PHYSICAL REVIEW B **69**, 041305(R) (2004)

Quantum well state of self-forming 3*C*-SiC inclusions in 4*H* SiC determined by ballistic electron emission microscopy

Y. Ding, K.-B. Park, and J. P. Pelz*
Department of Physics, The Ohio State University, Columbus, Ohio 43210-1106, USA

K. C. Palle, M. K. Mikhov, and B. J. Skromme
Department of Electrical Engineering and Center for Solid State Electronics Research, Arizona State University, Tempe, Arizona 85287-5706, USA

H. Meidia and S. Mahajan
Department of Chemical and Materials Engineering and Center for Solid State Electronics Research, Arizona State University, Tempe, Arizona 85287-6006, USA

(Received 13 November 2003; published 22 January 2004)

High-temperature-processing-induced double-stacking-fault 3*C*-SiC inclusions in 4*H* SiC were studied with ballistic electron emission microscopy in ultrahigh vacuum. Distinctive quantum well structures corresponding to individual inclusions were found and the quantum well two-dimensional conduction band minimum was determined to be approximately 0.53 ± 0.06 eV below the conduction band minimum of bulk 4*H* SiC. Macroscopic diode *I*-*V* measurements indicate no significant evidence of metal/semiconductor interface state variation across the inclusions.

DOI: 10.1103/PhysRevB.69.041305 PACS number(s): 73.21.Fg, 61.72.Nn, 61.72.Qq, 72.80.Jc

Quantum well (QW) structures in semiconductor materials have played an important role in the fabrication of semiconductor lasers and other devices. Most QW structures are fabricated by changing the chemical composition of epitaxial layers during growth. However, the polytypism of SiC has made possible a unique type of ''structure-only'' QW (with no change in composition, density, or nearest-neighbor stacking across the QW boundaries) involving thin layers of cubic 3*C* SiC (which has the smallest band gap among SiC polytypes) embedded in a higher band gap SiC host.[1] Recently, evidence of self-forming 3*C* inclusions in hexagonal SiC due to stacking fault formation along the (1000) hexagonal basal plane[2] has been observed in 4*H*- and 6*H*-SiC *p*-*n* diodes after high current operation,[3,4] and also in 4*H*-SiC materials with heavily *n*-type epilayers[5] or substrates[6,7] after high temperature processing. Observations of reduced-energy luminescence from these transformed materials and theoretical calculations of the band structure led to the proposal that the 3*C* inclusions in 4*H* and 6*H* SiC behave as electron QW's.[5,6,8–10]

In this Rapid Communication, we report high-resolution electronic characterization of individual 3*C* inclusions (of the ''double stacking fault'' type[5–7]) that intersect a metal-coated 4*H*-SiC wafer surface using ballistic electron emission microscopy (BEEM).[11] The results directly verify the QW nature of the inclusions. We find that the QW states are propagating two-dimensional (2D) states with a 2D conduction band minimum (CBM) energy 0.53 ± 0.06 eV lower than the 4*H*-SiC bulk CBM. Microscopic BEEM measurements as well as macroscopic diode *I*-*V* measurements show no evidence of significant metal/semiconductor (M/S) interface state variation across the inclusions. BEEM has previously been shown to be a powerful tool to investigate planar resonant tunneling structures located close to the M/S interface,[12] and our ''cross-sectional BEEM'' further extends its capability to probe propagating states in individual QW's.

The original 4*H*-SiC samples of this study were 35 mm diameter wafers purchased from Cree, Inc. and were processed and first studied using electrical, optical, and structural methods at Arizona State University.[6,13] They had a 2 μm lightly *n*-type *N*-doped $[(1-1.5)\times 10^{17}\ \mathrm{cm}^{-3}]$ epilayer on a heavily *n*-type *N*-doped $(\sim 3\times 10^{19}\ \mathrm{cm}^{-3})$ Si-face substrate with an 8° surface miscut from the basal plane. After being thermally oxidized at 1150 °C for 90 min in dry oxygen, these wafers appeared dimpled in the central region where the substrate had a higher doping level.[6] High-resolution cross-sectional TEM images of the central transformed region revealed 3*C* inclusions (all of the double-stacking-fault type) in the 4*H* lattice,[13] as shown in Fig. 1. Room and low temperature photoluminescence energies in the transformed central region of the wafer used for the BEEM measurements are reduced by about 0.74 eV relative to the untransformed peripheral region, similar to room temperature cathodoluminescence redshift measurements by

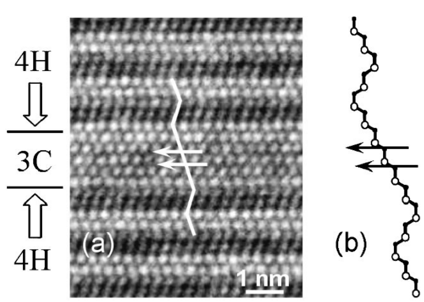

FIG. 1. (a) Cross-sectional TEM image of a 3*C*-SiC inclusion in 4*H* SiC. Arrows indicate the two successive stacking faults that formed the inclusion. (b) Schematic illustration of the atomic stacking along the zigzagged line in (a) (see Ref. 10).

