PERGAMON

Solid State Communications 112 (1999) 611–615

solid state communications

www.elsevier.com/locate/ssc

A BEEM study of the temperature dependence of the barrier height distribution in PtSi/n-Si Schottky diodes

S. Zhu[a,b], R.L. Van Meirhaeghe[a,*], C. Detavernier[a], G.-P. Ru[b], B.-Z. Li[b], F. Cardon[a]

[a]*Department of Solid State Sciences, University of Gent, Krijgslaan 281/S1, B-9000 Gent, Belgium*
[b]*Department of Electronic Engineering, Fudan University, Shanghai 200433, People's Republic of China*

Received 10 July 1999; received in revised form 23 August 1999; accepted 25 August 1999 by J.H. Davies

Abstract

Schottky barrier height distributions of a PtSi film on n-Si(100) are directly measured by ballistic electron emission spectroscopy at temperatures ranging from 180 to 300 K. At any temperature, the measured barrier height distribution can be fitted by a Gaussian function quite well. The mean barrier height decreases with increasing temperature almost linearly with a coefficient of $(-2.6 \pm 0.2) \times 10^{-4}$ eV/K, which is approximately equal to the temperature dependence of the energy band gap of Si, thus suggesting that the Fermi level at the interface is pinned to the valence band edge. The width of the Gaussian barrier distribution is 32 ± 4 meV, without clear dependence on temperature. The results are consistent with the values obtained from traditional *C–V* measurements.

Keywords: A. Semiconductors; A. Surfaces and interfaces; A. Thin films; D. Electronic states (localized)

The temperature dependence of the Schottky barrier height (SBH) in PtSi/Si contacts has been studied by several authors [1–5], due to its importance both for understanding the mechanism of Schottky barrier formation and for applications such as Schottky diodes and infrared detectors. It was found that the SBH of PtSi on both n and p type substrates decreases more or less linearly with increasing temperature between 150 and 300 K, but the reported temperature coefficients (α_Φ) were different. For example, Werner and Güttler [1] measured two PtSi/n-Si diodes using the capacitance–voltage (*C–V*) method and obtained $\alpha_\Phi = -2.52$ or -3.26×10^{-4} eV/K, while they reported $\alpha_\Phi = -0.95 \times 10^{-4}$ eV/K for PtSi/n-Si and $\alpha_\Phi = -1.26 \times 10^{-4}$ eV/K for PtSi/p-Si in another paper [2]. Chin et al. [3] obtained $\alpha_\Phi = -2.7 \times 10^{-5}$ eV/K for p-type PtSi Schottky diodes using the reverse bias *I–V* method, but McCafferty et al. [4] determined α_Φ for p-type PtSi as -1.21×10^{-4} eV/K, and Wittmer [5] stated that α_Φ of n-type PtSi was -4.04×10^{-5} eV/K. These contradictory results require more investigations on the SBH temperature dependence.

On the other hand, spatial imhomogeneity of the SBH at M–S contacts has been thoroughly discussed and many electrical anomalies observed in M–S contacts, such as the dependence of SBH on the measurement method, the temperature dependence of the idealtity factor and a curved Richardson plot, etc. can be explained by assuming a Gaussan distribution of SBH [1,6,7]. The temperature dependence of the mean SBH $\overline{\Phi}_B$ and its standard deviation σ_Φ can be obtained from the standard *I–V*/*C–V* data indirectly, but they have not been determined directly up to now.

Ballistic electron emission microscopy (BEEM) is a well-established method to determine the local SBH on the nanometre scale [8–10]. The spatial and statistical SBH distribution can be directly obtained by BEEM spectra (BEES) measurements. In this letter, the temperature dependence of the SBH distribution in PtSi/n-Si is reported by carrying out BEEM measurements at temperatures ranging from 180 to 300 K.

