can be made commensurate in one or two directions because a rigid commensurate lattice is always more stable than an incommensurate one. The energy gain is equal to the Fourier component of the substrate potential which corresponds to a reciprocal lattice parameter of the coincidence cell. As a rule, this energy gain will be larger as the size of the superperiod decreases. This so-called lock-in energy is opposed by strain contributions because, in general, there will always be a finite misfit. In the geometrical models these strain contributions are assumed to be of minor importance.

The simplest approach of this kind is to look for the nearest coincidence lattice. For both the 30° rotated islands and the twisted domains, we can find the supercell needed for coincidence with the substrate lattice by allowing some homogeneous strain in the adsorbate lattice. Following Bauer and van der Merwe,²⁰ coincidence is achieved if

$$N\mathbf{b}_i = \sum_{k=1}^2 n_{ik} \mathbf{a}_k , \qquad (12)$$

$$\sin\alpha = \frac{\sqrt{3}}{2} \frac{n_2}{(n_1^2 + n_1 n_2 + n_2^2)^{1/2}} .$$
 (13)

The unit-cell vectors of the adsobate are denoted by \mathbf{b}_1 and \mathbf{b}_2 , the unit cell vectors of the substrate by \mathbf{a}_1 and \mathbf{a}_2 , and N and n_{ik} are integers. The rotation angle is α . The orientation is completely determined by specifying one superlattice unit-cell vector: $N\mathbf{b}_1 = n_1\mathbf{a}_1 + n_2\mathbf{a}_2$. We define the strain parameter $s = (b - b_0)/b_0$, where b is the average Pb-Pb distance in the adsorbate layer and $b_0 = 3.5$ Å, which is the interatomic distance in bulk Pb. The substrate lattice parameter is equal to the average Pb-Pb distance in the 2D adlayer. This substrate lattice is assumed to be rigid. Although this approach only allows adsorbate relaxation, the results shown in Tables II-IV are quite instructive. The 30°-rotated islands on top of the Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) surface have a coincidence mesh of 5×5 atoms if the overlayer is allowed to expand 0.95% (Table II). These 30°-rotated Pb islands are also present on top of the Ge(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) surface but in that case, the 5×5 -coincidence mesh is only realized if the overlayers are compressed (Table III). Due to anharmonicity, expansion of the overlayer will be more favorable than compression. Note that the 30° rotated islands on the $\sqrt{3} \times \sqrt{3}$ surfaces are oriented parallel to the Si or Ge lattice $([1\overline{10}]_{Pb} \| [1\overline{10}]_{Si})$. For the Pb islands on a Ge(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) substrate, coincidence is also achieved for a 6×6 supercell with a twist angle of 4.7° (Table III). This rotation angle is in very good agreement with the observed rotation angle of $4.5^{\circ}\pm0.5^{\circ}$.²² Similarly, for the Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) interface another favorable rotation is $\pm 3^\circ$, which corresponds to a 9×9 coincidence mesh (Table II). This angle is very close to the experimental twist angle. Other possibilities for expanded overlayers with even a smaller coincidence mesh also exist, but then the twist angle is much larger. The 6×6 coincidence supercell might be unfavorable for the Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) interface because, in contrast to the Ge case, the overlayer has to be compressed. Finally, the experimental twist angle for the Si(111)(7 \times 7)-Pb interface is close to an 8 \times 8 coincidence mesh (Table IV).

We note that parallel orientations for the Pb islands with the intermediate Pb layers require a high compressive strain (2.9% and 4.0% for the $\sqrt{3} \times \sqrt{3}$ and the 7×7 interfaces, respectively). If the adsorbate lattice is fully relaxed, a coincidence mesh of 34×34 atoms is obtained for the $\sqrt{3} \times \sqrt{3}$ interface and a coincidence mesh of

TABLE II. Possible rotation angles obtained from the coincidence principle [Eqs. (12) and (13)] for epitaxial Pb(111) layers on top of the Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) interface. The restraint put on the maximum size of the coincidence mesh is a supercell of 9×9 atoms. The strain limit put on the overlayer is 3%. Negative strains correspond to compression of the overlayer; positive strains correspond to dilation.

n ₁	<i>n</i> ₂	Ν	α (deg)	b (Å)	s (%)
0	1	1	0	3.40	-2.86
9	1	9	5.2	3.60	2.96
8	2	9	10.9	3.46	-1.07
7	2	8	12.2	3.48	-0.61
6	2	7	13.9	3.50	0
5	2	6	16.1	3.54	1.11
4	2	5	19.1	3.60	2.81
5	3	7	21.8	3.40	-2.86
4	3	6	25.3	3.45	-1.52
6	5	9	27.0	3.60	2.96
3	3	5	30.0	3.53	0.95

TABLE III. Possible rotation angles on top of the Ge(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) interface. The limits on the size of the supercell and the strain in the overlayer are the same as in Table II.

