Variation of Contrast of H/pn-Si(100)
Imaged with Different Emission Electron Microscopies∗

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H-terminated Si(100) with lateral p+-n junction has been imaged with emission electron microscopies as a model system where surface electric field is inhomogeneously distributed. It is clarified that mirror electron microscope has a higher sensitivity to the electric field parallel to the surface, compared to photoemission electron microscopy (PEEM) with either Hg-lamp (UV-PEEM) or synchrotron radiation to emit secondary electrons (SE-PEEM). On the other hand, intensity contrast between p-region and n-region arising from the difference in band bending, i.e., an electric field normal to surface, can be detected by UV-PEEM. It has been found in SE-PEEM that the intensity contrast becomes lost with higher kinetic energies. [DOI: 10.1380/ejssnt.2006.539]

Keywords: Si; emission electron microscopy; photoemission electron microscopy; mirror electron microscopy

I. INTRODUCTION

Microscopic characterization of physicochemical properties of specimens for the applications to semiconductor devices and catalysts is highly needed. Scanning probe microscopy (SPM) is applied to microscopically characterize surfaces of specimens due to its high spatial resolution. The application of SPM to the microscopic characterization makes, however, sometimes complication in analyzing the images to extract surface properties. The complication arises from the strong interaction of probes with the specimen surface through, for example, spatially confined electric field and inelastic events in tunneling phenomena [1]. The information from SPM thus includes the interference of SPM probes with the surfaces.

On the other hand, emission electron microscopies can give the microscopic information with a small interference with the specimen, the interference due to an acceleration voltage between the objective and the specimen. During imaging with EEM, the acceleration voltage is in fact applied so small that the electric field does not seriously interfere with the surface, compared to SPM observation of surfaces. Although the electric field can affect the image contrast through the deflection of trajectories of emitted electrons in EEM, such effect of the electric field is predictable [2, 3]. Actually, recent reports about the image contrast of EEM demonstrate that a potential distribution parallel to the specimen surface can be estimated through the analysis of the image contrast of EEM under the application of the acceleration voltage [2, 3].

There exist different types of EEM, for instance, mirror electron microscope (MEM) can image the surface with electrons reflected just in front of the surface, and the images selectively contain information on the surface lateral potential distribution, in principle, without the interference with incident electrons and secondary electrons.

On the other hand, photoemission electron microscope (PEEM) can image the surface with photoelectrons ejected from the surface, and the PEEM image inevitably contains information on local variation of work function as well as perpendicular electric field of surface, i.e., band bending beneath the surface, including the surface photocurrent effect in the case of semiconductors surfaces. It is so natural to anticipate that the comparison between different emission electron microscopes, such as MEM and PEEM, can provide insight into the nature of physicochemical properties of semiconductor surfaces.

In this report, the laterally p+-n junctioned Si(100) has been used a model substrate where spatially inhomogeneous electric fields at p+-n junctions exist. The imaging of the surface with different emission electron microscopes has been performed to examine their availability of the inhomogeneous distribution of surface electric field.

II. EXPERIMENTAL

In our experiments, LEEMIII (Elmitec GmbH) installed at a branch of BL27SU in Spring-8 has been used as a spectroscopic photoemission and low energy electron microscope (SPELEEM) connected with a light source of synchrotron radiation. The detail of the SPELEEM system has been well described in detail elsewhere [4]. The SPELEEM system contains the energy analyzer that can select the kinetic energy of emitted electrons with an energy slit of 0.5 eV. Laterally p+-n junctioned Si(100), hereafter abbreviated as p+-n-Si(100), has been designated and manufactured at equipments of a semiconductor clean room of Toyota Technological Institute to fabricate p+-n layer ([B+]: 10¹⁸ cm⁻³) of 7 μm long, 100 μm long and 0.1 μm thick on n-Si(100) (~ 10¹⁵ cm⁻³) substrate [5]. The surface thus fabricated has been cleaned in a mixture of H₂SO₄ and H₂O₂ solutions, followed by a dip in