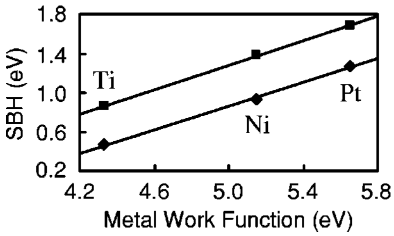

FIG. 2. The dependence of macroscopic SBH on metal work function, from conventional diode I-V measurements. Upper line: untransformed region, slope=0.625; lower line: transformed region, slope=0.605. The SBH value is actually an extrapolation to unity ideality factor, to account for discrete patches of low SBH due to defects other than the 3C inclusions (Ref. 6). These patches are commonly present even in the absence of any 3C inclusions (Ref. 14).

Okojie *et al.*[5] for the same type of inclusions. Figure 2 shows a comparison of the macroscopic Schottky barrier height (MSBH) measured by conventional diode I-V measurements on transformed (upper line) and untransformed regions (lower line) of similar wafers as a function of the metal work function. We see that the MSBH's are $\sim$0.41 eV lower on the transformed regions, but remarkably both regions exhibit a strong dependence on metal work function with essentially the same slope. This indicates that Fermi-level pinning by interface states is weak and not significantly affected by the transformation.

Cleaved and oxide-stripped pieces from the transformed region of a wafer were then studied by BEEM. The wafer surface was degreased, cleaned with two cycles of 30 min ultraviolet ozone oxidation and 2 min etching in 1:10 HF:H_2O, and then introduced into an ultrahigh vacuum (UHV) chamber and outgassed overnight at $<230\,^\circ$C. Two sets of Schottky diodes were made *in situ* by depositing $\sim$8 nm and $\sim$4 nm Pt films, respectively, through a shadow mask at room temperature using e-beam evaporation. After each deposition, the samples were transported in UHV into an adjacent chamber (base pressure $\sim 1\times10^{-10}$ Torr) where BEEM measurements were performed at room temperature.

BEEM is an extension of scanning tunneling microscopy (STM) that can probe the electronic transport properties of M/S interfaces with nm-scale spatial resolution and $<$10 meV energy resolution.[11] The STM tip (at a voltage$-V_T$ relative to the metal) injects hot electrons into a metal overlayer film with an energy distribution that depends on V_T. The BEEM signal consists of the fraction of injected electrons that crosses the metal film and local Schottky barrier and is ‘‘collected’’ from the semiconductor substrate as a BEEM current I_c. The local SBH and additional information of the semiconductor conduction band structure can be obtained by measuring a BEEM spectrum (i.e., a BEEM $I_c - V_T$ curve) and fitting it to the Bell-Kaiser model.[11] We have previously studied Pt diodes on n-type bulk 4H SiC using BEEM and found a SBH of 1.58 ± 0.03 eV and a second CBM at $\sim$0.14 eV higher energy.[15]

Most BEEM measurements on the transformed SiC samples measured at random locations show a local SBH of 1.54 ± 0.02 eV and a second CBM at $\sim$0.13 eV above the first one, which are close to our earlier results on bulk 4H SiC mentioned above. The slight difference in the SBH is probably due to lower signal-to-noise in our earlier study.[15] However, if we search for BEEM current at a $V_T=1.5$ V (just below the bulk 4H-SiC SBH), we can easily locate where the 3C-SiC inclusions intersect the Pt-SiC interface. Figure 3(a) is a $(100\text{ nm})^2$ STM topographic image of the top metal surface of a diode made with a 8-nm-thick Pt film, and shows no particularly distinctive features other than $\sim$6 nm diameter Pt crystallites, which are normal for polycrystalline thin metal films. Figure 3(b) is a simultaneously measured BEEM image (a plot of local BEEM current vs tip location) at $V_T=1.5$ V, and shows a straight stripe of strongly enhanced BEEM current. This indicates a region of reduced barrier height as compared with bulk 4H SiC.

