AIP Applied Physics Letters

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Citation: Applied Physics Letters **87**, 232103 (2005); doi: 10.1063/1.2138442
View online: http://dx.doi.org/10.1063/1.2138442
View Table of Contents: http://scitation.aip.org/content/aip/journal/apl/87/23?ver=pdfcov
Published by the AIP Publishing

APPLIED PHYSICS LETTERS **87**, 232103 (2005)

Quantum well behavior of single stacking fault 3C inclusions in 4H-SiC *p-i-n* diodes studied by ballistic electron emission microscopy

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(Received 4 October 2005; accepted 26 October 2005; published online 28 November 2005)

We show that "single" stacking fault 3C inclusions formed in 4H-SiC *p-i-n* diodes behave as electron quantum wells (QWs) with the QW energy depth of ~0.25 eV below 4H-SiC conduction band minimum, by measuring the Schottky barriers on and away from inclusions with ballistic electron emission microscopy (BEEM). The Schottky barrier on the 4H area ([11-20] oriented) is measured to be essentially the same as (0001) plane studied previously, indicating that the interface pinning effects on both crystal faces are almost identical. Additionally, BEEM current amplitude is observed to be very sensitive to subsurface damage induced by polishing. © *2005 American Institute of Physics*. [DOI: 10.1063/1.2138442]

SiC is a wide band gap semiconductor with unique physical and electrical properties suitable for high voltage, high temperature, and high frequency electronic device applications.[1] The recent availability of large diameter substrates of 4H- and 6H-SiC has made it possible to commercialize unipolar SiC devices such as Schottky barrier diodes and metal semiconductor field effect transistors.. However, the commercialization of 4H-SiC *p-i-n* diodes (bipolar devices) is hindered by the formation and propagation of stacking faults (SFs) in hexagonal basal planes during operation.[2] High-resolution transmission electron microscopy studies showed that the SFs formed this way are all of the "single-layer" Shockley type produced by the motion of a basal-plane partial dislocation[3,4] resulting in a structure that is equivalent to a ~0.5-nm-thick[5] planar inclusion with local cubic (3C) structure embedded in the 4H-SiC host. Based on redshifted luminescence[2,6] and calculations,[5,7] these 3C inclusions were proposed to behave as unique "structure-only" quantum wells (QWs) due to the ~0.9 eV lower conduction band energy of 3C-SiC relative to 4H-SiC. A temperature-dependent luminescence quenching measurement by Sridhara *et al.*[8] suggested a ~0.282 eV QW energy depth in this inclusion, consistent with the calculations that predicted an energy (depending on calculation method) between 0.2 and 0.3 eV.[5,7] To date, however, measurements have not demonstrated that these inclusions actually support *propagating* two-dimensional (2D) QW electron states, and no experimental confirmation of the reported ~0.282 eV QW energy has been made. Accurately determining this energy depth is important not only as a test of the calculations, but also because the thermodynamic energy gain as electrons fall into the SF QWs has been proposed as the driving force for SF propagation.[7]

In this letter, we report nm-resolution electronic characterization using ballistic electron emission microscopy (BEEM) of these single SF inclusions that directly confirms they are QWs with propagating 2D states, with a QW subband energy depth ~0.25 eV below the 4H-SiC conduction band minimum (CBM). We have also made the nanometer (nm)-resolution measurements of the Schottky barrier height (SBH) on the "*a*-face" (11-20) surface of 4H-SiC, and observed that the SBH (with Pt contacts) on this face is essentially the same as that on the more common (0001) surface. We further discovered that BEEM is locally sensitive to electron scattering from subsurface defects created during surface polishing.

