# Direct Three-dimensional Characterization of Buried Interface Morphology with Quantized Electron Waves

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**Abstract**

Experimental results on the direct three-dimensional characterization of the buried Pb/Si(111) interface are presented. A novel principle of characterization is based on the quantization of electron states in a thin metal film. Due to the unexpectedly high sensitivity of the quantized electron spectra on the thickness, metal film becomes "transparent" for scanning tunneling microscope (STM). STM images of the top surface of a Pb film show a sequence of the electron fringes. The geometry of the fringes exactly reproduces the buried interfacial steps on the Si(111) substrate. The absolute depth of the metal film can be found from the period of the quantized tunnel spectra. Three-dimensional characterization of the buried interface is achieved by combination of the STM and local tunnel spectroscopy.

Probing the buried interface is important for understanding the physical mechanisms of heteroepitaxy. In the past years a great progress in the characterization of the buried interfaces has been achieved. Imaging buried point defects has been demonstrated with a ballistic electron emission microscopy[1, 2]. Interfacial atomic steps have been observed with a low energy electron microscopy[3]. Reconstruction of the buried interfaces has been studied with an intense synchrotron light source and x-ray diffraction[4, 5]. However, a direct three-dimensional characterization of the morphology of buried interfaces still remains an unsolved problem. A new approach to the problem has been proposed in the recent experiments with a scanning tunneling microscopy (STM) of thin Pb films, demonstrated a unique sensitivity of the quantized tunnel spectra to the morphology of the buried metal/semiconductor interface [6].

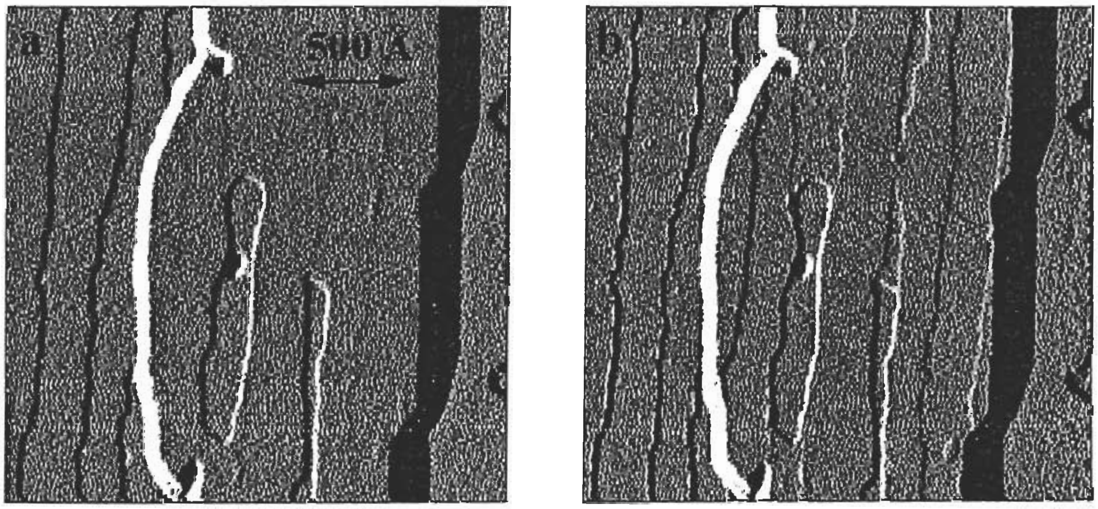

**Fig.1** Scanning tunneling microscopy images of the Pb wedge on the Si(111) substrate. The height of the wedge increases from 8 atomic layers at the left side to 15 atomic layers at the right side. Images are obtained in the constant-current mode of STM. The original STM data are differentiated with respect to the horizontal axis.
a. STM image acquired at the negative tip bias -5V shows the morphology of the top surface of the island.
b. STM image acquired at the positive tip bias +5V shows additionally the electron fringes coming from the buried interface.

