Nanometer-Scale Investigation of Schottky Contacts and Conduction Band Structure on 4H-, 6H-, and 15R-SiC using Ballistic Electron Emission Microscopy

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Abstract: We have performed ballistic-electron emission microscopy (BEEM) of Pd and Pt Schottky contacts on 6H- and 4H-SiC and Pd Schottky contacts on 15R-SiC. Measured Schottky barrier heights (SBH’s) appear spatially uniform up to the fitting error due to noise (~0.03 and ~0.1 eV for 6H- and 4H-SiC, respectively). In 4H-SiC, we observed an additional conduction band minimum (CBM) ~0.14 eV above the lowest CBM, which is in good agreement with our band theoretical calculation. Preliminary results on Pd/15R-SiC indicate a higher CBM ~0.5 eV above the lowest CBM, and possibly another higher CBM ~0.3 eV above the lowest CBM. Also, in Pd/15R-SiC, large variations in BEEM spectra at different locations were observed, suggesting an inhomogeneous interface. Additionally, we sometimes observed enhancement in ballistic transmittance over regions intentionally stressed by hot electron injection.

We report ballistic-electron emission microscopy (BEEM) measurements of Pd and Pt Schottky contacts on 6H- and 4H-SiC, and Pd contacts on 15R-SiC. The BEEM technique is an extension of scanning tunneling microscopy (STM) and can be used to probe local electronic properties of buried metal/semiconductor interfaces with nanometer-scale spatial resolution and high energy resolution [1,2]. Figure 1 shows the schematic experimental setup with corresponding energy-level diagrams for BEEM. The STM tip is used to inject hot electrons into a thin metal film, with the hot-electron peak energy controlled by the applied tip bias $V_T$. Provided the metal film is thin enough compared with the electron mean free path, a small fraction of these electrons can cross the metal film elastically and can enter the semiconductor conduction band if injected with sufficient energy. Hence, the local Schottky barrier height (SBH) [3] $qV_B$ can be directly determined by measuring BEEM $I_c-V_T$ curves (also called BEEM spectra) and evaluating the threshold voltage $V_{th}$ for

Fig. 1: (a) Physical setup of the BEEM experiment on SiC and (b) the corresponding energy level diagram (only the lowest CBM is shown). By measuring the dependence of $I_c$ (flux of ballistic electrons from the STM tip into the SiC) on tunnel voltage $V_T$ (at constant tunnel current $I_T$) we can probe the local Schottky barrier height and SiC band structure.
non-zero BEEM current. If higher conduction band minima (CBM’s) exist in the semiconductor band structure, each CBM will be associated with an onset of additional BEEM current $I_c$ at a tip bias corresponding to the energy of that CBM [2].

2 µm-thick epilayers of 6H-, 4H-, and 15R-SiC grown using chemical vapor deposition (CVD) were used in our experiments [4]. These samples consisted of a highly $n$-doped (using nitrogen) 5x5 mm$^2$ substrate ($N_D \sim 5 \times 10^{18}$ cm$^{-3}$) and $n$-doped epi-layers ($N_D \sim 3 \times 10^{16}$ cm$^{-3}$). The samples were cleaned by cycles of sacrificial oxidation and etching steps. After outgassing in ultra-high vacuum (UHV) at < 230 °C, a Pd or Pt film 6-10 nm thick was deposited by e-gun evaporation through a shadow mask producing an array of 0.5 mm diameter circular dots. The samples were then transported in UHV into the STM/BEEM chamber, where the dots were individually gently contacted with a thin Au wire. The dots exhibiting the best ideality factor [3] (< 1.1) were then used in our BEEM measurements [5].

BEEM $I_c-V_T$ curves were taken at different locations of the sample separated by 20 nm or more. We first consider possible spatial variation of the SBH, investigated by analyzing individual $I_c-V_T$ curves. The BEEM $I_c-V_T$ curves were fit using the Bell-Kaiser (BK) model to extract local SBH’s [2]. In the 6H-SiC sample, spatial inhomogeneity was measured to be ~0.03 eV which is roughly the same as the fitting error due to noise in the individual $I_c-V_T$ curves (See Fig. 2). Thus any “real” variations are less than ~0.03 eV. In 4H-SiC, the spatial inhomogeneity of SBH was estimated to be less than ~0.1 eV, with the larger uncertainty resulting from larger fitting errors for the 4H-SiC data [5].

In order to determine the average SBH more accurately, 125—175 $I_c-V_T$ curves are averaged together to improve signal-to-noise. Representative averaged BEEM spectra (open circles) for Pd are shown in Fig. 3 for 6H-SiC and 4H-SiC. Each spectrum shows distinct thresholds, the lowest of which represents the Schottky barrier height. Solid curves are fits to the BK model, and the arrows indicate the extracted threshold values [6]. Obtained SBH’s for Pd/ and Pt/6H-SiC are in general agreement with reported values using conventional techniques [7,8] although previously reported values measured with X-ray photoemission spectroscopy and conventional I-V curve analysis tend

![Fig. 2: Threshold distributions of (a) 10 nm Pd (grey bars) and (b) 6 nm Pt (transparent with dark borders) Schottky contacts on 6H-SiC as determined from individual BEEM $I_c-V_T$ curves. Standard deviations are ~0.03 V and ~0.04 V for (a) and (b), respectively.](image)

![Fig. 3: BEEM $I_c-V_T$ data (circles) and BK fits (solid curves) for 6—10 nm Pd Schottky contacts on (a) 6H- and (b) 4H-SiC. Arrows designate extracted thresholds. In (b), a best fit with only one threshold is plotted as well (lower solid curve). Pt Schottky contacts with 6H- and 4H-SiC indicate thresholds of 1.34 and 1.58 V, respectively.](image)
to be lower than our values. Our own conventional $I$-$V$ measurements on Pd/6$H$-, Pt/6$H$-, Pd/4$H$-, Pt/4$H$-, and Pd/15$R$-SiC indicate SBH' of 1.27, 1.26, 1.56, 1.48 eV, and 1.22 eV, respectively.

