Quantum-well energy of 3C-SiC inclusions embedded in 4H-SiC determined from capacitance-voltage curves and electrostatic potential modeling

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We have compared capacitance-voltage (C-V) measurements with finite element electrostatic modeling of process-induced double-stacking-fault 3C-SiC inclusions in 4H-SiC, which act as self-forming electron quantum wells. The modeling shows that the remarkable decrease in the Schottky barrier height observed by C-V measurements can be explained by the free carrier charging of the inclusions in the epilayer bulk. From the C-V measurements and the measured inclusion density, the energy of the quantum well conduction band is estimated to be ~ 0.51 eV below the host 4H-SiC conduction band.

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SiC is a wide band gap semiconductor which has a large potential in applications to high-temperature, high-frequency, and high-power electronic devices. Recently, it was found that stacking faults (SFs) lying in (0001) hexagonal basal planes can form in 4H- and 6H-SiC p-n diodes under high current operation,\textsuperscript{1,2} and also in 4H-SiC with heavily n-doped epilayers\textsuperscript{3} or substrates\textsuperscript{4,5} during high temperature processing. These SFs produce a local 3C (cubic) stacking, and hence behave as thin 3C planar inclusions embedded in hexagonal host material. Because of the large band gap difference (but very little difference in the valence band structure) between 3C and hexagonal SiC, the 3C inclusions are expected to behave as electron quantum wells (QWs). This QW nature of the inclusions was shown in luminescence measurements\textsuperscript{3,4,6} and electronic structure calculations,\textsuperscript{7} and recently confirmed by local ballistic electron emission microscopy (BEEM) measurements.\textsuperscript{8}

Epitaxial 4H layers are typically grown on substrates tilted 8\textdegree{} off axis to ensure polytype stability, so that the SF’s are “inclined” and they intersect the sample surface, as shown in Fig. 1(a). As a result, the inclusions can affect surface and interface behavior, as well as bulk behavior. Skromme \textit{et al.} recently reported that samples with “double-SF” type inclusions strongly reduce the Schottky barrier height (SBH) measured by both conventional current-voltage (\textit{I-V}) and capacitance-voltage (\textit{C-V}) methods by 0.37-0.47 eV.\textsuperscript{4} The \textit{I-V} result is not so surprising, since the local SBH was found to be locally reduced by \textasciitilde{}0.53 eV over the \textasciitilde{}2\% of the sample contact area where the inclusions intersect the metal interface,\textsuperscript{8} and it is known that even a small area fraction of low SBH will dominate \textit{I-V} measurements.\textsuperscript{9} However the similar reduction measured by \textit{C-V} profiling is more surprising, as \textit{C-V} determined values are generally assumed to be much more representative of \textit{average} barrier properties.\textsuperscript{9}
In this letter, we report finite-element modeling (FEM) of expected $C-V$ curves of Schottky diodes on 4H-SiC with inclined double-SF 3C inclusions, which are directly compared with in-situ $C-V$ and BEEM measurements. We show that the $C-V$ measurements are actually dominated by charging of the SF inclusions away from the interface, which is determined by the depth of the QW energy levels in SF inclusions. Hence $C-V$ measurements can be used to measure the two-dimensional (2D) conduction band minimum (CBM) energy of the QW inclusions deep in the bulk of the host 4H-SiC epilayer. If we assume that spontaneous polarization (SP) exists in the 4H host$^{10,11}$ with the strength recently reported by Bai et al.,$^{11}$ we estimate the 2D CBM of a double-SF QW inclusion to be at $\Delta E_{QW} \cong 0.51$ eV below the bulk 4H-SiC CBM. If we neglect SP in the 4H host, we estimate $\Delta E_{QW} \cong 0.59$ eV. These estimates of the QW energy are in good agreement with the $\sim 0.60$ eV estimate made from bulk electronic structure calculations,$^7$ and with the experimental estimate of $\sim 0.53$ eV measured on inclusions near the metal/SiC interface.$^8$ In general, this modeling shows that for a sample with this kind of inclined multi QW structure, $C-V$ measurements can be used to estimate the QW energy in the bulk of the host crystal.

