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Dopant and Potential Profiling with Atomic Resolution by Scanning Tunneling Microscopy

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1. Introduction

Nowadays, miniaturization of transistors requires reliable dopant profiling with a spatial resolution of a few nm. Moreover, to analyze the effect of statistical fluctuations of dopant distributions on device performance, we need to detect locations of individual dopant atoms.

In order to meet such requirements, we are employing scanning tunneling microscopy (STM). The advantage of STM is not only its high spatial resolution but capability of various measurement modes, which yield information on electronic structures in the sample. This feature enables STM to detect the surface potential and the individual dopant atoms on atomically flat and electrically inert semiconductor surfaces as discussed below.

2. Visualization of Surface Potential and Dopant Atoms

Usually, STM observes structure of a sample by mechanically scanning the probe tip while keeping the tunneling current constant. This measurement is called the constant-current topographic image mode of STM and is capable of atomic spatial resolution because the tunneling current depends very sensitive to the gap distance between the tip and the surface atoms. The tunneling current also depends on electronic structures in the sample and the voltage difference between the tip and the sample surface as well. Thus, if atomically flat and electrically inert surfaces are prepared, the topography image gives information on internal potentials of the sample.

For this purpose, we adopted the (111) surface of Si, instead of (001) or (110) surface, because the (111) surface can be atomically flattened by wet treatment in NH_4F aqueous solutions.[1] Although the (111) surface is not perpendicular to the (001) wafer surface, it will not be an essential problem in actual dopant profiling. This treatment in NH_4F renders the Si surface mono-hydride, well suited for STM analysis. The treatment also hydrogenates and deactivates dopant atoms, but heat treatment at moderate temperatures around 400°C can restore the dopant activity.

Figure 1 is an STM topograph thus obtained of a pn junction formed on a (111) surface.[2] The dark triangles seen on the left side (a large one at the upper left and a small one near the bottom) are etch pits with a depth of one bilayer, indicating that this surface is almost atomically flat. The p -type region in this figure appears dark, i.e. topographically lower. Note that the p and n regions are observed on a single atomic terrace, indicating that the apparent

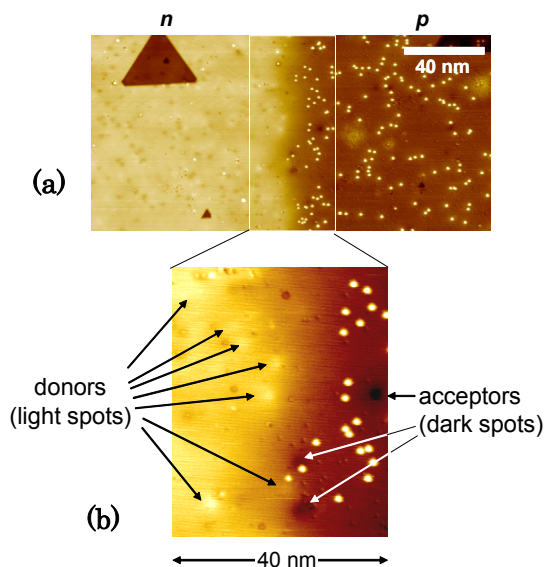


Fig. 1 An STM topographic image of a pn junction region taken with a positive sample bias voltage of 1.7 V (a) and a magnified view of the junction edge (b). Small bright spots are due to dangling bonds formed by hydrogen desorption.

height difference emerges from the potential variation between the two regions. This potential origin of the p/n imaging is confirmed by the fact that the contrast was reversed with the bias voltage polarity.

In this image, the many small bright spots with distinct boundaries are due to Si dangling bonds formed by hydrogen desorption. In addition, there are bright and dark spots extending for a few nm. We identify that the origin of these blunt spots are dopant atoms residing just below the surface because the contrast is again reversed by the polarity of bias voltage. Since an acceptor behaves as a negative charge in Si, for example, it enhances the voltage drop across the tip-sample gap when the sample bias is negative, and hence appears as a protrusion, while it reduces the gap voltage for the positive bias and hence looks as a depression. A donor atom, which is a positive charge center, gives opposite contrast. Thus in Fig. 1, which is taken with a positive sample bias, the blunt bright spots are donors and the dark ones are acceptors.

In Fig. 1 (b), the potential contour between the p and n regions is not straight. This variation correlates well with the donor fluctuation. For example, at the center of the image, several donors happen to be accumulated, where the potential deviates to the right hand side. This correlation

indicates that the potential fluctuation is caused by the statistical randomness in donor distribution.