In this paper we discuss a direct three-dimensional characterization of the buried interface morphology using tunnel spectroscopy of the quantized electron states in a thin metal film. The experiments were performed in ultra high vacuum (UHV) chamber with a basic pressure $3 \cdot 10^{-11}$ Torr. The UHV chamber is equipped with a surface preparation and analysis tools such as a RHEED, Auger spectrometer, ion gun sputtering, and a number of effusion cells for the deposition of metals. Lead atoms were deposited on the Si(111) substrate kept at the temperature 77K in order to eliminate the diffusion of Pb atoms on the surface. Measurements were performed with a low temperature scanning tunneling microscope (STM) in situ at the temperatures 77 and 4.8K.

As it was previously shown, STM images of thin epitaxial Pb films on a Si(111) substrate demonstrate series of fringes[6] (see Figure 1b). Fringes are observed in the wide range of the tunnel bias between -1V and +5V. The fringe boundaries exactly reproduce the geometry of the buried interfacial steps, and the period of the fringe pattern was found to be 2 atomic layers of height. Since the fringes originate from quantization of electron states across a thin metal film, the actual period of the electron interference pattern must be equal to the one half of the Fermi wavelength in Pb $\lambda_F = 3.8a_0$. Incommensurability between $\lambda_F$ and the period of a crystal lattice $a_0$ results in the periodic interrupts of the binary periodicity of the fringe pattern, as we can see in Figure 2. Remarkably, quantization of electron states makes metal film "transparent" for STM and allows to see in details the morphology of the interface buried under the tens of atomic layers of Pb. Upon increasing the negative tunnel bias above -1V the fringe pattern starts to disappears and, finally, at the large negative tip bias STM image reflects only the morphology of the top surface of the Pb film, as one can see on the Figure 1a. The reason of this lies in the dependence of the height of the tunnel barrier on the energy of the quantized state and has been in details explained in Ref[6].

Figure 2 shows that not only the stepped morphology of the interface but the buried voids as well can be imaged with STM. In Figure 2 the void on the Si(111) substrate is partially open and can be imaged in a conventional tunnel microscopy and partially buried under the Pb island, and, therefore, appears on STM images only at certain tunnel bias. Figure 3 shows the STM image of the void on Si(111) substrate separated from the edge of the terrace.

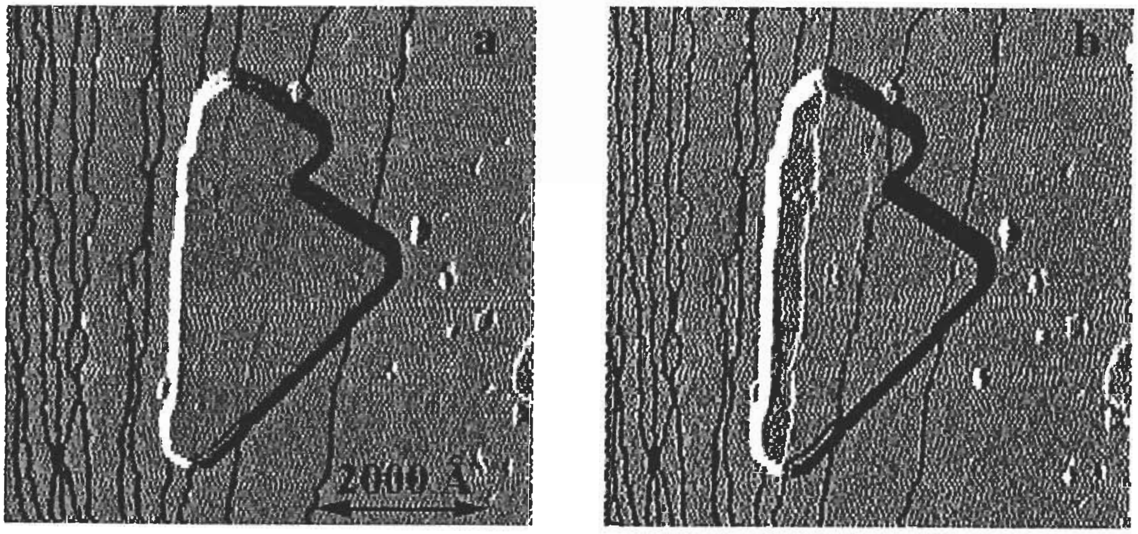

**Fig.2** STM image of the 10÷14 atomic layers height Pb island on Si(111). The original STM data are differentiated with respect to the horizontal axis.

a. STM image corresponding to the tip bias-5V. The void on the Si(111) is partially open and can be observed with STM at any tunnel bias.

b. STM image obtained at the tip bias +5V. Image shows the buried part of the void.