The fabrication and electrical stressing of the [11-20]-oriented *p-i-n* diodes used in this study have been described elsewhere.[4] Electric stressing caused single-SF basal-plane inclusions with typical 100–500 μm lateral extent and 10–50 μm separation to form in the n^-($\sim 10^{15}$ cm^{-3}) "intrinsic" blocking layer of the *p-i-n* diodes. To study these inclusions with BEEM, it was necessary to make a Schottky contact on a surface that *intersects the inclusions* in a cross-sectional geometry. We therefore used mechanical polishing to remove the top metal contacts, the top *p*+ layer, and part of the 30-μm-thick n^- blocking layer. The final surface was prepared by a chemimechanical polishing step resulting in cross-sectioned basal-plane inclusions oriented perpendicular to the polished (11-20) surface. The sample was then cleaned as described in Ref. 9, introduced into an UHV chamber (base pressure: $\sim 1 \times 10^{10}$) and outgassed overnight at <230 °C. A set of Schottky diodes with ~5 nm thickness and ~0.5 mm diameter was formed *in situ* by electron-beam evaporating Pt through a shadow mask at room temperature. The sample was then transferred in UHV to an adjacent scanning tunneling microscope (STM) chamber where BEEM measurements were done. Despite a number of surface polishing scratches (see later), we found these Pt Schottky diodes to be highly rectifying and nonleaky, very similar to diodes formed on epitaxially grown films.[9–11] This indicates that chemimechanical polishing could also be used to expose other kinds of extended defects for electronic studies by BEEM and other experimental techniques.

BEEM is an extension of STM that can probe the local electronic transport property across buried metal/semiconductor (M/S) interfaces with nm-scale spatial resolution and 10–20 meV energy resolution.[12] "Hot" electrons are injected from the STM tip (at a voltage of -V_T) into a thin metal film of a Schottky contact, and the BEEM "collector"

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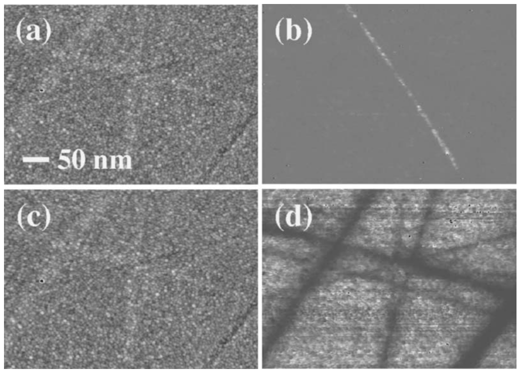

FIG. 1. (a) STM image of a 5-nm-thick Pt overlayer on chemimechanically polished (11-20) plane of 4H-SiC (gray scale: 4 nm) and (b) simultaneously taken BEEM image (gray scale: 1 pA), taken at V_T=1.55 V and I_T=5 nA. (c) STM image and (d) simultaneous BEEM image (gray scale: 9.5 pA) taken on the same area at V_T=2.00 V and I_T=5 nA. The straight stripe of enhanced BEEM current in (b) reveals where the 3C inclusion intersects the M/S interface.

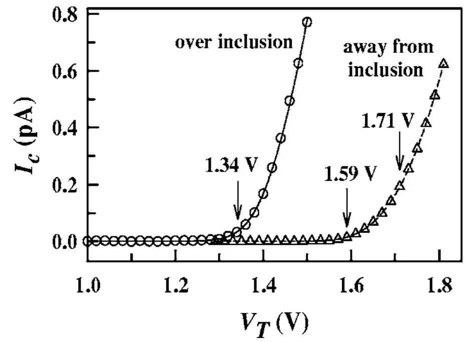

FIG. 2. Typical BEEM spectra (I_c-V_T curves) averaged over ~100 individual I_c-V_T curves on an 3C inclusion (open circle) and on the surrounding 4H-SiC ([11-20] oriented) away from it (open triangle). The solid and dashed lines going through the measured data are fitted curves with Bell-Kaiser model. The arrows indicate SBHs determined by fitting. On the surrounding 4H-SiC, the same two thresholds (local SBH and second CBM) as (0001) plane are observed and ~0.25 eV lower SBH was measured on the inclusion, representing the QW energy depth in the inclusion.

current I_c is measured from the substrate. I_c is due to the fraction of injected electrons that crosses the metal film, surmounts the Schottky barrier, and enters propagating states in the conduction band of the semiconductor substrate. A separate "base" contact to the metal film removes any injected electrons that do not enter the substrate. The local SBH (energy difference between the semiconductor CBM *at the M/S interface* and the metal Fermi level E_F) can be determined by using a "BEEM spectrum," i.e., measuring I_c as a function of V_T and determining the "threshold" tip voltage at which electrons start to enter the semiconductor conduction band. One can also make a "BEEM image" to search for local regions with lower conduction band energy, i.e., plotting I_c versus tip position with V_T held fixed, and looking for regions with high I_c. We have previously shown that BEEM can be used in this way to locate cross-sectioned QWs at a M/S interface, and measure the local conduction subband energy in "double-SF" cubic inclusions SiC (Ref. 9) and in cross-sectioned AlGaAs/GaAs/AlGaAs QWs.[13]