The samples have been prepared in the following manner: n-type Si(100) wafers with a resistivity of 5–8 Ω cm ($N_d \sim 1 \times 10^{15}$ cm^{-3}) were loaded into a DC magnetron sputtering system immediately after a standard RCA cleaning

* Corresponding author.
E-mail address: roland.vanmeirhaeghe@rug.ac.be (R.L. Van Meirhaeghe)

0038-1098/99/$ - see front matter
PII: S0038-1098(99)00404-4

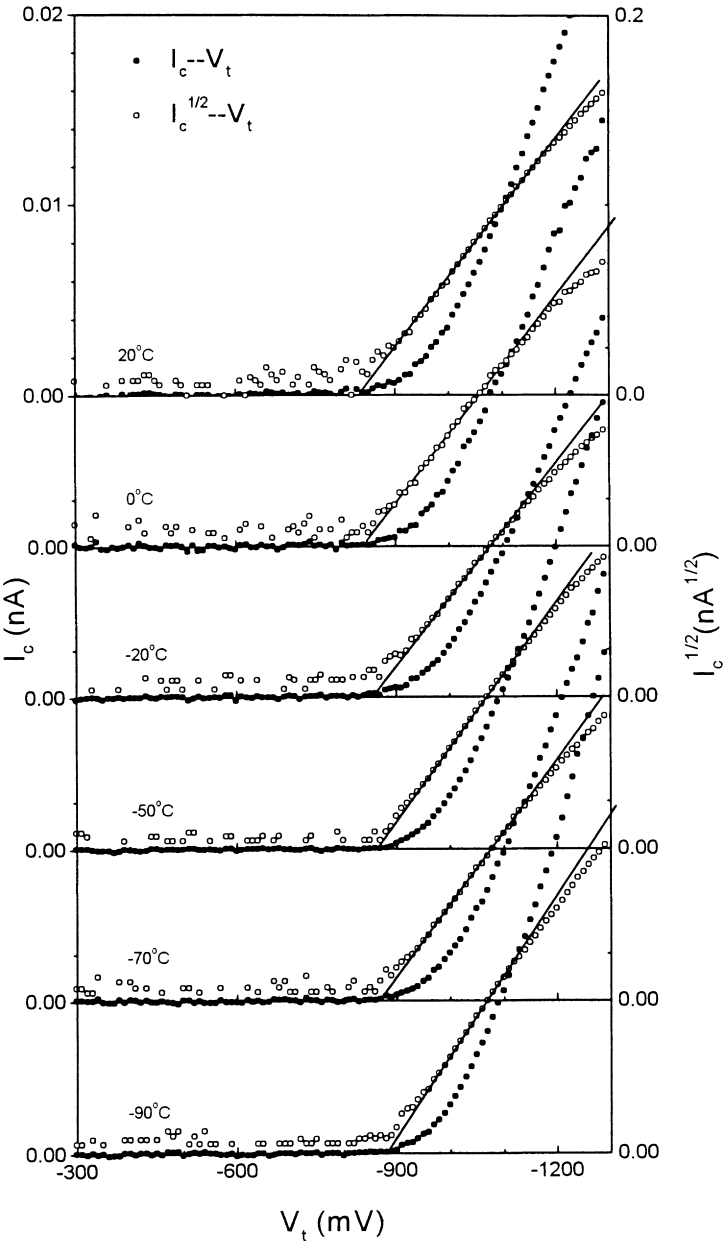

Fig. 1. Typical $I_c(V_t)$ BEEM spectra at different temperatures (solid dot), the local SBHs were extracted from the intercepts of linear extrapolation of the $\sqrt{I_C} \sim V_t$ plots (open dot) on the voltage axis, and adding k_BT for thermal broading correction: 863 meV (20°C); 870 meV (0°C); 877 meV (−20°C); 884 meV (−50°C); 888 meV (−70°C); 896 meV (−90°C).

followed by a diluted HF dip. A tens of nanometer thick Pt layer was deposited. An ultra-thin PtSi film was formed by a two-step process with controlled reaction [11]. Ohmic contact was formed by evaporating a 100 nm thick Ti layer on the backside. Finally, the wafers were cut into small pieces with an area of typical 0.1–0.4 cm^{-2} to obtain PtSi/n-Si Schottky barrier diodes (SBD) for BEEM and *I–V*/*C–V* measurements.

