Semicond. Sci. Technol. **18** (2003) 642–646 PII: S0268-1242(03)60611-5

The barrier height inhomogeneity in identically prepared Pb/p-type Si Schottky barrier diodes

Ç Nuhoğlu, Ş Aydoğan and A Türüt

Atatürk University, Faculty of Sciences and Arts, Department of Physics, 25240 Erzurum, Turkey

E-mail: aturut@atauni.edu.tr

Received 10 March 2003, in final form 23 April 2003
Published 21 May 2003
Online at stacks.iop.org/SST/18/642

Abstract
We have studied the experimental linear relationship between barrier heights (BHs) and ideality factors for Pb/p-type Si(100) Schottky contacts with a doping density of about 10^{15} cm^{-3}. The BH for the Pb/p-type Si(100) diodes from the current–voltage (I–V) characteristics varied from 0.686 to 0.735 eV, the ideality factor n varied from 1.054 to 1.191, and from capacitance–voltage (C^{-2}–V) characteristics the BH varied from 0.751 to 0.928 eV. The experimental BH distributions obtained from the I–V and C^{-2}–V characteristics were fitted by a Gaussian function, and their mean BH values were found to be 0.709 and 0.799 eV, respectively. The laterally homogeneous BH value of approximately 0.741 eV for the H-terminated Pb/p-type Si(100) Schottky diodes was obtained from the linear relationship between experimental effective BHs and ideality factors.

1. Introduction

During recent years, the application of surface and interface science techniques has shown that interfaces between metals and semiconductors are complex regions whose physical properties strongly depend on the preparation conditions of the surface [1–6]. Although Schottky interfaces have been well studied for over 50 years, it is only in the past decade that an inhomogeneous contact [4–14] has been considered as an explanation for a voltage-dependent barrier height (BH). As mentioned in [6–15], the BH is likely to be a function of the interface atomic structure, and the atomic inhomogeneities at the metal-semiconductor (MS) interface which are caused by grain boundaries, multiple phases, facets, defects, a mixture of different phases, etc. The existence of small local regions ('patches') with different BHs was evidenced experimentally by using ballistic electron emission spectroscopy (BEES) [15–17]. In the model of Tung *et al* [11, 12], small regions or patches with a lower BH than the junction's main BH were assumed to exist at the junction. As mentioned in the model of Tung *et al* [11] and Sullivan *et al* [12], since the variation in BH may occur even at a scale much smaller than the depletion region width, the interaction between patches should invariably lead to pinch-off of the conduction path of small low BH regions that are surrounded by regions with high Schottky barrier height (SBH). In such cases, the current across the MS contact may be greatly influenced by the presence of the BH inhomogeneity [7–14]. Some studies [6–14] have shown that a variety of inhomogeneity models can be applied to describe the non-ideal Schottky barrier diode (SBD) [7–11]. First, Song *et al* [7] have introduced an analytical potential fluctuation model (a Gaussian distribution of the BHs). Recently, the temperature dependence of the BH and ideality factor in some studies [8–10, 16, 17] has been successfully explained on the basis of a thermionic emission mechanism with a Gaussian distribution of the BHs.

The experimental effective BHs and ideality factors obtained from the current–voltage (I–V) and capacitance–voltage (C–V) characteristics differ from diode to diode even if they are identically prepared (on the same sample). It has been reported theoretically by Tung and co-workers [11, 12] and experimentally by Mönch and co-workers [13, 18–21] that the linear relationship between effective BHs and ideality factors may be explained by the BH inhomogeneity. That is, the BHs become smaller as the ideality factors increase. This finding has been attributed to patchy interfaces, i.e., to lateral inhomogeneities of the BH [11, 21]. Tung [11] says that these results are hard to explain with interface gap states because the gap states are usually assumed to have implications for the magnitude of the BH and ideality factor of a SBD diode.