We next consider the shape of the measured BEEM spectra, and what this can tell us about conduction band structure in SiC. The BEEM spectra on 6$H$-SiC are fit quite well by the BK model assuming a single threshold, with no evidence of any higher thresholds within ~1 V of the lowest threshold. As discussed above, this indicates there is only a single CBM exists within ~1 eV of the lowest CBM. In contrast, for 4$H$-SiC we observe an additional threshold ~0.14 V above the lowest threshold, suggesting an additional CBM at an energy ~0.14 eV above the lowest CBM. These results are in reasonable quantitative agreement recent band structure calculations done by us [6] and other groups [9,10], providing direct experimental verification of these calculations.

BEEM spectra measured at certain locations on a Pd/15$R$-SiC sample [shown in Fig. 4(a)] suggest the existence of an additional CBM ~0.5 eV above the lowest CBM. However, there is also an indication of another possible CBM at ~0.3 eV above the lowest CBM, as shown by the middle arrow in Fig. 4(a). We should emphasize that these measurements are preliminary, so more data need to be taken and a more thorough comparison with band structure calculation should be done.

In this particular Pd/15$R$-SiC sample, we also observed a very interesting spatial variation of the BEEM spectra. Figures 4(a) and 4(b) show that two qualitatively different BEEM spectra were found at different sample locations. We note that the spectrum shown in Fig. 4(b) looks qualitatively similar to the 6$H$-SiC spectrum shown in Fig. 3(a), with a slightly shifted threshold. A possible scenario is that the sample consists of mostly 15$R$-SiC with occasional inclusions of a 6$H$-SiC polytype. In this regard, we note that this epitaxial SiC sample was actually grown on a substrate which had macroscopically separated regions of the 15$R$- and 6$H$-SiC polytypes. It is possible that there might be some microscopic intermixing of these polytypes as well, which can be resolved using BEEM.

![Fig. 4: BEEM $I_c$-$V_T$ data (circles) and BK fits (solid curves) for 6 nm-Pd/15$R$-SiC taken at two different locations showing (a) “true” 15$R$-type spectrum and (b) “6$H$-like” spectrum. Arrows designate extracted thresholds. In (a), best fits with one and two thresholds are plotted as the first and the second curve from the reference line, respectively.](image)

![Fig. 5: (a) 150x150 nm$^2$ topographic image and (b) corresponding BEEM image of 6 nm Pt/4$H$-SiC contact, measured with $V_T = 2$ V and $I_T = 10$ nA. Grey-scale range is ~5 nm for (a) and ~2 pA for (b). A 40-minute “stressing” scan with $V_T = 10$ V and $I_T = 10$ nA was then done over region outlined by dashed box. (c) and (d) show “post-stress” topography and BEEM image, respectively, and indicate slightly enhanced BEEM current in stressed region.](image)
We also used BEEM to perform preliminary microscopic investigations of hot-electron-induced interface modification of Pt/4H-SiC. We occasionally observed enhanced ballistic electron transmittance (but little change in barrier height) over a region intentionally stressed by injecting high kinetic energy (~10 eV above metal $E_F$) electrons, behavior which may be of importance in certain high-voltage, high-current device applications. Figures 5(a) and 5(b) show the topography of top metal layer and simultaneously taken BEEM image, respectively. A 40-minute long stressing scan was performed over the region designated by a dashed box at tip bias $V_T = 10$ V and tip current $I_T = 10$ nA. Figures 5(c) and 5(d) show “post-stress” topography and BEEM image, respectively. While the surface topography reveals no noticeable change except for small drift, the corresponding BEEM image show a small enhancement over the stressed region. We have not measured noticeable change in SBH over the stressed region. Hallen and co-workers have reported similar enhanced ballistic transmittance on stressed Au/Si Schottky contacts, which was attributed to thinning of an interfacial layer [11]. A similar mechanism may be effective in our experiment.

In summary, we performed BEEM measurements on SiC Schottky contacts and determined local SBH’s from the data. The measured BEEM spectra indicate the existence of higher energy conduction band minima (in addition to the lowest CBM) in 4H-, and 15R-SiC, in agreement with band theoretical calculations. Spatial inhomogeneities of 6H- and 4H-SiC SBH’s were shown to be smaller than the instrumental uncertainties. However, on a particular Pd/15R-SiC sample, we observed indications of a “15R-like” and “6H-like” BEEM spectrum, depending on the sample location. Preliminary microscopic investigations of hot-electron-induced interface modification were performed on Pt/4H-SiC and instances of enhanced ballistic transmittance over a stressed region were observed.

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References:

[4] The SiC epi-layers were grown by L. Rowland at Northrop-Grumman Co.

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