BEEM measurements were performed in an AIVTB-4 system of Surface/Interface using a Pt–Ir tip in air at temperatures ranging from 180 K to room temperature (300 K). The statistical distribution of SBH was obtained by collecting a total of 156 BEEM spectra measured at different points, randomly spread over the contact area with a separation larger than 2 nm. The variation of temperature was less than ±3 K during those

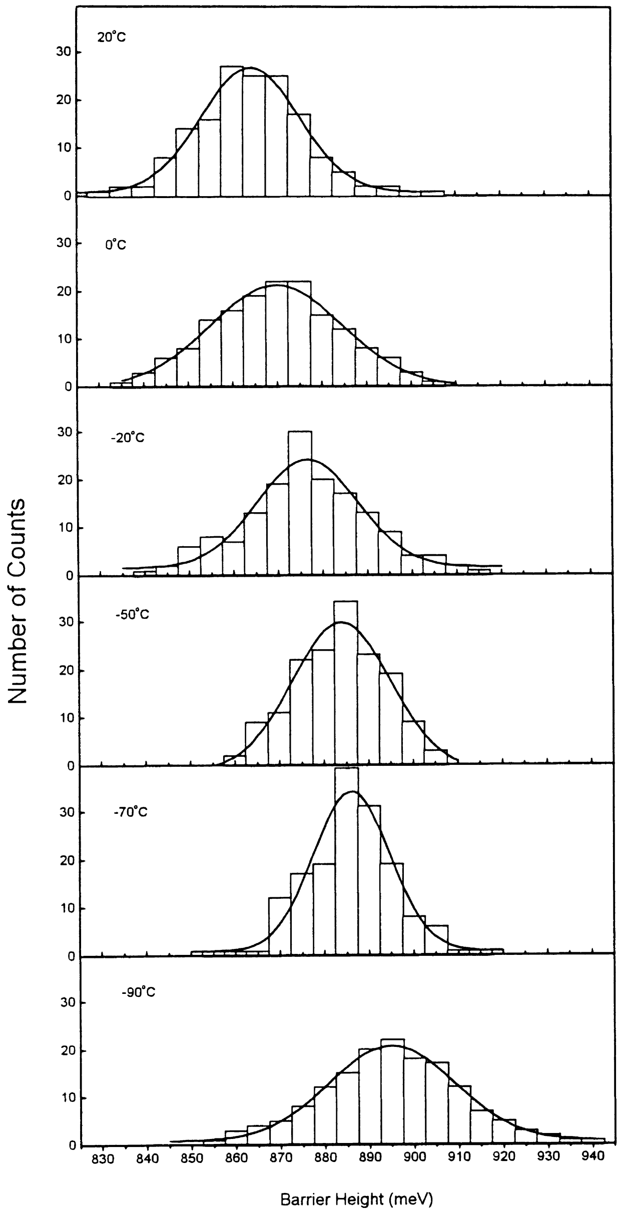

Fig. 2. Statistical distributions of Schottky barrier height of a PtSi/n-Si SBD and their Gaussian fits at different temperatures, the total number of measurements is 156 for each distribution.

measurements. For each spectrum, the tunnel current I_t was maintained constant at 1.5 nA and the tip bias V_t was varied from 300 to 1300 mV with a step of 10 mV. The collector current I_C was measured without an external substrate bias. Typical $I_c(V_t)$ spectra at different temperatures are shown in Fig. 1: (solid dot). To improve the signal/noise ratio, 10–12 scans were taken at the same point. The local SBHs were extracted by linearly fitting the $\sqrt{I_c} \sim V_t$ plots (also shown in Fig. 1: open dot) near the threshold region and adding $k_B T$ (k_B is Boltzmann's constant) for thermal broadening correction, according to a Kaiser–Bell quadratic law [8].