Our purpose is to experimentally confirm the theoretical prediction for the linear region with large BHs and low patch density below $n \cong 1.2$ in figure 7 of [19], that is, for a Si substrate with a doping density of 1.4×10^{15} cm^{-3}. For this purpose, H-terminated Pb/p-type Si(100) Schottky diodes (70 dots) with a doping density of about 10^{15} cm^{-3} have been prepared. The effective BHs and ideality factors from the experimental forward bias *I*–*V* and reverse bias *C*–*V* characteristics of these diodes have been calculated. The previously polished p-type Si wafer was cleaned by using traditional RCA cleaning with the final dip in diluted hydrofluoric acid (HF) for 30 s. The RCA cleaning procedure was as follows: a 10 min boil in NH_3+H_2O_2+6H_2O followed by a 10 min boil in HCl+H_2O_2+6H_2O. The RCA cleaning with HF dip shows a predominant coverage of the surface with hydride groups. Grundner and Jacob [22] have shown that a hydrophobic surface (called RCA cleaning) is mainly achieved by the 'HF' dip with consecutive water rinsing. In the same way, Gräf *et al* [23] have reported that, immediately after the HF treatment, high-resolution electron energy loss spectroscopy (HREELS) shows a predominant coverage of the surface with hydride groups. Pietsch *et al* [24] have found that after HF etching the surface is predominantly terminated by various hydrides. This hydrogen termination is well established and fluorine termination can be removed efficiently by a short final rinse with water. The predominant termination with hydrogen is responsible for a variety of remarkable properties of the silicon surface after HF treatment. Chemically, the H-terminated surface behaves in a completely hydrophobic manner and is passivated against reoxidation which allows a short handling time before regrowth of the oxide. Electronically, it is remarkably inactive with a largely reduced density of surface states in the Si energy bandgap due to the covalent satisfaction of all surface bonds. The surface after HF treatment is unreconstructed with an undisturbed bulk-like arrangement of surface atoms [24]. Heating to about 850 °C for 2 or 5 min leads to desorption of hydrogen [13, 24]. Furthermore, Kampen and Mönch [13] have also indicated that such treatments remove the native oxide layer and result in H-terminated clean Si surfaces. That is, Si atoms at the cleaned Si wafer surface are terminated by hydrogen. As is known, the intrinsic surface states present at the semiconductor–vacuum interface before contact with the metal are an important factor in Schottky barrier formation or Fermi level pinning at the interface. Briefly, hydrogen is well known to saturate the dangling band of the Si surface [17–26]. As mentioned in [21], Si surfaces may be easily terminated with hydrogen by HF dips, and the hydrogen persists under Pb films evaporated on to H-terminated Si surfaces at room temperature.

2. Experimental procedure

The diodes were prepared using p-type Si(100) wafers. An average doping concentration of $N_A = 5.313 \times 10^{15}$ cm^{-3} for the Si wafer was found from *C*–*V* measurements, and the corresponding resistivity value was $\rho_p = 2.62\ \Omega$ cm. The wafer was chemically cleaned using the RCA cleaning procedure. The native oxide on the front surface of the substrate was removed in HF:H_2O (1:10) solution and finally the wafer was rinsed in deionized water for 30 s. Then, low resistivity ohmic back contact to p-type Si(100) wafers was made by using Al, followed by a temperature treatment at 570 °C for 3 min in N_2 atmosphere. The Schottky contacts were formed by evaporation of Pb dots with a diameter of about 1.0 mm (diode area = 7.85×10^{-3} cm^2). The thickness of the Pb film was 800–1200 Å. All evaporation processes were carried out in a turbo molecular fitted vacuum coating unit at about 10–5 mbar. The *I*–*V* and *C*–*V* characteristics were measured using a HP 4140B picoampermeter and a HP model 4192A LF impedance analyser, respectively, at room temperature and in the dark.

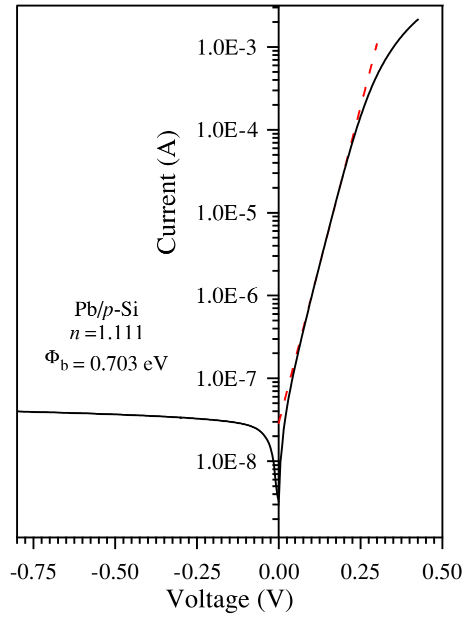

Figure 1. The forward and reverse bias *I*–*V* characteristics of one of the 70 Pb/p-Si SBDs at room temperature.

