

PEEM Imaging of Dopant Contrast in Si(001)

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Abstract

We report on a quantitative investigation of doping-induced contrast in photoelectron emission microscopy (PEEM) images of Si devices. The calibration samples were fabricated using standard photolithography and focussed ion beam (FIB) writing, and consisted of p-type (B) stripes of different nominal dopant concentrations (10^{18} - 10^{20} cm⁻³) and line separations, written on n-type ($N_d=10^{14}$ cm⁻³) Si(001) substrates. Using a near-threshold light source, we find that the signal intensity increases monotonically with B concentration over the measured range of doping. The measured intensity ratios are in good agreement with a calculation based on photoemission from the valence band.

KEYWORDS: Electron Microscopy; Surface electronic phenomena (workfunction, surface potential, surface states, etc.); Semiempirical models and model calculations; Silicon; Photoelectron emission; Photoemission (total yield)

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Spatial variation in photothreshold is one of several possible contrast mechanisms in photoelectron emission microscopy (PEEM). For instance, the photothreshold of a metal is equal to the work function and varies slightly with crystallographic orientation to produce PEEM contrast for poly-crystalline metals¹. Similarly, in a semiconductor, the photothreshold can be changed by varying the level of doping² which can also lead to contrast in PEEM³.

It has been known since the 1960s that the photothreshold of clean, cleaved Si(111) decreases when the sample is heavily to degenerately doped^{2,4,5}. The reason for this is that surface-state associated Fermi level pinning results in band bending, which for p-doping reduces the photothreshold for electrons excited from sufficient depth in the bulk. The magnitude of the band bending is determined by the doping level, the position of the surface states relative to the bulk Fermi level and the density of surface states. For a small number of surface states, the energy bands will be flat upto the surface and PEEM contrast due to doping should not occur. To control the surface state characteristics, we have used a wet-chemical oxidation as a standard preparation. Scanning tunneling spectroscopy observations of pn devices fabricated on Si(001) prepared in this way indicated a small enough density of interface states to allow tip induced band bending⁶. Previous PEEM observations on the same devices, however, indicated that this interface state density was large enough to result in observable contrast³. In this letter, we report a quantitative investigation of the contrast available in PEEM images of pn junctions as a function of silicon dopant concentration, and the sensitivity of the contrast to overall band bending.

A commercial PEEM (Staib PEEM-350) mounted in a UHV stainless steel chamber was used to image the Si devices. Prior to loading the samples, a wet chemical etch is done leaving a thin oxide on the sample⁷. All imaging is done in a vacuum of approximately 10^{-9} Torr. The samples are mounted approximately 4 mm from the aperture lens. The sample holder has 5 degrees of freedom (3 linear and 2 angular) and heating capability. The light source is a 100 W mercury short-arc lamp which produces a continuous spectrum up to approximately 5.15 eV, just above the nominal photothreshold

for Si. A chevron-type multichannel plate is used to intensify the images approximately a million times. The images are recorded using a 12-bit CCD camera which produces a 1280 x 1024 bitmap. Image files are stored in 16-bit tif format.

The samples used for the study were initially fabricated using standard photolithography techniques. A lateral array of pn junctions was formed by implanting boron ions (10^{18} cm^{-3} , 190 keV) through a mask into an n-type Si(001) substrate ($P 10^{14} \text{ cm}^{-3}$). Two hundred 1 um p^+ stripes spaced 30 um apart were fabricated. The pn junction devices were then modified using focussed ion beam (FIB) writing to allow a systematic variation of the doping levels. Two different FIB writing systems were utilized. One system utilized a 120 keV beam of boron ions for the implant while the second system produced a beam of boron ions with an energy of 34 keV. In both cases, three sets of 9 lines were produced, each perpendicular to the pre-existing photolithography lines. The first set of lines was produced with nominal p-type doping levels of 10^{18} , 10^{19} , 10^{20} cm^{-3} and nominal line widths of 200 nm . The second set of lines was produced at nominal p-type doping levels of 6×10^{18} , 6×10^{19} , $6 \times 10^{20} \text{ cm}^{-3}$ and nominal line widths of 750 nm . The line spacing was varied from 0 to 10 um for both sets of lines.

PEEM images of the samples show that the photoyield from the p-stripes indeed increases as the amount of doping is increased, as expected based on the measurements of photothreshold for cleaved Si surfaces^{2,4,5}. In figure 1, a PEEM image of the 120 keV FIB implants is shown. The bright horizontal lines on the left side of the image are p-type 10^{20} cm^{-3} FIB lines, while the dimmer horizontal lines on the right are FIB lines at 10^{19} cm^{-3} . The vertical p-type lines (produced by photolithography) are nominally 10^{18} cm^{-3} p-type. The 10^{18} cm^{-3} FIB lines yield a significantly lower intensity. As discussed below, this is due to differences in the vertical implant profile in the three implantation procedures.