The 4H-SiC samples used in this study$^{4,8}$ had a 2 µm lightly $n$-type N-doped ($1 - 1.5 \times 10^{17}$ cm$^{-3}$) epilayer on a heavily N-doped ($\sim 3 \times 10^{19}$ cm$^{-3}$) $n$-type Si-face substrate, with a surface miscut by 8° from the basal plane. Some of the double SF’s formed in the substrate during a 90 min. thermal oxidation$^4$ at 1150 °C extend into the epilayer and up to the sample surface, as illustrated in Fig. 1. The $I-V$ and initial $C-V$ SBH measurements made with different metals on similar wafers were presented elsewhere.$^4$ For the measurements presented here, samples were stripped of their oxide and cleaned,$^8$ introduced into our UHV chamber, and then $\sim 8$ nm thick,
0.5 mm diameter Pt dots were electron-beam evaporated through a shadow mask to form Schottky diodes. The BEEM and C-V measurements were done in-situ after Pt deposition.

Figure 2 shows a typical C-V measurement made on one of these Schottky diodes, plotted as 

\( \frac{1}{C^2} \) vs. applied reverse bias \( V_r \). For a uniform Schottky barrier, the slope of this line is related to the semiconductor doping, and the intercept voltage \( V_i \) is related to the SBH.\(^{13}\) We measured the “C-V determined” reduction in the SBH (as compared to similarly prepared diodes made on a peripheral part of the wafer without inclusions\(^4,8\)) to be \( \Delta \phi_{SBH-CV} \approx 0.48 \) V and 0.43 V for two different Schottky diodes, which we denote as Diode A and Diode B, respectively. These values for \( \Delta \phi_{SBH-CV} \) are consistent with the reduction reported by Skromme et al.\(^4\) We also measured \( \Delta \phi_{SBH-CV} \) for ~10 Ni Schottky diodes at various locations on a similar wafer, with a varying density of inclusions which we could estimate from secondary electron images of inclusions around the Ni diodes.\(^{14}\) We observed a strong, nearly linear decrease of up to ~0.58 V in the C-V determined SBH with increasing relative inclusion density. These Ni diode data will be described in detail elsewhere.

Figure 1(b) shows a BEEM image of Diode A, which reveals the subsurface inclusions as bright lines in the image.\(^8\) We measured a large number of such BEEM images across each diode, from which we estimated the average lateral spacing between the intersections of inclusions with the sample surface to be \( s \approx 570 \) nm and 680 nm for Diode A and Diode B, respectively.\(^{15}\)

Finite element electrostatic modeling (using the commercial software package FlexPDE\(^{16}\)) was used to calculate expected potential profiles through the sample, and also expected C-V curves. The sample geometry is illustrated in Fig. 1. We define the total “electron potential” in the 4H-SiC host and QW regions respectively as \( \phi_{tot-4H} = \phi(x,y,z) + \phi_{4H} \) and \( \phi_{tot-QW} = \phi(x,y,z) + \)
\( \phi_{QW} \), where \( \phi(x,y,z) \) is the electrostatic electron potential determined by solving the Poisson Equation
\[
\nabla^2(\phi) = -\rho(x, y, z) / \varepsilon \varepsilon_0 ,
\]
where \( \rho(x,y,z) \) is the charge distribution inside the epilayer, and \( \phi_{4H} (\phi_{QW}) \) is a fixed offset potential when an electron is in the 4H (QW) regions of the epilayer. Note that \( \phi_{QW} \) includes quantum confinement energy. We choose the Fermi level in the metal as the reference potential, so \( \phi(x,y,0) = 0 \) at the metal interface. The local SBH (which is the energy of the CBM at the metal/semiconductor interface) is then given by \( q \phi_{4H} \) and \( q \phi_{QW} \) over the 4H and QW regions, respectively. The energy difference \( \Delta E_{QW} \) between the lowest allowed conduction band states in the 4H and QW regions is \( \Delta E_{QW} = (q \phi_{4H} - q \phi_{QW}) \). We choose \( q \phi_{4H} = 1.60 \text{ eV} \) to match the measured SBH from the C-V curves on 4H-SiC regions of the metal/SiC interface far from any QW.\(^{17} \) The single free parameter in our modeling is \( \Delta E_{QW} \), which we adjust in order to match the measured C-V curves. Here, \( \varepsilon \) is the static dielectric constant of SiC (\( \sim 9.7 \) for both 3C- and 4H-SiC\(^{18} \)), \( \varepsilon_0 \) is the vacuum permittivity, \( \rho(x,y,z) = q[N_d - n_s(x,y,z)] \), \( N_d \) is the donor density (measured from C-V curves), and \( q \) is the elementary charge. The free carrier (electron) density in the 4H-SiC host is given by\(^{13} \)
\[
n_e (x,y,z) = \left( M_c / 4 \right) \left( 2m^* k_B T / \pi h^2 \right)^{3/2} \exp \left[ (E_F - q \phi_{tot-4H}) / k_B T \right],
\]
where \( M_c = 3 \) is the number of equivalent minima\(^{19} \) in the conduction band of 4H-SiC, \( m^* \approx 0.39 \) \( m_0 \) is the effective electron density-of-states mass in 4H-SiC,\(^{19} \) \( m_0 \) is the free electron mass, \( T \) is the sample temperature, \( h \) is the reduced Planck’s constant, and \( k_B \) is Boltzmann’s constant. Inside the QW’s, we have
\[
n_e (x,y,z) \approx \sigma_{QW} / d , \text{ where } \sigma_{QW} = \left( M_c m^*_i k_B T / \pi h^2 \right) \ln \left[ 1 + \exp \left( (E_F - q \phi_{tot-QW}) / k_B T \right) \right] \text{ is the sheet electron density in a QW},
\]
and \( m^*_i \approx 0.36 \) \( m_0 \) is the in-plane effective density-of-states mass in 3C-SiC.
inclusions in the hexagonal basal plane. Here we assume the QW electron density is uniformly spread throughout the \( d \approx 1.25 \) nm width of the double SF QW.