Fig. 2 shows statistical distributions of SBH at different temperatures. The histograms were made by taking the number of counts in intervals of 5 meV. Using other intervals (1–10 meV) did not influence the resulting fits. In all cases, the distribution can be fitted by a Gaussian function quite well. Then $P(\Phi_B)$, the probability of local SBH, has the form [1,3,6,7]: $P(\Phi_B) = (1/(\sigma_\Phi\sqrt{2\pi}))\exp[-((\Phi_B - \overline{\Phi}_B)^2/(2\sigma_\Phi^2))]$, where $\overline{\Phi}_B$ is

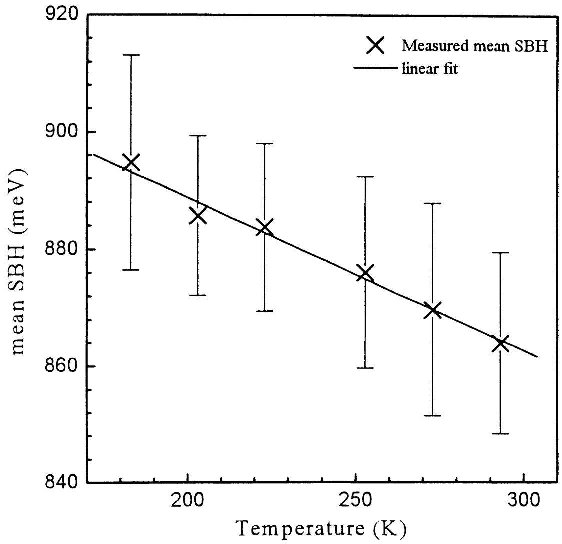

Fig. 3. The mean SBH obtained from Fig. 2 as a function of temperature and a linear fit, the standard deviations were used as error bars.

the mean value of SBH and σ_Φ is its standard deviation.

Fig. 3 gives the $\overline{\Phi}_B$ obtained from Fig. 2 as a function of temperature with the standard deviations (σ_Φ) used as error bars. The $\overline{\Phi}_B$ decreases with increasing temperature almost linearly. Using a straight-line least-square fit, the $\overline{\Phi}_B$ at any temperature can be written as: $\overline{\Phi}_B = \overline{\Phi}_B(0) + \alpha_\Phi T$, where $\alpha_\Phi = (-2.6 \pm 0.2) \times 10^{-4}$ eV/K is the temperature coefficient of the mean SBH, and $\overline{\Phi}_B(0) = 941 \pm 4$ meV is the barrier height extrapolated towards zero temperature, then

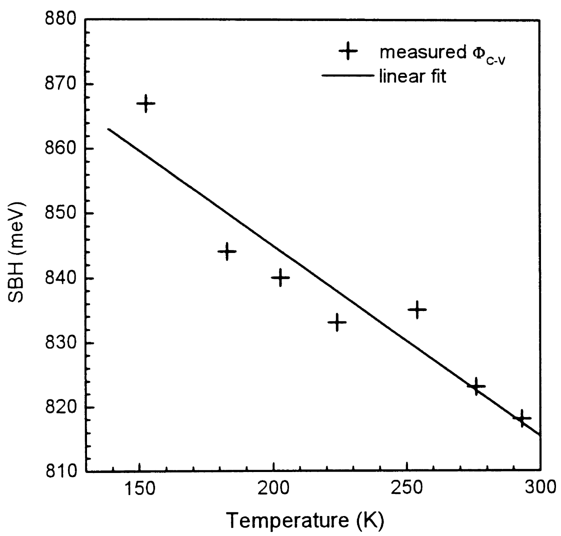

Fig. 4. Barrier heights obtained from C–V measurements ($\Phi_{C\text{–}V}$) as a function of temperature and a linear fit.

the SBH at room temperature is calculated as 0.86 eV, which is in good agreement with the published data (0.87 eV) [12].

