Semiconductor surface characterization by scanning probe microscopies

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ABSTRACT

Besides the well-known 3-dimensional surface topography, scanning probe methods give access to a whole world of local physical information on solid surfaces. Here, we demonstrate opportunities given by scanning tunnelling spectroscopy (STS) and scanning electrical force microscopy/spectroscopy (SEFM/SEFS). In this paper, we compare the wide-spread UHV-STM/STS technique with ambient SEFM/SEFS. After short description of the methods, some applications to semiconductor surfaces are discussed. Possibly SEFS has a great potential for local electronic spectroscopy in near future.

Keywords: Scanning probe microscopies; Semiconductor surfaces; Local electronic spectroscopy

1. INTRODUCTION

Scanning probe microscopies have fastly developed to standard methods in solid surface microscopy and analysis. When the scanning tunneling microscope (STM) was invented in 1981\textsuperscript{1} there has been started a rapid development of near-field microscopies allowing extremely high spatial resolution and approaching also highly-resolved mappings of various surface properties. The most famous representatives of these microscopies are the STM and the atomic force microscope (AFM)\textsuperscript{2}.

The common feature typical to all of these methods is a sharp probing tip which is approached to a very short distance to the surface and raster scanned within this distance across the surface. Due to tip-sample interaction local physical properties of the sample surface can be imaged. For a more detailed representation we refer to\textsuperscript{3,4}.

In this paper, we restrict us to applications concerning semiconductors, especially the Si(111) surface, to demonstrate the opportunities offered by the scanning probe methods. Actually the whole world of semiconductor materials and structures studied meanwhile has lead to a hardly to overview amount of publications.

2. SCANNING TUNNELING MICROSCOPY AND SPECTROSCOPY

In scanning tunneling microscopy a sharp metallic tip is approached to the sample till to a distance typically smaller than 1 nm. If a bias is applied between tip and sample there occurs an electrical current due to the quantum mechanical tunnel effect which allows electrons to overcome the narrow gap between both electrodes. This current $I_T$ depends according to

$$I_T \propto \exp\left(\text{const.} \sqrt{\Psi z}\right)$$

extremely sensitive on the width $z$ of this gap ($\Psi$ – energetic “height” of the potential barrier made of the gap). In the constant current mode a feedback circuit controls the movement of the tip during the raster scan in such a way that the tunnel current remains constant. For a homogeneous sample, the tip then follows the surface profile with very high accuracy which can even reach atomic dimensions.

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Si(111)7x7 was the first surface imaged with atomic resolution in real space. Fig. 1 shows an image of this surface with the characteristic rhombohedral surface unit cell marked by 4 corner holes. In combination with theoretical simulations the detailed atomic arrangement in this complex surface reconstruction could be determined. This image demonstrates also the advantage of imaging in real space: detailed surface structure including local defects is visible. (An disadvantage is, on the other hand, that only a very small area of the surface is investigated and one has carefully to proof all generalizations made from such images.)

Fig. 1: STM images of a 7x7 reconstructed Si(111)-surface.

Besides pure surfaces, adsorbate structures, processes of epitaxial growth, influence of technological surface treatment, and device structures can be imaged.

In many cases, one obtains slightly different images from semiconductor surfaces at different applied voltages U. This is due to the imaging of different electronic states. Applying a positive bias (sample on positive potential) unoccupied states of the sample are imaged whereas applying a negative bias (sample on negative potential) allows the investigation of occupied sample states. Actually the constant current mode image reflects contours of constant local density of states (LDOS). In the case of Si(111)7x7 for positive U appears the image already seen in Fig. 1 whereas at negative U an asymmetric unit cell is observed.

Local spectroscopy (STS) is performed by measuring I(U) characteristics over fixed positions on the sample surface. These characteristics allow directly a local imaging of energy gaps and Schottky barriers. A more elaborate analysis shows that actually $d \ln I / dU$ reflects the LDOS.

STM/STS is a pure surface method. It visualizes surface bands instead of bulk bands, reflects band bending at the surface, and is influenced also by the tip (the electric field in the tunnel gap influences the surface bands).

Extensions of STM include scanning tunneling potentiometry (STP) and ballistic electron emission microscopy (BEEM) which allow mapping of lateral surface potential and local subsurface Schottky-barrier heights, respectively.

3. ATOMIC FORCE MICROSCOPY AND SCANNING ELECTRICAL FORCE MICROSCOPY AND SPECTROSCOPY

Atomic force microscopy allows direct imaging without electrical current. In this case a sensitive miniaturized tip-cantilever system is scanned across the surface. In the contact modus there is a very small distance between tip and sample atoms leading to a repulsive interaction. Keeping the interaction force constant (via the cantilever deflection) one can image the sample surface topography till to atomic resolution.