3. Results and discussion

It is assumed that the current in SBDs is due to thermionic emission current and this can be expressed as [4, 5]

$$I = I_0 \exp\left(\frac{qV}{nkT}\right)\left[1 - \exp\left(-\frac{qV}{kT}\right)\right], \qquad (1)$$

where

$$I_0 = AA^*T^2 \exp\left(-\frac{q\Phi_b}{kT}\right), \qquad (2)$$

is the saturation current density, Φ_b is the effective barrier height at zero bias, A^* is the effective Richardson constant and equals 32 A cm^{-2} K^2 for p-type Si, A is the diode area and n is an ideality factor. Figure 1 shows the room temperature forward and reverse bias *I*–*V* characteristics of one of the Pb/p-Si(100) SBDs. We fabricated 70 dots (Schottky contacts) for the Pb/p-Si(100) SBDs on the same p-type semiconductor substrate. The SBH Φ_b for the diodes ranged from 0.686 to 0.735 eV, and ideality factor n varied from 1.054 to 1.191.

The ideality factor determined by the image-force effect alone should be close to 1.01 or 1.02. Our data clearly show that the diodes have ideality factors that are considerably larger. The high values of n can be attributed to the presence of

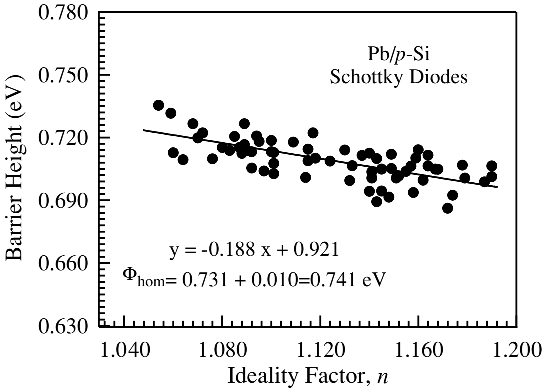

Figure 2. The plot of experimental BH versus ideality factor of the Pb/p-type Si SBDs at room temperature.

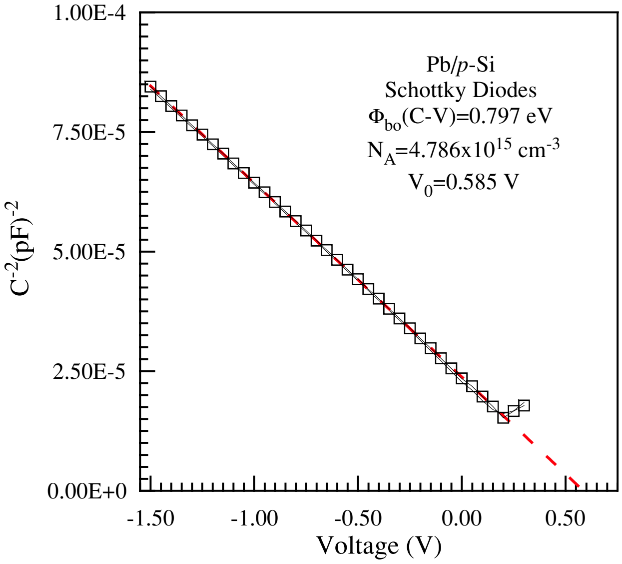

Figure 3. The room temperature reverse bias C^{-2}–V characteristic of one of the Pb/p-type Si SBDs at 1.0 MHz.