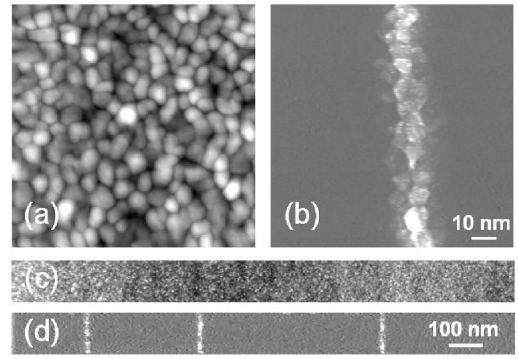

FIG. 3. (a) $(100\text{ nm})^2$ STM image of an 8-nm-thick Pt film on transformed 4H SiC, taken at $V_T=1.5$ V, $I_T=5$ nA. Gray scale: 4 nm. (b) Simultaneous BEEM image. Gray scale: 1 pA (the gray areas have zero BEEM current). (c) 1500 nm$\times$125 nm STM image on the same metal film. (d) Simultaneous BEEM image. The bright stripes in (b) and (d) correspond to low-SBH regions.

Many similar stripes of reduced barrier height were observed on the sample. They were all straight, parallel to each other [as shown in Fig. 3(d)], and longer than our largest BEEM images of $\sim$1.6 μm. The measured orientation and average spacing ($\sim$500–600 nm) of these stripes agrees well with expectations based on the known surface miscut (c-axis tilted 8° toward the wafer minor flat) and the $\sim$77 nm average separation between the planar inclusions in the bulk (the expected spacing along the wafer surface is $\sim$77 nm/sin 8°$\approx$550 nm). The orientation of the stripes also matches that of the bright stripes observed in secondary electron images of the transformed part of the bare wafer.[6] A small ($<$0.5 nm) topographic depression was often observed to coincide with the bright stripes in BEEM. However, similar depressions were also observed at locations with no extra BEEM current or reduced barrier height, and are probably due to atomic steps that existed on the vicinal wafer surface before Pt deposition.

BEEM spectra measured away from the stripes (rightmost curve in Fig. 4) were always like those of normal Pt/4H-SiC contacts with a local SBH of 1.54 ± 0.02 eV, confirming that most of the sample surface ($\sim$95%) looks just like untransformed, bulk 4H SiC. However, directly over the stripes (leftmost curve in Fig. 4), BEEM spectra yielded a local SBH of 1.01 ± 0.03 eV. Around the stripe boundaries

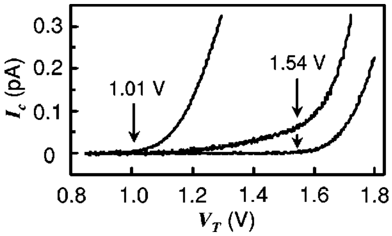

FIG. 4. Typical averaged BEEM I_c-V_T curves (average of 53 to 95 individual $I_c - V_T$ curves taken at the same locations with 10 nA tunnel current). Left: Measured on an enhanced-BEEM stripe (scaled by a factor of 0.25). Right: away from a stripe. Middle: on the boundary of a stripe. Arrows indicate SBH's determined by fitting the data. Fitted curves are not shown here because they are almost completely overlapped by the measured data.

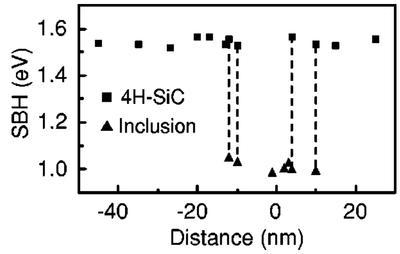

FIG. 5. SBH measured at different distances from enhanced-BEEM stripe center. No significant SBH variation is observed across the stripe. Dashed lines indicate where $4H$ and QW SBH's were simultaneously measured.

(middle curve in Fig. 4), BEEM data appear to be a superposition of the two spectral types above, probably due to the finite spatial resolution of the BEEM technique caused by multiple elastic scattering of hot BEEM electrons in the metal film.[16] If we fit these boundary spectra as a superposition of two spectra, we obtain essentially the same two SBH's ($\sim$1.54 eV and $\sim$1.01 eV) as found far from the inclusions and directly over them, respectively. Our measured local SBH reduction of $\sim$0.53 eV is fairly close to the $\sim$0.41 eV reduction observed by *macroscopic* diode I-V measurements (Fig. 2) on transformed regions.[6]

We believe that our measured $\sim$0.53 eV local reduction in SBH over the $3C$ inclusions represents a direct local estimate of the lowest quantum well state energy, with respect to the bulk $4H$-SiC CBM. First, we note that to measure a BEEM current over the inclusions, the hot BEEM electrons *must enter a propagating state* in order to reach the substrate interior and be collected as BEEM current. Hence our measurements of a reduced SBH on the inclusions are not simply due to a localized interface state close to the inclusions. Second, the inclusions and surrounding $4H$ regions are both entirely in depletion close to the M/S interface. Hence there is negligible screening by free carriers near the interface that would affect the local interface potential (this is not true deep in the bulk beyond the depletion region, where the QW should be filled with electrons[9]).