To check the above results, a second PtSi/n-Si SBD was measured at 24°C (116 points) and −82°C (170 points). The distribution of SBH can be fitted by one Gaussian function very well for each case with $\overline{\Phi}_B = 854$ meV, $\sigma_\Phi = 36$ meV at 24°C and $\overline{\Phi}_B = 881$ meV, $\sigma_\Phi = 35$ meV at −82°C, respectively. The temperature coefficient can be calculated as $\alpha_\Phi = -2.54 \times 10^{-4}$ eV/K, which is in good agreement with the above result.

The same PtSi/n-Si SBD was also measured by standard I–V/C–V methods at a frequency of 100 KHz between 150 and 300 K. The results are shown in Fig. 4. The barrier height obtained from C–V measurements ($\Phi_{C\text{–}V}$) gives the average barrier height in the contact area without image force lowering. If we ignore the temperature dependence of the Schottky effect lowering, the temperature coefficient of the SBH obtained from C–V measurement ($\alpha_{C\text{–}V}$) is equal to α_Φ. In our experiments, $\Phi_{C\text{–}V}$ decreases with increasing temperature approximately linearly with the temperature coefficient $\alpha_{C\text{–}V} = (-2.9 \pm 0.4) \times 10^{-4}$ eV/K, which is in good agreement with the BEEM results within the experimental error. The I–V characteristics show relatively large ideality factor ($n = 1.4 \sim 1.8$), the SBH derived from the I–V data (Φ_{I-V}) gradually decreases (and the ideality n increases concomitantly) when the diode is cooled, thus the temperature coefficient is positive. This apparent coefficient does not reflect an intrinsic temperature dependence of the SBH but results from the inhomogeneities of the Schottky contact [1,4,7,13,14].

The temperature dependence of the mean SBH is normally explained within the frame of the Fermi-level pinning concept [2,15,16]. According to the band position where the Fermi level is pinned to the temperature coefficient α_Φ will vary from 0 to $\mathrm{d}E_g^i/\mathrm{d}T$, where E_g^i is the energy gap of Si, and $\mathrm{d}E_g^i/\mathrm{d}T \approx -2.4 \times 10^{-4}$ V/K for temperatures between 150 and 300 K [17,18]. Our measured temperature coefficient of PtSi/n-Si is equal to the full band gap value within the measuremental error, which suggests that the barrier height is pinned to the valence band edge. This result is in agreement with the results reported in Refs. [1,3], since the sum of the temperature coefficient for PtSi SBD on n-type and p-type is approximately equal to $\mathrm{d}E_g^i/\mathrm{d}T$, thus makes a negligible small temperature coefficient of PtSi/p-Si SBD.

The standard deviation σ_Φ is another important parameter obtained from BEEM measurements. The average value of σ_Φ is 32 ± 4 meV, and there is no simple dependence of σ_Φ on temperature. According to the pinch-off model [13,14], the low SBH patch is pinched off and the potential at the saddle point which determines the measured SBH increases with increasing temperature, which makes the overall SBH more smooth, thus decreases the standard deviation σ_Φ slightly. However, the thermal uncertainty of the BEEM measurement will increase with increasing temperature, which increases σ_Φ slightly. It can be expected that only a very weak temperature dependence of σ_Φ will result. On the other hand, the σ_Φ is also influenced by the selection of the measurement points, the variation of temperature, the uncertainty of SBH determined from BEES fitting, etc. to that the relatively large uncertainty of σ_Φ obtained from BEEM measurements makes it impossible to determine the relatively weak temperature dependence of σ_Φ.