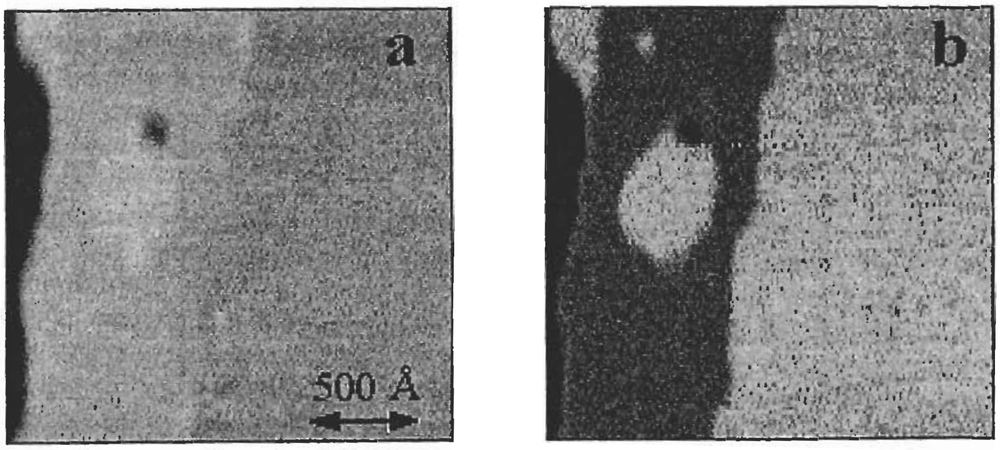

**Fig.3** STM image of the void on the Si(111) surface buried under 15 atomic layers of Pb. Figures a and b are obtained at the tip bias -5V and +5V, respectively.

Tunnel spectra measured over the different fringes demonstrate the stepped dependence between the tunnel current and tip bias, as shown in Figure 4. The origin of the steps on the tunnel I-V characteristics lies in the quantum size-effect predicting that for large thickness *H* period of quantization must be inversely proportional to H[7] and near the Fermi level

$$\Delta = \frac{\hbar v_F}{H} \qquad (1)$$

where $\hbar$ is a Plank's constant, and $v_F$ is a Fermi velocity of electron. In the nanometer regime, however, the tight-binding calculations predict that the energy of quantization

$$\Delta = \frac{\hbar v_F}{a_0(N+1)} \qquad (2)$$

where N is the number of atomic layers in a film, and $a_0$ is a separation between the atomic layers in a crystal lattice. Thus, for the ultrathin metal film the effective thickness in the quasiclassic Eq. (1) must be increased by one atomic layer height. In Figure 4 the inverse of the period of quantization observed on thin Pb films[6] is plotted as a function of the number of atomic layers in a film. The offset of the linear dependence in Figure 4 indicates that the height of Pb islands found from STM measurements is by two atomic layers smaller that the actual thickness of the metal film. The "missing" atomic layers are most likely the two wetting layers of Pb uniformly covering Si(111) substrate. Remarkably, a similar conclusion also followed from the RHEED measurements[8].