a wide distribution of low-SBH patches. Figure 2 shows a plot of the experimental BHs versus the ideality factors at room temperature. As can be seen from figure 2, there is a linear relationship between experimental effective BHs and ideality factors of Schottky contacts. That is, the BHs become smaller as the ideality factors increase. This finding may be attributed to lateral inhomogeneities of the BHs in Schottky diodes [11–14, 18–21]. In addition, it has been mentioned by Tung [11] and Mönch and co-workers [18–21] that, among identically prepared diodes, higher ideality factors were often found to accompany lower observed BHs and that the observed behaviour of the ideality factor can be explained by means of the bias dependence of the saddle-point potential of an inhomogeneous Schottky barrier (SB). We conclude that the data on the H-terminated Pb/p-type Si contacts are interesting, being a good experimental illustration of the theoretical predictions in [19]. The theoretical prediction in [19] (their figure 7) shows the simulation of the effective BH as a function of the ideality factor for three different homogeneous BHs with the Si substrate assumed to have a doping density of 1.4×10^{15} cm^{-3}. The $\Phi_b(n)$ curves become nonlinear above $n \cong 1.2$ for large BHs and small standard deviation of the patch parameter. The BH curve in [19] may be divided into three regions. The first region allows for extrapolation to $n = 1$ to determine the laterally homogeneous BH. In the second region, the curve exhibits a strong downward bend. It is eventually followed by a third and almost linear part for large ideality factors. In the third region with high n, the behaviour of the diodes is completely determined by the characteristics of the patches, due to a very high density of patches. The extrapolation to $n = 1$ for this third region does not result in a meaningful number. Thus, looking at the data in our own figure 2, and comparing with figure 7 in [19], it seems clear to us that the data on the H-terminated Pb/p-type Si samples allow meaningful extrapolation to $n = 1$ which determines the laterally homogeneous BH because its ideality factors n vary from 1.054 to 1.191 for large BHs. The laterally homogeneous BH value of approximately 0.741 eV for the H-terminated Pb/p-type Si(100) SBDs was obtained from the linear relationship between experimental effective BHs and ideality factors (figure 2). Kampen and Mönch [13] have obtained a value of 0.71 eV for Pb/H/p-type Si(111) contacts from their plot of experimental BHs versus ideality factors at room temperature. The laterally homogeneous BH value of 0.741 eV that we have obtained for the H-terminated Pb/p-type Si(100) SBDs is in close agreement with the expected value of 0.78 eV theoretically evaluated for the H-terminated Pb/p-type Si(111) contacts by Kampen and Mönch [13].

In Schottky diodes, the depletion layer capacitance, C, can be expressed as [5]

$$C^{-2} = 2(V_0 + V)/q\varepsilon_s A^2 N_A, \tag{3}$$

where A is the area of the diode, V_0 is the diffusion potential at zero bias and is determined from the extrapolation of the linear C^{-2}–V plot to the V-axis, ε_s is the dielectric constant of the semiconductor, and N_A is the acceptor concentration of p-type semiconductor substrate. Figure 3 shows the room temperature reverse bias C^{-2}–V characteristic of one of the devices at 1.0 MHz. The BH and carrier concentration values for each diode were extracted from its individual C^{-2}–V characteristic. The SBH obtained from C^{-2}–V characteristics varied from 0.751 to 0.928 eV.

As can be seen from the data, the effective SBH from I–V and C–V characteristics varied from diode to diode. Therefore, it is common practice to take averages [16–21]. Figures 4(*a*) and (*b*) show the statistical distribution of the BHs and ideality factors from the forward bias I–V plots (70 dots), respectively. Figures 5(*a*) and (*b*) show the statistical distribution of the BHs and the doping concentrations calculated from the reverse bias C^{-2}–V plots of the diodes, respectively. The experimental distributions of the effective BHs were fitted by the Gaussian function. The statistical analysis of the I–V BHs has yielded a mean BH value of 0.709 eV with a standard deviation of $\sigma = 9.2$ meV, and $\bar{n} = 1.121$ eV and $\sigma = 0.048$ for the ideality factors. The Gaussian distribution of barrier heights from the reverse bias C^{-2}–V characteristics has yielded $\bar{\Phi}_b = 0.799$ eV with $\sigma = 29$ meV, and $N_A = 5.313 \times 10^{15}$ cm^{-3} with $\sigma = 0.947 \times 10^{15}$ cm^{-3} for carrier concentration. The difference between the mean SBH values from the C^{-2}–V and I–V characteristics is larger than the image force lowering value of 0.02 eV for this device. The image force lowering