For clean semiconductor surfaces as Si(111) atomic resolution in UHV is relatively difficult due to strong interaction of the cantilever with the dangling bonds. It could be achieved only in the non-contact modus. In this modus of operation, the cantilever is externally excited to oscillations near to its eigenfrequency. Approaching the sample surface the tip reaches the
range of attractive van der Waals interaction. The corresponding force gradient influences the effective spring constant and so the eigenfrequency of the cantilever. Experimentally this leads to a change of the stationary oscillation amplitude and phase. Imaging is performed by keeping one of these quantities constant.

In general the AFM allows nm-resolution imaging of surfaces and devices. An essential advantage with respect to scanning electron microscopy is that really three-dimensional images are obtained. Additional contrast may be included using lateral (frictional) forces.

\begin{equation}
U = U_{d} + U_{ac} \sin \omega t.
\end{equation}

The additional electrostatic force between cantilever-tip and sample is

\begin{equation}
F_{el} = -\frac{1}{2} \frac{\partial C U^{2}}{\partial z} = -\frac{1}{2} \frac{\partial C}{\partial z} \left[ \left( U_{d}^{2} + \frac{1}{2} U_{ac}^{2} \right) + 2U_{d} U_{ac} \sin \omega t - \frac{1}{2} U_{ac}^{2} \cos 2\omega t \right]
\end{equation}

It contains components independent of time and such oscillating with frequencies \(\omega\) and \(2\omega\) but only the first of them depends on \(U_{d}\). According to

\begin{equation}
x(t) = \frac{1}{k} F(t)
\end{equation}

(k - spring constant of the cantilever) these components can be obtained from the complex cantilever movement (which always includes the movement due to the external mechanical excitation from the usual non-contact modus too) by use of lock-in technique. The additional information which can be obtained from the oscillating components concerns the potential drop across the sample surface (via \(U_{d}\)) and the vertical component of the local capacitance gradient of the tip-sample system. According to this analysis SEFM allows a simultaneous mapping of topography and local electrical properties.

The interpretation turns out to be quite complex. This is due to the complex character of \(\delta C/\delta z\). We remember the expression of a parallel plate capacitor

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**Fig. 2: Principle of SEFM operation.**

Scanning electrical force microscopy (SEFM)\(^{13,14}\) is based on non-contact atomic force microscopy. Fig. 2 demonstrates the principle of operation. An additional modulated bias is applied between the conducting cantilever-tip and the sample

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\[ C = \frac{Q}{U} = \varepsilon_0 \varepsilon A / d. \]

Fig. 3: Cross-section through a poly-silicon resistor. Left: Topography. Right: Capacitance. Scan range: 3 \( \mu \text{m} \times 3 \mu \text{m}. \) 

First of all, topographic features are reflected in C via the variation of the effective area A when the tip is positioned above a valley (relatively large A) or above a hill (relatively small A). This makes interpretation of images from samples with topographic profiles quite difficult. Plane sample surfaces and especially polished cross-sections are much better suited for SEFM investigations. Fig. 3 shows a cross-section through a poly-Si resistor. In this case, the contrast from the \( 2\omega \) signal reflects local variations in carrier density (that means in the induced charge Q) between the poly-Si channel, the insulating layer and the Si substrate.

\[ U_\infty = 5 \text{V}, f_c = 49 \text{kHz}, f_r = 67 \text{kHz}. \]

Fig. 4: \( C(U_\text{dc}) \)-characteristics on a hydrogenated silicon (100)-surface detected in several distances.

There can also be measured local characteristics \( C(U_\text{dc}) \) with \( U_\infty \) as a constant parameter. Fig. 4 shows such characteristics for a hydrogenated Si(100) surface. There is a step-like increase of \( \delta C/\delta z \) at some threshold voltage which increases with \( U_\infty \) that means with increasing field strength. This phenomenon reflects the gap and the band bending on the surface which consists of the original bending at the sample and the additional bending due to the local electric field between tip and sample.

We would like to draw attention to the fact that such characteristics can be measured at ambient conditions which is in contrast to STS which allows electronic structure investigations only in UHV.
4. CONCLUSIONS

We have demonstrated the broad field of applications accessible by using various scanning probe methods in semiconductor research and technology. The local character of information available allows high-resolution mapping of surface topography supplemented in some cases by detailed physical properties of the (tip-) sample (system). The full potential offered by these methods has not yet been exhausted.

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