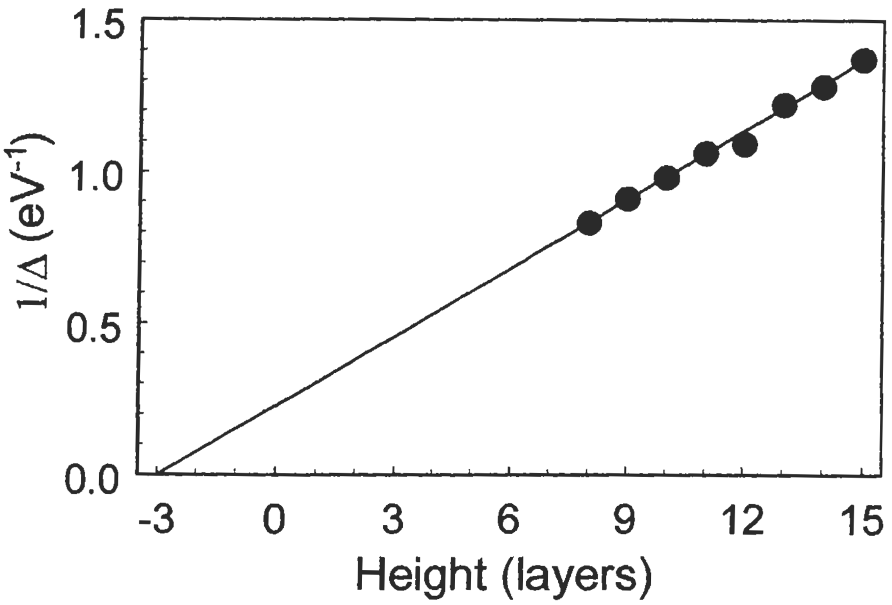

**Fig.4** The inverse of the separation between the steps on tunnel I-V characteristics of thin Pb films vs. number of atomic layers in a film. Thickness has been measured from the top of the wetting Pb layers.

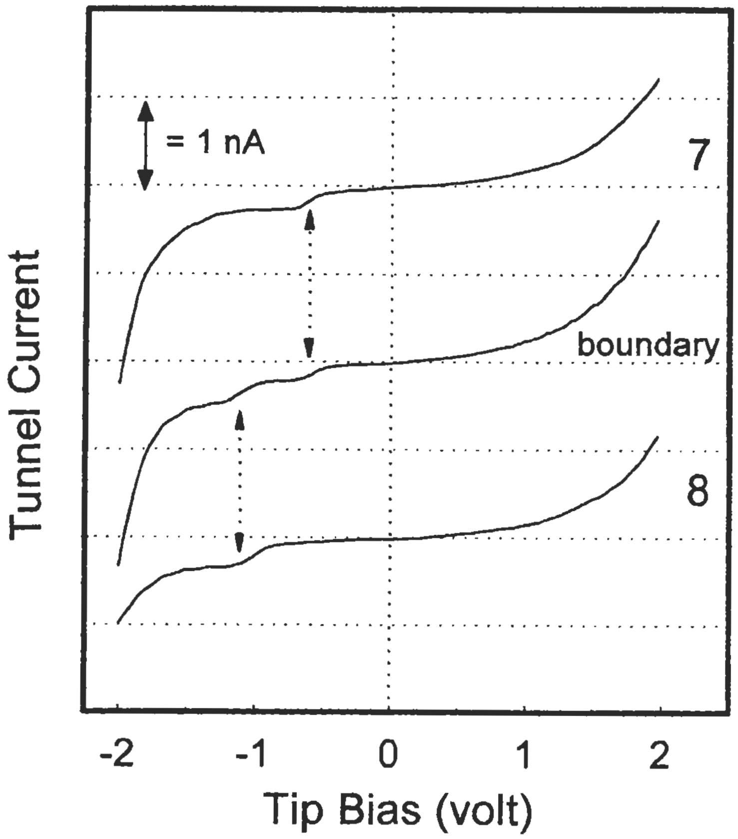

**Fig.5** Curves 7 and 8 are the tunnel I-V characteristics measured on the neighboring fringes with a thickness of a metal film 7 and 8 atomic layers, respectively . The middle curve is a tunnel I-V spectrum corresponding to the fringe boundary.

Figure 5 shows the tunnel I-V curves measured over the two neighboring fringes. One can see that the steps corresponding to the odd and even numbers of atomic layers are shifted with respect to each other, and as it was shown in Ref[6] the shift.

$$\delta \approx \Delta 2a_0/\lambda_F \approx \Delta/2 \qquad (3)$$

Interestingly, we also found that the tunnel spectra measured exactly on the boundary between the fringes include both series of steps. This observation indicates that scattering on the edge of a buried step does not affect strongly the motion of electrons in a Pb film. Thickness dependence of $\Delta$ shown in Figure 4 combined with the oscillations of the tunnel spectra between the odd and even fringes allows to identify precisely the number of atomic layers in each point of a metal film.

In conclusion, we have demonstrated that scanning tunneling microscopy of thin metal film combined with a tunnel spectroscopy of the quantized electron states can identify the morphology of the buried interface in all three dimensions with a precision of one atomic layer. The precise information about the depth of a film is provided from the quantized tunnel spectra, while the two-dimensional contours of equal depth can be directly imaged with a STM.

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