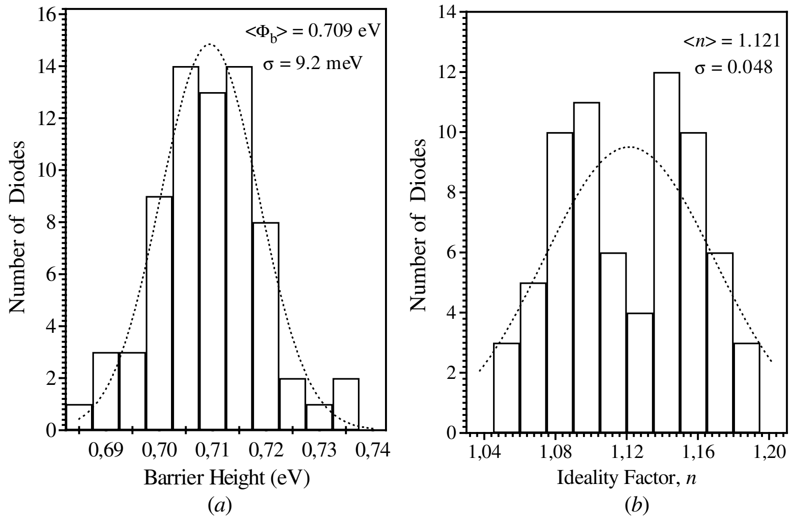

Figure 4. The Gaussian distribution of BHs from the forward bias *I–V* characteristics of the Pb/p-type Si SBDs at room temperature: (*a*) the Gaussian fits yields $\bar{\Phi}_b = 0.709$ eV and $\sigma = 9.2$ meV for the barrier heights; (*b*) $\bar{n} = 1.121$ eV and $\sigma = 0.048$ for the ideality factors.

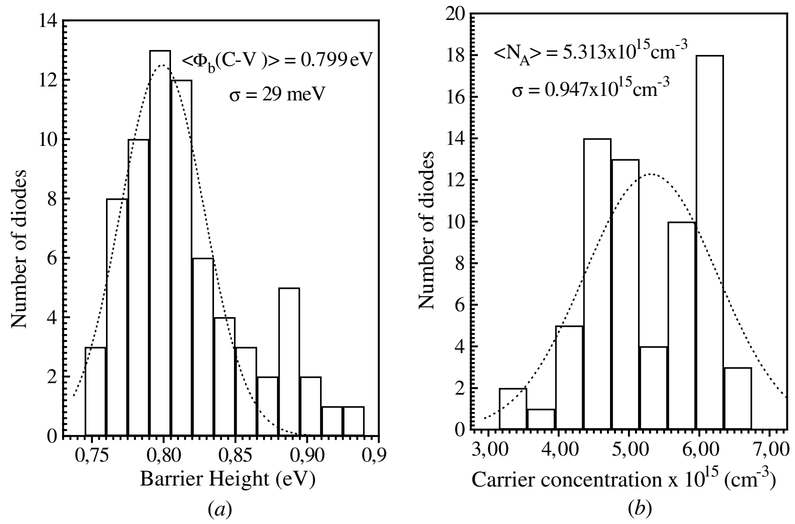

Figure 5. The Gaussian distribution of BHs from the reverse bias C^{-2}–V characteristics at 1.0 MHz and room temperature: (*a*) Gaussian fits yield $\bar{\Phi}_b = 0.799$ eV and $\sigma = 29$ meV; (*b*) $N_A = 5.313 \times 10^{15}$ cm^{-3} and $\sigma = 0.947 \times 10^{15}$ cm^{-3} for carrier concentration.

value for the barrier height was determined by using equation (19.7) in [21].