An important third issue is whether the M/S interface near the inclusions has a different pinning strength and/or charge neutrality level than the rest of the M/S interface, because this could cause the measured SBH reduction at the inclusions to differ from the actual QW binding energy. As discussed earlier, however, the data in Fig. 2 indicate that interface pinning is essentially the same (and rather weak) on both the transformed and untransformed parts of the sample. Since diode I-V measurements are dominated by low barrier-height regions of a sample,[17] Fig. 2 gives strong evidence that any interface-state pinning is nearly the same near the inclusions as it is over the rest of the M/S interface. Theoretical calculations also indicate that stacking-fault-induced inclusions (and polytypism in general) affect only the conduction band (and not the valence band) energy relative to the vacuum level,[10] suggesting that changes in the SBH should track changes the lowest conduction band energy. This conclusion is consistent with earlier BEEM measurements that indicate that the SBH's on different SiC polytypes indeed track their band gaps to within $\sim$0.05 eV.[15] We use this and our BEEM uncertainties in measured SBH's to roughly estimate an $\sim$0.06 eV uncertainty in our extracted QW energy. On a related issue, a large local variation in fixed charge could also shift the local SBH relative to the rest of the M/S interface. To check for local fixed charge, we measured systematic profiles of the $4H$-SiC SBH as a function of distance from an inclusion (see Fig. 5). These profiles show no significant systematic lateral variation in the $4H$-SiC SBH as the inclusion is approached, even for BEEM spectra measured over the boundary region where the $4H$ and QW SBH's can be measured simultaneously. We also note that no significant accumulation of dopant atoms at inclusions is expected during the 1150 °C oxidation step since diffusion of N atoms in SiC is known to be extremely slow even up to 1700 °C.[18]

Fourth, although it has been predicted that spontaneous polarization in $4H$ SiC (Ref. 19) produces an electric depolarization field across a $3C$ inclusion,[1,20] electrostatic considerations indicate that such a depolarization field should produce the same QW energy (relative to the local $4H$ CBM) close to a M/S interface as in the bulk. Finally, we note that our measured QW energy of $\sim 0.53 \pm 0.06$ eV below the CBM of $4H$ SiC is fairly close to a QW energy of $\sim$0.60 eV below the $4H$ CBM calculated recently by Iwata *et al.*[10,20] for this kind of double-stacking-fault $3C$ inclusion.

BEEM measurements with a 4-nm-thick Pt film yielded the same $4H$ and QW SBH's as with an 8-nm-thick film, but had BEEM current magnitudes more than twice as large in general. We also found that the apparent average width of the enhanced BEEM stripes (average full width at half maximum at $V_T = 1.5$ V) was $\sim$8 nm with the 4 nm-thick Pt film, as compared with $\sim$10 nm with the 8-nm-thick film. This is an indication that the apparent width of the enhanced BEEM stripes is broadened by multiple quasielastic scattering in the metal overlayer, and that the true width of the QW opening at the Pt/SiC interface is significantly smaller than 8 nm. Determining the true size of the QW opening is a topic of ongoing measurement and modeling.

In summary, we have used BEEM to directly identify and characterize individual QW structures formed by double-stacking-fault $3C$-SiC inclusions in $4H$ SiC, and find the 2D

CBM of these QW states to be ~0.53 eV below the bulk 4*H* CBM. Macroscopic diode *I-V* and microscopic BEEM measurements indicate that there is little variation of interface state density or fixed charge across the inclusions. Our study also suggests that BEEM measurements made on manually-cross-sectioned semiconductor heterostructures may be able to probe 2D conduction bands of individual QW's, even if they are not accessible to ''plan-view'' BEEM.

The authors thank H. Iwata for helpful discussions. The work at The Ohio State University was supported by the Office of Naval Research under Grant No. N00014-93-1-0607 and the National Science Foundation under Grant No. DMR-0076362. The work at Arizona State University was supported by the National Science Foundation under Grant No. ECS-0080719, and by a Motorola Semiconductor Products Sector Sponsored Project.

*Electronic address: jpelz@mps.ohio-state.edu

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