<i>n</i> ₁	<i>n</i> ₂	N	α (deg)	b (Å)	s (%)
0	1	1	0	3.46	-1.01
8	2	9	10.9	3.53	0.81
7	2	8	12.2	3.55	1.29
6	2	7	13.9	3.57	1.98
5	2	6	16.1	3.61	3.04
7	3	9	17.0	3.42	-2.24
6	3	8	19.1	3.44	-1.78
5	3	7	21.8	3.46	-1.01
4	3	6	25.3	3.51	0.36
3	3	5	30.0	3.43	-2.02
3	3	5	30.0	3.43	-2.0

 24×24 atoms is obtained for the 7×7 interface.

Recently, Grey and Bohr proposed a simple symmetry principle for epitaxial rotation.²⁶ They suggested that domain walls, produced by the beating of the adsorbate and substrate lattices, tend to align along high-symmetry directions of either the substrate or adsorbate. Based on the moiré pattern generated by the overlap of two crystal lattices, they deduced expressions for the rotation angle as a function of the misfit. This model can only be applied to the 7×7 interface (the $\sqrt{3} \times \sqrt{3}$ interface is complicated by the two rotations of 30°). Taking the substrate lattice parameter of the two-dimensional 7×7 adlayer, we obtain twist angles of 4.0° or 4.8° if the domain walls are aligned along the close-packed rows of the substrate or adsorbate, respectively. The experimental value is 6.1° \pm 0.4°, which is closer to the 5.8°-rotated 8×8 coincidence mesh derived from Eq. (13). Therefore, the prediction based on the coincident superlattice is much closer to the experimental value. Unfortunately, in many cases different coincident superlattices can be found, which makes it almost impossible to predict the orientation of epitaxial overlayers.

However, if the adsorbate is allowed to relax, epitaxial rotation can also be understood by applying a generalized row-matching principle. Row matching is, for instance,

TABLE IV. Possible rotation angles on top of the $Si(111)(7 \times 7)$ -Pb interface. The limits on the size of the supercell and the strain in the overlayer are the same as in Table II.

$\overline{n_1}$	<i>n</i> ₂	N	α (deg)	b (Å)	s (%)
9	1	9	5.2	3.56	1.74
8	1	8	5.8	3.59	2.52
8	2	9	10.9	3.42	-2.25
7	2	8	12.2	3.44	- 1.79
6	2	7	13.9	3.46	- 1.12
5	2	6	16.1	3.50	0
4	2	5	19.1	3.56	1.58
7	4	9	21.1	3.60	2.85
4	3	6	25.3	3.41	-2.69
6	5	9	27.0	3.56	1.74
3	3	5	30.0	3.49	-0.25

used to explain the occurrence of the well-known Kurdjumov-Sachs and Nishiyama-Wasserman orientations for fcc metals on bcc substrates.²⁰ In the case of row matching, the total energy is lowered because all the atoms are sitting in a corrugation-potential ditch, without the requirement that individual atoms along the rows must match with the substrate lattice sites. We generalize the row-matching principle by demanding that instead of all atoms, a large fraction of atoms is sitting in the corrugations. Then there are two possibilities: (a) one out of n corrugations between substrate rows is filled with an adsorbate row; (b) the atoms of one out of n rows of adsorbate atoms are sitting in a set of parallel ditches, which is illustrated in Fig. 16. Then the difference vector Δa between the substrate and adsorbate lattices is parallel to a symmetry direction which is also the case for the symmetry principle of Grey and Bohr. However, an additional requirement is that the difference vector should be commensurate with the substrate lattice; otherwise, the arrangement will remain fully incommensurate.

Table V shows possible twist angles on the 7×7 surface for different relaxations of the overlayer based on this generalized row-matching principle. The twist angle is obtained from simple geometrical considerations (Fig. 16)

$$\cos \alpha = \frac{3}{4}r \pm \frac{1}{4}\sqrt{4 - 3r^2} . \tag{14}$$

r is the ratio of the substrate and adsorbate lattice parameter. In all cases $N \Delta a$ is coincident with the substrate lattice. It is clear that smaller values for N result in a higher degree of commensurability at the expense of lattice strain in the overlayer. The rotation angle of 5.8° is closest to the experimentally found angle, which indicates that the overlayer is slightly expanded (nearest-neighbor distances of 3.57 Å). Of course, the solutions in Table V correspond to $N \times N$ coincidence meshes which are also obtained from Eqs. (12) and (13), but these solutions are very special ones because stabilization is not only achieved by coincidence but also by row matching. Therefore, the row-matching argument makes it possible to select only a few particular coincidence meshes out of many other possible solutions, therefore improving the predictive power of geometrical considerations. So the experimentally found twist angles for the crystallites on

FIG. 16. Illustration of the generalized row-matching principle. One particular atom row of the adsorbate is sitting in a set of parallel ditches of the substrate. In order to achieve some coincidence, it is not necessary that each atom row sits in such a set of parallel ditches, but this configuration should be repeated over a period of several substrate lattice constants.