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a dilute HF solution to remove a sacrificial oxide (20 nm thick) and to simultaneously H-terminate the surface. Immediately after the HF treatment [6], the sample has been transferred to the chamber of the SPELEEM system. The pressure of the analysis chamber in the system has been \( \sim 1 \times 10^{-7} \) Pa during imaging the surface. Hg-lamp is used to acquire PEEM images composed of photoelectrons from near the top of valence bands of Si substrates (abbreviated as UV-PEEM). In getting the PEEM images with secondary electrons (SE-PEEM) by synchrotron radiation, a photon of 300 eV has been used to emit photoelectrons from the surface.

### III. Results and Discussion

Figure 1(a) shows a bright-field low energy electron microscope (LEEM) image of H/pm-Si(100) surface. In the images, darker and brighter regions are the \( p^+ \)-region and the \( n \)-regions, respectively. The observed contrast is embodied in a cross-sectional intensity profile across the line marked in Fig. 1(a), as shown in Fig. 1(b). In the images, peculiar inhomogeneity exists in upper left and lower right sides of Fig. 1(a). This arises from the blur of the microchannel plate. In imaging surfaces with LEEM, surface crystallinity may be one of determining factors in the image contrast, so that the \( p^+ \)-layer may be darker because of the degradation arising from the amorphous layer owing to the heavy B+ implantation, while H-termination of Si surface without ion implantation can possess the high degree of surface order [7]. Surface morphology may be another cause of the difference in the LEEM images. As shown below in the MEM observation sensitive to surface morphology as well as surface potential, however, the remarkable difference in surface morphology between \( p^+ \)-region and \( n \)-region could not be observed. Surface crystallinity might be thus more probable than surface morphology.

Figure 2(a) shows the MEM image of the pm-Si(100). In the image, \( p^+ \)-region looks brighter while \( n \)-region darker. To analyze concretely this observed contrast, Fig. 2(b) shows the intensity profile along the line A-B marked in Fig. 2(a), with the fitted curve calculated from the surface potential distribution shown in the bottom of Fig. 2(b). The intensity profile clearly indicates that the intensity in the \( p^+ \)-region is larger than that in \( n \)-region. In addition to this intensity contrast, the asymmetrical line shape in \( p^+ \)-region can be clearly seen, a bump in \( n \)-side and a bulge in \( p^+ \)-side. It is to be noted that the asymmetrical lineshape is not remarkable on the intensity profile of the LEEM image as shown in Fig. 1(a). This can be attributed to a fact that surface potential distribution is not the principal factor in the LEEM imaging [8].

The asymmetrical lineshape has been theoretically analyzed and concluded to be the result from the deflection of electron trajectories due to the local electric field parallel to the surface [2]. In imaging with MEM, the incident electrons are reflected from the surface, and then they can be greatly influenced by the parallel electric field just outside the surface \( \phi(x) \). The shift of electron on the screen due to a deflection of electron trajectories under the influence of unidimensional microfields can be written as [2]:

\[
S(x) = \frac{\sqrt{l(f + 2l)}}{2\sqrt{2V_0}} \int_{-\infty}^{\infty} \frac{\phi'(x - \xi)}{\sqrt{|\xi|}} d\xi, \tag{1}
\]

where \( V_0 \), \( l, f \) is the acceleration voltage, the distance between the objective and the specimen, and the focal length, respectively. Equation (1) can be rewritten for a point perturbation (charge) that can be regarded as \( \phi(x) \) in the form of Dirac’s \( \delta \)-function as [2]:

\[
S(x) = -\frac{\sqrt{lf + 2l}}{2\sqrt{2V_0}} \frac{x(2h + \sqrt{h^2 + x^2})}{2(h^2 + x^2)^{3/2} \sqrt{h + \sqrt{h^2 + x^2}}} \tag{2}
\]