To make a quantitative assessment of the PEEM intensity from each set of doping levels, line scans were measured from the image data. In a given image, a single p-type FIB line, a photolithography line and the surrounding n-type region were defined and a series of line scans perpendicular to the FIB line were averaged. Typically, 20 to 25 lines were averaged to produce an intensity profile with a rms fluctuation that is less than 1%

of the average intensity from the n-type region. The intensity from the photolithography

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lines was used to normalize the intensities from the FIB lines to correct for detector gain and incident light intensity variations. As shown in figure 2, for the 120 keV FIB implants the average ratio of the heights of the intensity profiles is 6.3:2.5:1.0 for the nominal 10^{20} : 10^{19} : 10^{18} p-type doping, respectively. The results for the six different FIB doping levels are summarized in Table I. Also shown in Table I (column 2) are the doping levels in the near surface region, calculated using SUPREM-IV⁸.

Using theory developed by Kane⁹, photoyield ratios were calculated. The photoyield Y from the valence band for an indirect optical excitation near threshold can be expressed as

$$Y \propto \int (h\nu - E_T(x))^{5/2} e^{-x/l} dx$$

where $h\nu$ is the photon energy and $E_T(x)$ is the depth dependent threshold energy. The reduced escape depth l is given by $1/l=1/l_\alpha+1/l_e$ where l_α is the absorption length and l_e is the electron escape depth. We use values of $l_\alpha = 62 \text{ \AA}$ for $h\nu = 5.15 \text{ eV}$ and $l_e = 25 \text{ \AA}$ for near threshold photoelectrons⁴. The energy threshold is equal to the surface value, $E_T(0)$, minus the band bending profile $\Delta E(x)$. For Si(111), $E_T(0)$ is approximately 5.15 eV which we initially assume is the same for our Si(001) surface. The band bending profile $\Delta E(x)$ is uniquely determined by the potential at the surface relative to the potential in the bulk, V_s , which in turn is determined by the interface state density and the bulk doping. Given v_s (defined as qV_s/kT), the band bending profile can be determined by numerically solving Poisson's equation in the space charge region^{10,11}. It has been shown that formation of an oxide layer on Si will lower the density of surface states^{6,12,13}. We find that if the density of pinning states is at least few percent of the clean surface state density, surface band bending leading to behavior qualitatively like that seen in Fig. 2 will result. As a specific example, for a density of $5 \times 10^{13} \text{ cm}^{-2}$ interface states, the values of v_s range from 11.9 to 13.7 for p-type doping levels of 10^{18} to 10^{20} cm^{-3} when the surface states are 0.29 eV above the surface valence band¹⁴. For these values of v_s , with electrons emitted just at threshold, the resulting calculated intensity ratios are approximately 24:8:1 for 10^{20} , 10^{19} , 10^{18} cm^{-3} doping. This is substantially higher than the experimental ratios listed in Table I.

If the number of interface states is too small, the calculated intensity ratios will not increase as the doping level is increased over the entire range we have studied. We have found that the interface state density must be approximately $5 \times 10^{13} \text{ cm}^{-2}$ for the calculated intensity ratios to increase monotonically with doping concentration. This provides a lower bound on the density of interface states necessary for surface band bending to occur. By changing the position of the pinning states relative to the surface valence band from 0.15 to 0.33 eV, we have found that the lower bound on the number of interface states does not change significantly, which results in monotonic intensity ratios independent of the interface state position.

A plausible explanation for the discrepancy between the calculation (curve marked by open squares in Fig.3) and our measurements is that we are imaging with a range of electron energies above threshold. The effect of increasing the difference in energy between the absorbed photon and the threshold $E_T(0)$ on the calculated intensity ratios was therefore tested. The calculated ratios are sensitive to the energy difference $\Delta E = h\nu - E_T(0)$. The results of the calculation when ΔE is increased from 0 (Box) to 180 meV (bigtriangledown) are shown in figure 3. The agreement with the measured ratios is good for ΔE approx. 150 meV. The calculation suggests that doping-contrast in PEEM will increase by imaging closer to threshold. In practice this could be done by utilizing a tunable light source.

In the calculations done here, emission from surface states to the photoyield has been neglected. Spatially averaged photoemission measurements from cleaved Si surfaces of different dopant concentrations⁵ suggested that the contribution of surface states to the photoemission yield is independent of type and doping level. We note that at doping levels higher than 10^{18} cm^{-3} , which includes most of the range we have investigated, the surface state contribution is small compared with the valence band contribution.