In conclusion, we have found that the data on the H-terminated Pb/p-type Si(100) samples allow meaningful extrapolation to $n = 1$ to determine the laterally homogeneous BH. The laterally homogeneous BH value of approximately 0.741 eV for the H-terminated Pb/p-type Si SBDs was obtained from the linear relationship between experimental effective BHs and ideality factors which can be explained by lateral inhomogeneities. In addition, we have shown experimentally that the data on the H-terminated Pb/p-type Si contacts become an interesting experimental illustration of the theoretical predictions in [19].

References

[1] Keffous A, Zitouni M, Belkacem Y, Menari H and Chergui W 2002 *Appl. Surf. Sci.* **199** 22

[2] Lu X, Xu X, Wang N Q, Zhang Q and Lin M C 2001 *J. Phys. Chem.* B **105** 10 069

[3] Abdelghani A, Hleli S and Cherif K 2002 *Mater. Lett.* **56** 1064

[4] Şafak H, Şahin M and Yű ksel Ő F 2002 *Solid-State Electron.* **46** 49

[5] Rhoderick E H and Williams R H 1998 *Metal-Semiconductor Contacts* (Oxford: Clarendon) pp 20, 48

[6] Jones F E, Hafer C D, Wood B P, Danner R G and Lonergan M C 2001 *J. Appl. Phys.* **90** 1001

[7] Song Y P, Van Meirhaeghe R L, Lafl´ere W H and Cardon F 1986 *Solid-State Electron.* **29** 633

[8] Werner J H and Güttler H H 1991 *J. Appl. Phys.* **69** 1522

[9] Chand S and Kumar J 1997 *J. Appl. Phys.* **82** 5005

[10] Zhu S, Van Meirhaeghe R L, Detavernier C, Cardon F, Ru G, Qu X and Li B 2000 *Solid-State Electron.* **44** 663

[11] Tung R T 2001 *Mater. Sci. Eng.* R **35** 1–138

[12] Sullivan J P, Tung R T, Pinto M R and Graham W R 1991 *J. Appl. Phys.* **70** 7403
Tung R T 1992 *Phys. Rev.* B **45** 13 509

[13] Kampen T U and Mönch W 1995 *Surf. Sci.* **331–3** 490

[14] Dobrocka E and Osvald J 1994 *Appl. Phys. Lett.* **65** 575
[15] Hecht M H, Bell L D, Kaiser W J and Grunthaner F J 1980 *Appl. Phys. Lett.* **55** 780
Olbrich A, Vancea J, Kreupl F and Hoffmann H 1997 *Appl. Phys. Lett.* **70** 2559
[16] Formen S, Van Meirhaeghe R L, De Vrieze A, Strubbe K and Gomes W P 2001 *Semicond. Sci. Technol.* **16** 975
Zu S, Detavernier C, Van Meirhaeghe R L, Qu X, Ru G, Cardon F and Li B 2000 *Semicond. Sci. Technol.* **15** 349
[17] Detavernier C, Van Meirhaeghe R L, Donaton R, Maex K and Cardon F 1998 *J. Appl. Phys.* **84** 3226
Vanalme G M, Van Meirhaeghe R L, Cordon F and Van Daele P 1997 *Semicond. Sci. Technol.* **12** 907
[18] Mönch W 1988 *Phys. Rev.* B **37** 7129
[19] Schmitsdorf R F, Kampen T U and Mönch W 1997 *J. Vac. Sci. Technol.* B **15** 1221
[20] Mönch W 1999 *J. Vac. Sci. Technol.* B **17** 1867
[21] Mönch W 2001 *Semiconductor Surfaces and Interfaces* 3rd edn (Berlin: Springer) pp 389, 421, 485
[22] Grundner M and Jacob H 1986 *Appl. Phys.* A **39** 73
[23] Gräf D, Grundner M, Schulz R and Mühlhoff L 1990 *J. Appl. Phys.* **68** 5155
[24] Pietsch G J, Köhler U and Henzler M 1993 *J. Appl. Phys.* **73** 4797
[25] de Nijs J M M, Druijf K G, Afanas'ev V V, van der Drift E and Balk P 1994 *Appl. Phys. Lett.* **65** 2428
[26] Pardo R S, Perez R, Vidal F J G, Whittle R and Flores F 1999 *Surf. Sci.* **426** 26