Figures 1(a) and 1(b) show a STM topographic image of the Pt film top surface and a simultaneously taken BEEM image respectively, measured at V_T=1.55 V. The STM image shows the characteristic ~5-nm-diam. metal grains of the polycrystalline Pt film but no sign of the buried cross-sectioned SF inclusion. Most of the BEEM image [Fig. 1(b)] exhibits zero BEEM current, since the Pt contact on this 4H-SiC substrate was measured to have a SBH of ~1.59 eV, which is larger than the 1.55 V tip bias. However, we clearly see a long line of nonzero BEEM current in this image, indicating that on the line injected hot electrons can locally enter *propagating conduction band states* (at energies lower than the ~1.59 eV CBM energy of the surrounding Pt/4H-SiC interface), propagate through the wide depletion zone near the Pt/SiC interface, and be collected from the SiC substrate. Many such linear features were observed, all with an orientation and average spacing corresponding to the cross-sectioned SF inclusions. We therefore conclude that the lines represent where the inclusions intersect the interface, and that these inclusions are electron QWs with propagating 2D conduction band states.[9,13]

We next measured the CBM energy of the QW by positioning the STM tip over the SF inclusion and measuring BEEM spectra. The circular data points in Fig. 2 show an average of 96 such spectra, and the solid line shows a single-threshold fit to the Bell-Kaiser model[12] with a best-fit threshold voltage of 1.34±0.01 V, indicating the QW CBM at the metal interface is 1.34±0.01 eV above E_F. The triangular data points in Fig. 2 show an averaged BEEM spectrum measured with the tip located >20 nm away from the SF, over the normal 4H-SiC host material. The dashed line shows a "two-threshold" Bell-Kaiser fit, indicating a lowest CBM of 1.59±0.01 eV. Two thresholds are required here because 4H-SiC has a second CBM at ~0.12–0.14 eV above the lowest CBM.[10,11]

These measurements indicate that the QW energy depth (i.e., the QW/4H-SiC conduction band offset) is E_{QW} =0.25±0.01 eV *at the metal interface*. As discussed previously,[9,10] there is evidence that the differences in CBM between 4H, 6H, and 15R SiC polytypes *measured at a metal interface with BEEM* are equal (within ~±30 meV) to the corresponding differences in CBM *in the SiC bulk*. We have recently made "hole BEEM" measurements[14] of the *p*-type Schottky contacts on 4H- and 3C-SiC which support this conclusion. The *p*-type SBH was found to be ~0.060 eV larger on 3C- than on 4H-SiC, very consistent with the calculated ~0.050 eV lower valence band energy of 3C-SiC.[15] Furthermore, the interface pinning strength of 4H-SiC with cubic inclusions has been found to be nearly the same as 4H-SiC without inclusions,[16] indicating that any conduction band *shift* due to interface pinning would be nearly the same for the inclusions as for 4H-SiC.

We therefore also take $E_{QW} \cong 0.25$ eV±0.03 eV as our estimate of the QW depth far from the metal interface, consistent with the previous measurement[8] of 0.282 eV and the calculated range of 0.2–0.3 eV.[5,7] As a further check, we estimated the expected QW energy by numerically solving the time-independent Schrödinger equation for the simple potential profile illustrated in Fig. 3, assuming a QW width of 0.5 nm for a single SF,[5] and the parameter values assumed by Bai *et al.*[17] for the 4H/3C conduction band offset $\Delta E_c \cong 0.925$ eV, the 3C electron effective mass $m_{eff} \cong 0.313 m_0$ (m_0: free electron mass), and the spontaneous polarization (SP) induced electric field in the SF of $\sim 1.3 \times 10^6$ V/cm. Solving this simple one-dimensional model gives an estimate of ~0.245 eV for the QW energy, very close to our measured value of ~0.25 eV.