\( h \) is a height where the incident electrons reflect in front of the surface of specimen, and is defined as:

\[
h = \frac{\Delta V - W/e}{E_0} \tag{3}
\]
FIG. 2: (a) a MEM image of pn-Si(100) (16 µm × 10 µm), and (b) the intensity profile of the image along the line A-B shown in (a). The intensity profile is normalized, so as to set the value of n-region to be 1. In Fig. 3(b), the solid line on the upper side is the fitted curve to the experimental line profile according to the analysis described in the text, and the solid line in the bottom of the figure is the assumed potential on surface for the fitting displayed on the upper side of the figure. (c) shows the deflection of electron trajectories on the surface. The dotted line shows the deflected electron trajectories due to the attraction from the positive charge on the surface of p+-region. The sample potential is more negative than the potential of the cathode of e-gun by 1.2 V.

where ΔW, W, and E₀ are a bias voltage between the specimen and the gun cathode, additional energy of an incident electron, and the acceleration field of the objective lens, respectively [2]. Positive values of h indicate that the incident electrons reflect in front of the specimen surface, while negative values of h indicate that the incident electrons penetrate into the specimen.

Summing up S(x) with Eq. (2) in the interfacial region in the p-n junction enables us to simulate the cross section of MEM images (Fig. 2(b)) with the help from the following equation,

\[ j(x + S) = \frac{j_0}{1 + dS/dx}, \]  

where \( j(x+S) \) and \( j_0 \) are intensity profiles with or without the influence of the surface potential [2, 3].

With Eqs. (2) and (3), the experimental data is fitted as with the line shown in the upper part of Fig. 2(b), and the extracted surface potential distribution from the fitting is shown in the bottom of Fig. 2(b). In this calculation, the potential profile is, to a first approximation, assumed as a smoothly varying function, \( \varphi_n(x) = \left( \varphi_0 / \pi \right) \arctan(x/a) \), for the interfacial region in the n-side (\( x < 0 \)), while the sharply varying function, \( \varphi_p(x) = \varphi_1 \cdot \delta(x - 0.01) \) for the interfacial region in the p-side (\( x > 0 \)) [2, 3]. As a result of the calculation, it is demonstrated as expected in advance that the intensity profile can be well reproduced in the interfacial region by the fitted curve, and that the potential profile extracted from the calculation varies smoothly in n-region and sharply in p-region. It is also shown by the fitted curve that the intensity in the p-region away from the interfacial region is larger than that in n-region away from the interfacial region.

In the fitting, h has been estimated about +100 nm, on both n-region and p-region. This indicates that almost all the incident electrons reflect in front of the specimen surfaces on both regions, which can be supported by the warrant claiming that the absolute value of (negative) sample bias to the cathode of electron gun (1.2 V) is large enough to neglect the variation of surface potential at the surface (\( \sim 0.1 \) V), about the total amount of reflected electrons from the surface. Almost all the reflected electrons leaving from the surface can be collected by the objective lens, owing to the strong acceleration field (\( \sim 10^4 \) V/cm) between the objective lens and the surface. The contrast in MEM therefore arises from the redistribution of reflected electrons due to surface electric field parallel to the surface, not by the amount of reflected electrons.

This situation in MEM as stated above is different from that in the scanning electron microscopy (SEM), in which voltage contrast can be observed. Due to low acceleration electric field between the sample and the detector of sec-
ondaries, the voltage contrast arises from the apparent decrease of the detected secondaries because of the easiness to deflect trajectories of the secondaries [9]. It is safely to conclude that the mechanism of the contrast in SEM is different from that in MEM. Therefore, it is not so unnatural to observe the contrast in MEM that is different from the voltage contrast in SEM.

A probable origin of the potential profile examined above is discussed here. Hydrogen-termination of Si(100) surface cannot completely passivate the surface, and a pinning of Fermi level can therefore occur. Because of the Fermi level pinning, bands in n-region are bent upwards by electron transfer with surface acceptors, resulting in negative charging at the surface, while bands in p-region are bent downwards with the electron transfer with surface donors, resulting in positive charging at the surface [10, 11]. This spatial variation of surface charging due to the Fermi level pinning produces the microscopically inhomogeneous potential profile just outside the surface [12], so that the trajectories of reflected electrons to form MEM images are deflected, as schematically shown in Fig. 2(c).