Figure 3 shows calculated profiles (assuming SP in 4H-SiC with the reported value\(^{11}\) of \( 1.1 \times 10^{-2} \) C/m\(^2\)) of the total electron potential energy along a particular path perpendicular to the M/S interface (shown as the dotted line in Fig. 1(a)), for a pure 4H-SiC epilayer (dashed line) and for an epilayer with inclusions (solid line). Since the symmetry of 3C-SiC forbids SP, there should exist a large “depolarization” electric field across the thin cubic inclusions.\(^{11,12}\) Note that the solid line represents the \textit{three-dimensional} (3D) CBM for bulk 4H- and bulk 3C-SiC, while the horizontal dotted lines represent the 2D CBM of the QW states, including quantum confinement energy. We see that the band bending in the sample with inclusions is decreased overall with respect to the pure 4H-SiC sample, so that the conduction band of the 4H-SiC host is held well above the semiconductor Fermi level far from the interface, and is therefore depleted of electrons.\(^{20}\) This is due to \textit{charging} of the 2D QW conduction band at a depth where its CBM approaches the Fermi level \( E_F \), until the net QW negative charge effectively balances the surrounding positive donor charge.\(^{20}\) In essence, the QW charging reduces the \textit{effective depletion width} \( L_{\text{eff}} \) (Fig. 1) and overall band bending as compared to the sample without inclusions, and hence \textit{decreases the intercept voltage} \( V_i \) \textit{measured from C-V curves} (Fig. 2). If one uses the standard relation\(^{13}\) for a \textit{uniform} SB: \( \phi_{\text{SBH-CV}} = V_i + V_n + k_B T/q \) (where \( qV_n \) is the doping-dependent energy difference between the CBM and \( E_F \), deep in a \textit{uniform} semiconductor material), then it \textit{appears} that the SBH is reduced. However, the true SB at the metal interface actually has the full 4H value over \( \sim 98\% \) of the interface.

Since the measured value \( \phi_{\text{SBH-CV}} \) depends on the energy \( \Delta E_{\text{QW}} \), we should be able to quantify \( \Delta E_{\text{QW}} \) from \( C-V \) measurements, provided we know the average inclusion spacing. To do
this, the finite element program was used to calculate the net charge $Q$ that accumulates on the metal film as a function of the reverse bias voltage, then $C$ was determined from $C = (dQ/dV)$.