In conclusion, we find that differences in relative PEEM intensities in images of devices show a systematic variation with p-type dopant concentration. Within the range $10^{17} - 2 \times 10^{20} \text{ cm}^{-3}$, we find decreasing intensity at a rate of a factor of approximately 2 per decade, in good agreement with calculations of photoemission from the valence band for a

photothreshold slightly below our maximum photon energy. However, the calculated intensity ratios are quite sensitive to the difference between the photon energy and the photothreshold. By making PEEM intensity measurements relative to a known reference sample, the ratio of intensities should provide a robust measure of the p-type dopant concentration at high levels. Below 10^{17} cm^{-3} p-type, or for n-type material, the contrast decreases significantly and measurement of the doping concentration from PEEM image intensities is expected to be difficult.

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1. Doping (cm-3)	Doping at Surface (cm-3)	I_{FIB}	i_F	$i_F/i_{F,min}$
6.00E+20	2.00E+20	3158	4.9	12
1.00E+20	3.00E+19	2292	2.5	6.3
6.00E+19	7.00E+18	3269	1.8	4.5
1.00E+19	1.00E+18	1212	1	2.5
6.00E+18	8.00E+17	2478	1	2.5
1.00E+18	1.00E+17	1076	0.4	1

Table I: Nominal implant value, corresponding value of doping level at the surface (calculated with SUPREM-IV), measured intensity at peak of PEEM line profile, intensity normalized to intensity of standard (photolithography) line, intensities normalized to lowest doping level.

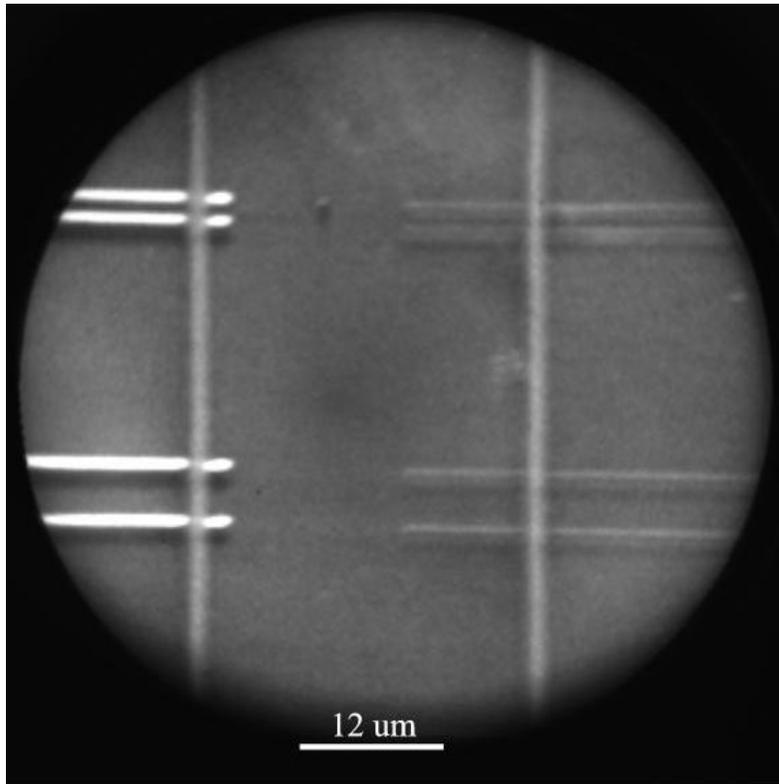


Figure 1. PEEM image of lateral array of pn junctions. The horizontal stripes are nominally 10^{20} cm^{-3} (bright) and 10^{19} cm^{-3} (dimmer) p-type FIB lines. The vertical lines are p-type 10^{18} cm^{-3} lines produced with photolithography. The upper line pair is separated by 2 μm and the lower pair by 5 μm . Image was averaged 16x with 0.5 s exposure.