2. Quantitative Measurement of Potential Distribution Scanning Tunneling Spectroscopy

The STM enables us to quantitatively analyze potential distribution by measuring the tunneling current vs bias voltage I - V relation at each point on the sample area. This kind of measurement is well known under the name of scanning tunneling spectroscopy (STS). An example of STS analysis is shown in Fig. 2 for the pn junction sample of Fig. 1. The negative and positive onset voltages of the tunneling current are extracted from the I - V curve, which correspond respectively to the valence band maximum (VBM) and the conduction band minimum (CBM) in the sample. Accordingly, we can draw the potential distribution by repeating the I - V measurements across the pn junction. Although the obtained profile looks plausible, it does not completely reproduce the original built-in potential.

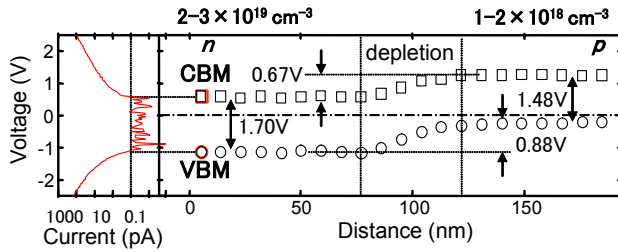


Fig. 2 Tunneling current I_t vs sample bias voltage relation taken in the n -type region, and the positive (square) and negative (circle) onset voltages, at which I_t reaches 0.1 pA, plotted against measured positions across a pn junction.

There are two major difficulties for quantitative STS measurements on semiconductor surfaces. One is that the applied bias voltage distorts the potential distribution and the measured profile is not the original but the resultant one. Another one is that the applied bias voltage is shared by the voltage across the vacuum gap V_{gap} and the band bending in semiconductors. The tunneling current is determined not by the applied bias but by V_{gap} . Thus, the correct potential profile should be plotted using the values of V_{gap} .

To solve these problems, we are developing a simulation program to calculate the potential distribution and tunneling current under the measurement conditions of STM. By comparing the measured STS profiles with the calculation results, we can estimate the original potential distributions.

Resonance tunneling spectroscopy using a marker molecule

Another method to separate the bias voltage into V_{gap} and the band bending is to introduce a suitable energy level in the tunnel junction as a marker in the energy axis.[3] This marker level can be detected by resonance tunneling using STM as shown in Fig. 3. This was actually done by using monolayers of fullerene C_{60} molecules deposited on top of oxidized Si layers. The monolayer can be formed by depositing sufficient amount of C_{60} , and re-evaporation of excess materials by heat treatment. When the C_{60} is not introduced onto the sample surface, there is no peak in the

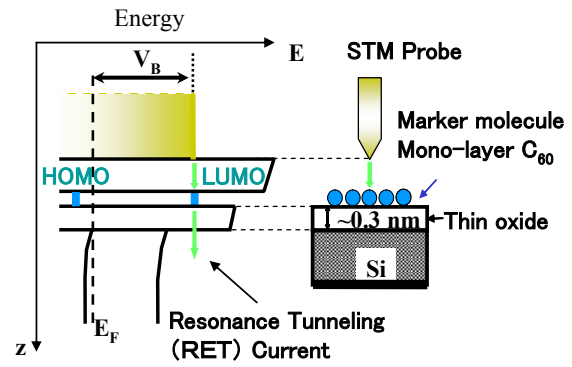


Fig. 3 Principle of scanning resonant tunneling measurement of local potential using C_{60} deposited on oxide as a marker molecule.

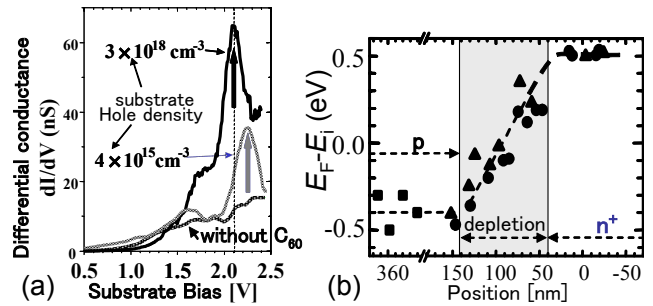


Fig. 4 (a) Differential tunnel conductance of oxidized surfaces with and without C_{60} layers. Two substrates with different boron concentrations are compared. (b) Position dependence across a pn junction of local Fermi level, $E_F - E_i$ measured by the resonance peak position of C_{60} molecular level, where E_i is the intrinsic Fermi level.

STM conductance spectrum, but the C_{60} deposition gives rise to the resonance tunneling peaks, the position of which depends on the hole density of underlying substrate (Fig. 4 (a)). This peak position reflects the Fermi level of the substrate[3], and enables us to measure the potential distribution across a pn junction as shown in Fig. 4 (b). This technique has been actually applied to quantitative analysis of doping profiles on cross sections of MOSFETs.[4]

3. Summary

We have demonstrated that STM is not a peculiar tool for surface science but a useful technique for quantitative analysis of local electrical properties in semiconductors. Actual profiling on device cross sections will be presented.

Acknowledgements

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References

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