The small temperature dependence of the apparent SBH obtained from I–V measurements reported by Wittmer [5] and the positive temperature coefficient of Φ_{I-V} observed from our I–V measurements can be partly explained by using a Gaussian distribution of SBH and the parallel conduction model. The apparent SBH obtained from I–V characteristics has the form [1,6]: $\Phi_{I-V} = \overline{\Phi}_B - (\sigma_\Phi^2/(2k_B T/q))$. Using the values of $\overline{\Phi}_B$ and α_Φ obtained from this letter, the temperature coefficient around 260 K is calculated as $\alpha_{I-V} \approx -1.7\times 10^{-4}$ eV/K, which is much smaller than α_Φ. Note that $\overline{\Phi}_B$ and α_Φ are all bias dependent, and taking the effect of a diode series resistance into account, the real apparent $\alpha_{I-V}(\alpha_{I-V} = -4.04\times 10^{-5}$ eV/K, as reported by Wittmer [5]) will be smaller than the above value.

In conclusion, the temperature dependence of the SBH distribution on PtSi/n-Si was directly determined by BEEM measurements. At all temperatures, a Gaussian distribution of SBH was obtained, and the mean SBH decreases with increasing temperature almost linearly with a coefficient close to that of the energy gap of Si, which means that the Fermi level at the interface is pinned to the valence band. The standard deviation shows no clear trend with temperature.

Acknowledgements

The authors would like to thank Mr L. Van Meirhaeghe for his technical support. This work is supported by a bilateral cooperation project Bil 96/74/B017 from the Flemish Ministry of Science and Technology and Technology Ministry of China. C. Detavernier thanks the “Fonds voor Wetenschappelijk Onderzoek—Vlaanderen” (FWO) for a scholarship.

References

[1] J.H. Werner, H.H. Güttler, J. Appl. Phys. 69 (3) (1991) 1522.
[2] J.H. Werner, H.H. Güttler, J. Appl. Phys. 73 (3) (1993) 1315.
[3] V.W.L. Chin, J.W.V. Storey, M.A. Green, J. Appl. Phys. 68 (8) (1990) 4127.
[4] P.G. McCafferty, A. Sellai, P. Dawson, H. Elabd, Solid State Electron. 39 (4) (1996) 583.
[5] M. Wittmer, Phys. Rev. B 43 (5) (1991) 4385.
[6] Y.P. Song, R.L. Van Meirhaeghe, W.H. Laflere, F. Cardon, Solid State Electron. 29 (6) (1986) 633.
[7] S. Chand, J. Kumar, J. Appl. Phys. 82 (10) (1997) 5005.
[8] W.J. Kaiser, L.D. Bell, Phys. Rev. Lett. 60 (14) (1988) 1406.
[9] H. Palm, M. Arbes, M. Schulz, Phys. Rev. Lett. 71 (14) (1993) 2224.
[10] C. Detavernier, R.L. Van Meirhaeghe, R. Donaton, K. Maex, F. Cardon, J. Appl. Phys. 84 (6) (1998) 3226.
[11] R.A. Donaton, S. Jin, H. Bender, M. Zagrebnov, K. Baert, K. Maex, A. Vantomme, G. Langouche, Microelectron. Engng 37/38 (1997) 507.
[12] E.H. Rhoderick, R.H. Williams, Metal-Semiconductor Contacts, 2nd Edition, Clarendon Press, Oxford, 1988, p. 201.
[13] R.T. Tung, Phys. Rev. B 45 (23) (1992) 13509.
[14] J.P. Sullivan, R.T. Tung, M.R. Pinto, W.R. Graham, J. Appl. Phys. 70 (12) (1991) 7403.
[15] J. Tersoff, Phys. Rev. Lett. 52 (1984) 465.
[16] J. Tersoff, Phys. Rev. B 32 (10) (1985) 6968.
[17] W. Bludau, A. Onton, W. Heinke, J. Appl. Phys. 45 (1974) 1046.
[18] C.D. Thurmond, J. Electrochem. Soc. 122 (1975) 1133.