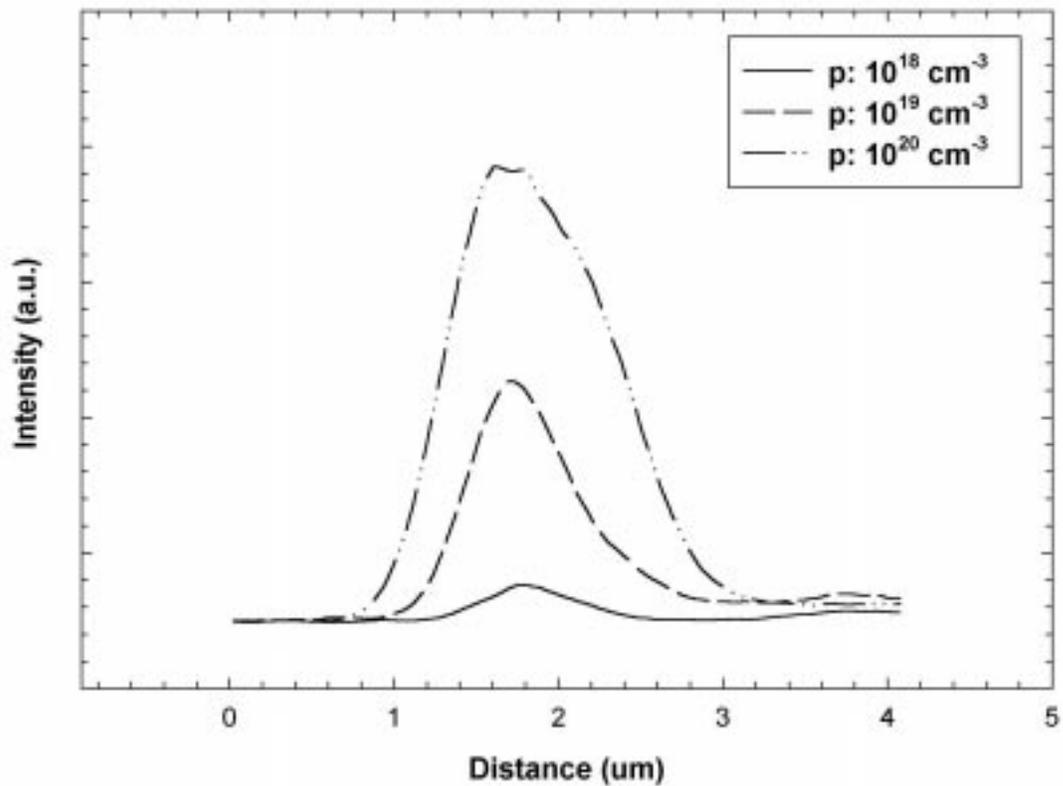


Figure 2. Normalized intensity profile of single FIB lines from the 120 keV implant. The intensity peak of the nominal 10^{20} cm^{-3} line is roughly 5 times the intensity peak of the nominal 10^{18} cm^{-3} line. The intensity of the nominal 10^{19} cm^{-3} line is approximately 2 times that of the nominal 10^{18} cm^{-3} line.

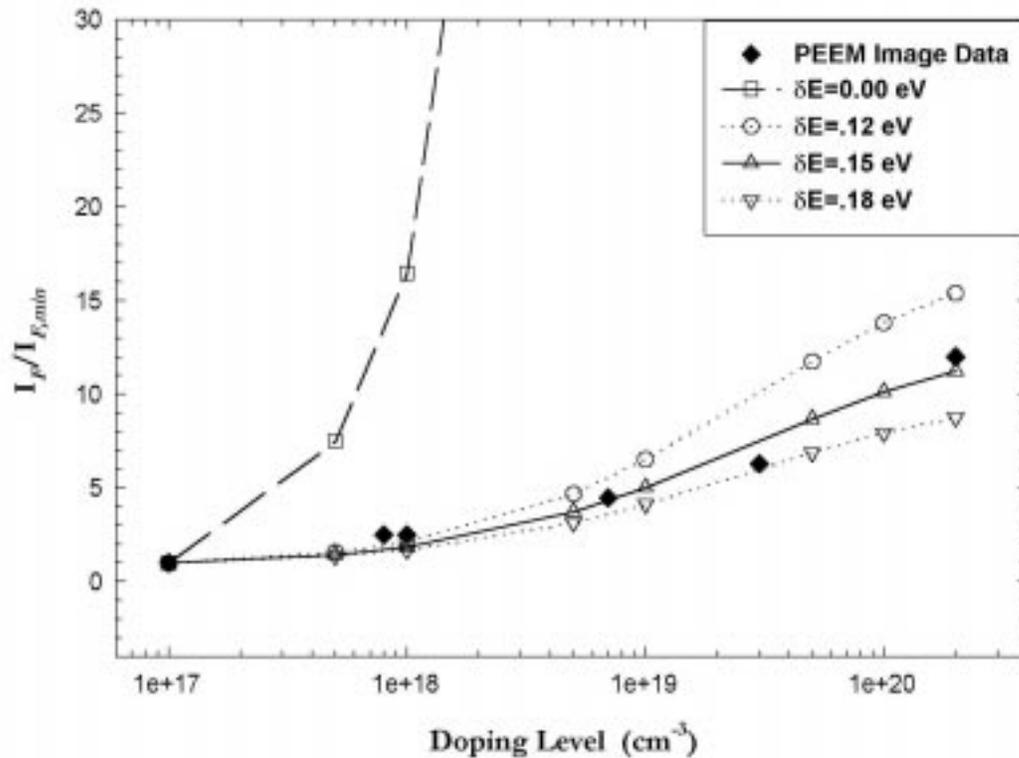


Figure 3. Calculated threshold photoyields from Si(001) vs. doping level at the surface (Column 2 in Table I). The curves marked with connecting lines show the calculated intensity ratios for photon energies upto 0.18 eV above threshold. The diamonds show the measured relative values of the PEEM intensities (column 5 of Table I)