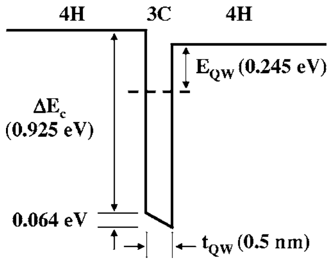

FIG. 3. Schematic view of conduction band profile of single SF 3C inclusion QW (~0.5 nm wide) embedded in 4H-SiC with the QW energy depth (E_{QW}) indicated. The SP of 4H-SiC causes a strong electric field in the inclusion resulting in a potential drop across the inclusion. Literature values were used for the SP and the conduction band offset of 3C- and 4H-SiC.

We note this Pt/4H-SiC sample has a (11-20) interface orientation while earlier BEEM studies of Pt/4H-SiC Schottky contacts deposited in the same way had a (0001) on-axis interface orientation,[10,11] or a (0001) interface miscut by 8° toward the [11-20] direction.[9] We can therefore compare the SBH (measured away from any inclusions) on these three samples to investigate the influence of interface orientation on SBH. The (11-20) sample (with $\sim 1 \times 10^{15}$ cm^{-3} *n*-type doping) had a measured SBH of ~1.59 eV, compared with ~1.58 eV for the (0001) on-axis sample ($\sim 3 \times 10^{16}$ cm^{-3} *n* type),[10,11] and ~1.54 eV for the 8° miscut (0001) sample ($\sim 1.5 \times 10^{17}$ cm^{-3} *n*-type).[9] To compare the measured SBH, we must correct for the small *image force lowering* of the SBH, which depends on doping.[18] This lowering is estimated to be ~0.022, 0.052, and 0.077 eV for these three samples, respectively, resulting in corrected SBHs of ~1.61, ~1.63, and ~1.62 eV, respectively. The values are nearly the same, indicating that the effect of any interface pinning on the SBH is almost the same for the (11-20) and (0001) interface orientations. We also note that the *shape* of the Pt/4H-SiC BEEM spectra is nearly the same for both orientations, i.e., they are both best described by two thresholds separated by ~0.12–0.14 eV. This is analogous to the well-known observation that BEEM spectra on Au/Si(001) and Au/Si(111) have nearly the same shape.[19]

Finally, we note that the BEEM current amplitude appears to be very sensitive to polishing scratches produced during the mechanical polishing step preceeding final chemi-mechanical polishing. Figures 1(c) and 1(d) show simultaneously measured STM and BEEM images of the same sample region as Figs. 1(a) and 1(b), respectively, except now with V_T=2.00 V instead of 1.55 V. The two STM images appear essentially the same, but the two BEEM images show striking differences. Since the Pt/4H-SiC SBH is ~1.59 eV, a tip voltage V_T=2.00 V should result in BEEM current everywhere over the sample, and not just over the inclusions. We do indeed observe BEEM current everywhere in Fig. 1(d), but we also see long lines of strongly *reduced* BEEM current with various orientation, width, and intensity. Careful inspections of the STM images show faint linear topographic features corresponding to most (but not all) of the dark lines in the BEEM image, probably due to shallow polishing scratches on the SiC surface present before Pt deposition. BEEM spectra measured over these dark features were found to have a ~1.55 V threshold voltage, fairly close to regions between the scratches. It is known that scratches on SiC produce subsurface defects.[20] We propose that the reduced BEEM current over the scratches is due to scattering of injected electrons off subsurface defects, which causes a fraction of these electrons to be scattered back into the metal film. We are currently working to verify this proposal, and investigating whether BEEM is sensitive to other subsurface defects.

In summary, we have used BEEM to characterize the electronic properties of "single-layer" Shockley SF 3C inclusions formed in 4H-SiC *p-i-n* diodes, and directly confirmed that they behave as QWs with propagating states. The QW energy depth was measured to be ~0.25 eV below the surrounding 4H-SiC CBM, which is close to estimations from the luminescence measurements and the theoretical calculations. The SBHs measured for Pt contacts on (11-20) and (0001) crystal planes of 4H-SiC are essentially the same, indicating the identical interface pinning on these two crystal faces. We also observed that BEEM is locally very sensitive to SiC polishing damage, likely due to local electron scattering off subsurface defects.

The authors thank Cristian Tivarus for helpful discussion. The work at the Ohio State University was supported by the Office of Naval Research Grant No. N00014-93-1-0607, monitored by Dr. Colin Wood. The initial diode preparation done by Joe Sumakeris of Cree, Inc. and the additional sample processing done at Carnegie Melon University were supported by ONR Contract No. N00014-02-C-0302, monitored by Dr. Harry Dietrich.

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