The solid line in Fig. 2 shows a calculated $C-V$ curve assuming $\Delta E_{QW} = 0.50$ eV and the average perpendicular inclusion spacing $s_{\perp} = \sim 95$ nm (in the bulk) we measured for Diode $B$. The value $\Delta E_{QW} = 0.50$ eV was chosen to give the same calculated intercept voltage as measured for Diode $B$. The dashed curve shows a $C-V$ curve calculated in the same way, but assuming a pure 4H-SiC epilayer. We see that the two curves are both nearly straight lines with essentially the same slope, but with different intercepts. For Diode $A$ (with a measured perpendicular inclusion spacing $s_{\perp} = \sim 79$ nm) we found the best fit value $\Delta E_{QW} = 0.52$ eV. These estimates are close to the calculated value $\Delta E_{QW} = 0.60$ eV, and the measured value $\Delta E_{QW} = 0.53$ eV determined by BEEM. We note that the BEEM estimate represents the QW energy measured very close to the metal/SiC interface, while the $C-V$ estimate is for the QW energy deep in the bulk. To check for self-consistency, we took the FEM-calculated profile of $\phi_{tot}$ (assuming SP is present) across an inclusion deep in the bulk (along a path perpendicular to the plane of the inclusion), and then numerically solved the one-dimensional Schrödinger equation to find a value $\Delta E_{QW}$ of $\sim 0.55$ eV. This result is in good agreement with the value determined from $C-V$ measurements.

Although theory and experiments indicate that SP exists in 4H-SiC, we have also done FEM calculations assuming that no SP exists in the 4H host. In this case the calculated $C-V$ curves match the measured data with $\Delta E_{QW} = 0.60$ eV for Diode $A$, and $\Delta E_{QW} = 0.58$ eV for Diode $B$. We see that the value of $\Delta E_{QW}$ obtained from $C-V$ measurements depends rather weakly on assumed strength of SP in the 4H-SiC host.

In summary, we have used finite element electrostatic modeling of a 4H-SiC with embedded double-SF cubic inclusions to explain the remarkable decrease in the macroscopic SBH observed
in C-V measurements. We further showed that these C-V measurements can be used to
determine the energy depth of the QW conduction band deep in the host epilayer. The obtained
estimates of ~0.51 eV (with SP) or ~0.59 eV (neglecting SP) are quantum mechanically self-
consistent, and agree well with calculations and with the estimate of ~0.53 eV measured close to
the metal/SiC interface by BEEM.8

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REFERENCES


Considering the 8° miscut, the average perpendicular spacing between inclusions in the bulk is $s_\perp \sim 79$ nm (Diode A) and $s_\perp \sim 95$ nm (Diode B).

The SBH measured from BEEM is smaller (~1.54 eV) due to image force lowering (Ref. 13).

References:


FIG. 1. (a) Schematic cross-sectional view of sample showing the 3C inclusions (grey+black lines) which start to fill with electrons at the depth $L_{\text{eff}}$ below the interface, while the surrounding 4H area remains depleted even in the bulk. (b) BEEM image (taken with –1.5 V tip voltage) of a Pt/4H-SiC sample with embedded 3C inclusions. The bright straight lines show reduced SBH where the 3C QW inclusions intersect the metal/SiC interface. More details are given in Ref. 8.
FIG. 2. Measured (□) and calculated (→) C-V curve on Diode B. C-V calculation done assuming SP at a level of ~1.1×10^{-2} C/m² in the 4H-SiC host crystal, doping \( N_d = 1.38 \times 10^{17} \text{ cm}^{-3} \), inclusion spacing \( s_\perp = 95 \text{ nm} \), and \( \Delta E_{QW} = 0.50 \text{ eV} \). The dashed line is the calculated C-V curve for 4H-SiC without inclusions, assuming the same doping. Essentially identical calculated C-V curves are obtained if SP is not present, but with \( \Delta E_{QW} = 0.58 \text{ eV} \).
FIG. 3. Calculated electron potential energy profiles for Diode A along the particular path perpendicular to the metal/SiC interface shown as a dotted line in Fig. 1(a). The solid line represent the three-dimensional CBM for bulk 4H- and 3C-SiC, while the horizontal dotted lines represent the two-dimensional CBM of the QW states, including quantum confinement energy. The overall band bending is decreased with respect to pure 4H-SiC (dashed line) by charging of the QWs deep in the bulk, with a corresponding reduction in $C-V$ measured SBH. Inset: close-up view of QW profile around an inclusion.