The deflection of electron trajectories is determined by magnitude as well as width of the potential distribution. Though not shown, S' reaches its maximum at \( x = 0.01 \) where the potential jump occurs due to the very narrow space charge layer in p-side. Because the strength of electric field at the depleted region in p-side, the region where the intensity profile is deviated from that under no electric field in p-side is larger than that of the physical width of the depleted region in p-side estimated from the dopant concentration. The difference in the intensity in p-region away from the interfacial region between the experimental intensity profile and the calculated one may arise from the fact that the width of local surface band bending of degenerated p-layer in the real p-n junction has been measured to be larger than that expected from the ideal (abrupt) p-n junction [13]. The more rigorous calculation concerning the potential on surface by the use of PEEM with X-ray excitation will be published elsewhere.

Figure 3(a) shows the UV-PEEM image of H/pn-Si(100), and the intensity profile along the line A'–B' is shown in (b). The intensity profile is normalized, so as to set the value of n-region to be 1. The kinetic energies of electrons has not been selected by an energy analyzer in the image.

To launch the discussion about the image contrast of the UV-PEEM images, it should be firstly mentioned that the equation for the quantum yield of photoemission from semiconductors can be expressed as,

\[
Y \propto (h\nu - E_{\text{gap}} - \chi + \Delta E(x))^5/2
\]

where \( h\nu, E_{\text{gap}}, \chi, \) and \( \Delta E(x) \) represent the incident photon energy, the band gap, the electron affinity, and the valence band profile [14, 15]. If \( \Delta E(x) > 0 \) \((<0)\), the bands are bent downwards (upwards). From this scenario, the \( p^+ \) region is imaged as the brighter region in UV-PEEM.

In the intensity line profile in Fig. 3(b), the asymmetrical lineshape does not remarkably appear. As discussed above, the image contrast in UV-PEEM is primarily determined by the probability of photoemission due to band bending that arises from the electric field normal to the surface, and then the deflection of electron trajectories due to surface electric field parallel to the surface becomes the secondary factor. In other words, the asymmetrical lineshape is hidden by the presence of the intensity contrast due to the band bending. Because the intensity contrast is strongly temperature-dependent [5], the asymmetrical lineshape becomes remarkable at low temperatures. The detail of the temperature dependence of the contrast will be published elsewhere [16].

Figures 4(a) and (b) show the SE-PEEM images with selected kinetic energies of 0.5 eV and 5 eV, respectively. The principle of the contrast of SE-PEEM images is similar to UV-PEEM images. Though weak, the intensity contrast can be seen in the images with the selected kinetic energy of 0.5 eV, as shown in Fig. 4(c). On the other hand, no image contrast can be seen on Fig. 4(b) with a selected kinetic energy of 5 eV. This is because, with high kinetic energy, the difference in the potential barrier due to the band bending becomes less influential to the probability of photoemission of electrons.
FIG. 4: (a, b) SE-PEEM images of \textit{pm}-Si(100) (22 μm×22 μm), and (c) the intensity profile of the image along the line A”–B” shown in (a). The intensity profile is normalized, so as to set the value of \textit{n}-region to be 1. The kinetic energies of electrons contributing to the formation of (a) and (b) that has been selected by the energy analyzer whose energy resolution is 0.5 eV are 0.5 eV and 5 eV, respectively.

IV. CONCLUSIONS

In this report, the various types of imaging with emission electron microscopes are shown to try to get the information of surface electric field parallel and perpendicular to the surface with and without UV irradiations. The results shown in this report is being analyzed together with the simultaneously acquired microspectroscopic data of the same sample. The combined analysis of these data will make it possible to do a quantitative characterization of the inhomogeneously distributed electric field on surfaces, and be published elsewhere.

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