TABLE V. Possible rotation angles on top of the
Si(111)(7×7)-Pb interface obtained from the row-matching
principle (see text). The parallel orientation ($\alpha = 0^\circ$) is a trivial
case of row matching. $\overline{\alpha}$ (deg) Δa (Å)Nb (Å)1440.10343.40

x (ucg)	 (11)	11	0 (11)
1.44	0.10	34	3.40
2.02	0.14	24	3.42
2.54	0.18	19	3.44
3.00	0.21	16	3.46
3.42	0.24	14	3.48
3.67	0.26	13	3.49
4.71	0.33	10	3.53
5.20	0.37	9	3.55
5.81	0.42	8	3.58
6.58	0.48	7	3.61
7.59	0.56	6	3.66

top of the 7×7 interface point towards an 8×8 coincidence mesh, stabilized by row matching. Because the row-matching principle and the symmetry principles are only applicable in the case of small mismatches, the epit-axial rotation on top of the $\sqrt{3} \times \sqrt{3}$ interfaces can only be understood from the more general coincidence principle.

The foregoing discussion is based on the assumption that the first Pb layer is rigid and does not change after being covered with Pb islands. This assumption is very crucial in connection to the different Schottky-barrier heights at these interfaces. A grazing incidence x-ray diffraction study of a 7×7 interface already confirmed that the 7×7 symmetry is preserved below the islands.²² Another observation which favors the above assumption is the occurrence of different epitaxial rotations on top of the $\sqrt{3} \times \sqrt{3}$ and 7×7 surfaces. As already pointed out by Grey *et al.*, this phenomenon provides useful information about the structures of deeply buried interfaces, which are otherwise difficult to probe by experimental means.²²

V. SUMMARY AND CONCLUSIONS

We characterized three different monolayer phases of Pb on Si(111). The earlier proposed structural models for the $\sqrt{3} \times \sqrt{3}$ and 7×7 monolayers⁹ are largely corroborated. In addition, from the analysis of our RHEED patterns we argued that the Pb sites of the incommensurate $\sqrt{3} \times \sqrt{3}$ layer are spatially modulated by the substrate corrugation potential. We also investigated the high-temperature Si(111)(1×1)-Pb phase and we concluded that it can be described as a 2D liquid.

At higher coverage, the Pb atoms agglomerate into three-dimensional islands. Their morphology strongly depends on the substrate temperature and is different for the 7×7 and $\sqrt{3} \times \sqrt{3}$ interfaces. These islands are oriented either parallel to the Si lattice or twisted. The twist angles are different for the 7×7 and $\sqrt{3} \times \sqrt{3}$ interfaces, which indicates that structural differences at the deeply buried interfaces still exist. This observation is very important for understanding the differences in SBH. We propose a new generalized row-matching model for explaining the epitaxial rotation of the metastable Pb crystallites on top of the Si(111)(7×7)-Pb surface. The rotated islands on top of the $\sqrt{3} \times \sqrt{3}$ structure may be stabilized by a coincident superlattice.

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FIG. 10. Scanning electron microscope image of epitaxial Pb films on top of (a) the Si(111)(7×7)-Pb interface, and (b) the Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) interface. The nominal coverage is 35 ML in both cases.



FIG. 11. LEED pattern of the Si(11)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) surface, covered with 35-ML Pb. For an explanation of this pattern, see text.



FIG. 12. Scanning electron microscope image of epitaxial Pb films on top of (a) the Si(111)(7×7)-Pb interface, and (b) the Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) interface. The nominal coverage is 210 ML in both cases.



FIG. 13. Scanning electron microscope image of epitaxial Pb films on top of (a) the Si(111)(7×7)-Pb interface, and (b) the Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) interface. The nominal coverage is 840 ML in both cases.



FIG. 14. LEED pattern of the $Si(111)(7 \times 7)$ -Pb surface, covered with 840-ML Pb. The diffraction spots only originate from the adsorbate layer. The twisted domains are easily recognized. The twist angle is about 6°.



FIG. 15. Scanning electron microscope image after deposition of 35 ML of Pb onto a hot $Si(111)(\sqrt{3} \times \sqrt{3})R 30^\circ$ -Pb(β) substrate (300 °C).



FIG. 3. LEED pattern of the Si(111)(7×7)-Pb surface at a beam energy of 31.8 eV. Fractional-order spots are visible around each integer order spot and along the hexagonal axes of the reciprocal lattice.



FIG. 5. RHEED pattern (15 kV) of the high-temperature 1×1 phase. Near the center, very faint diffuse streaks can be observed, which remain at the same position after rotation around the surface normal. The incident electron beam is along an intermediate azimuth.



FIG. 6. RHEED pattern (15 kV) of the Si(111)($\sqrt{3} \times \sqrt{3}$)R 30°-Pb(β) phase. The incident beam is parallel to the [112] azimuth of the Si lattice. The fat streaks near the center correspond to the (0,0) and incommensurate (0.65, 0.65) reflections.