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Microelectronic Engineering 85 (2008) 721–726
MICROELECTRONIC ENGINEERING
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Correlation between barrier heights and ideality factors of H-terminated Sn/*p*-Si(1 0 0) Schottky barrier diodes

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Received 22 October 2007; received in revised form 24 December 2007; accepted 8 January 2008
Available online 15 January 2008

Abstract

Schottky barrier diodes (SBDs) were prepared by evaporation on H-terminated *p*-Si(1 0 0) surfaces. The Si(1 0 0)-H surfaces were obtained by wet chemical etching in diluted hydrofluoric acid. The current–voltage (*I–V*) characteristics of real SBDs are described by using two fitting parameters that are the effective barrier height (EBH) Φ_b^{eff} and ideality factor *n*. They were determined from *I–V* characteristics of SBDs (30 diodes) fabricated under experimentally identical conditions. The obtained values of EBHs varied from 0.729 to 0.749 eV, and the values of ideality factors varied from 1.083 to 1.119. The results showed that both parameters of SBDs differ from one diode to another even if they are identically prepared. The EBH distributions were fitted by two Gaussian distribution functions, and their mean values were found to be 0.739 ± 0.003 eV and 0.733 ± 0.001 eV, respectively. The homogeneous barrier height of SBDs was found to be 0.770 eV from the linear relationship between EBHs (Φ_b^{eff}) and ideality factors (*n*).

Keywords: Schottky barriers; Metal–semiconductor interfaces; Thermionic emission; Silicon; Barrier inhomogeneities

1. Introduction

The major semiconductor devices contain one or more metal–semiconductor contact. Most metal–semiconductor contacts are rectifying. This behavior is explained by a depletion layer formed on the semiconductor side of contact. The electronic properties of such contacts are characterized by their barrier height [1]. The recent impetus (motivation) for studying Schottky barrier formation is due to the recognition that both electronic and chemical equilibrium have to be considered together across a reactive interface between metal and semiconductor. The classical Schottky theory of an abrupt interface [1,2] and subsequent theoretical refinements [3–6] from an electronic viewpoint, dealing with surface states and metal induced state failed to take into consideration the chemical equilibrium at the interface. The chemical equilibrium will motivate the interfacial atomic rearrangement, interdiffusion, and intermetallic compound formation, which should have a propound effect on the electronic equilibrium producing the Schottky barrier [7]. The measured values of Schottky barrier height in the published literature are vastly scattered [8–11]. This may be due to the sensitivity of the Schottky interfaces to preparation procedures and to different techniques of measuring barrier height. Generally speaking, parallel contact (or diode) is formed whenever a non-uniform interfacial reaction occurs on a semiconductor. Existing treatments of SBH inhomogeneity assume the various patches of different local SBHs to be non-interacting [12]. Possible lateral variations of the SBH have been analyzed using the parallel conduction model [12]. Regions with different local SBHs are assumed to be electrically independent and the total junction current is simply a sum of currents flowing through all individual areas. When two different phases with high and low Shottky barrier heights coexist

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doi:10.1016/j.mee.2008.01.005

at the interface, namely, in the so-called parallel silicide contacts, the apparent SBH which is obtained from forward I–V characteristics as an average of high and low SBH weighed by the area of the low barrier phase and a combination of the two SBH's [13].

It is well known that the interface properties of the metal–semiconductor (MS) contacts have a dominant influence on the performance, reliability and stability of the device [8–11]. In recent years, several articles dealing with inhomogeneous barriers of the MS contacts have been published [14–36]. Freeouf et al. [14,15] analyzed the influence of small patch with low barrier height within the contact area on the ideality factor and the importance of the contact area size in this effect. Song et al. [16] reported that barrier height difference over the contact area occurs due to variations in the interfacial layer thickness and/or chemical composition and also because of non-uniformity of the interfacial charges. Tung and co-workers [11,17–19] showed that non-ideal behavior of the SBHs could be quantitatively explained by assuming a set of small patches with appropriate parameters inserted into the contact area. These approaches underline the interaction between regions with different SBHs and are based on the so-called pinch-off effect that takes place when the SBH varies laterally on a scale comparable to the width of the depletion layer [19]. The existence of barrier height non-uniformities is shown to provide a simple explanation of the following abnormal experimental results, routinely observed from various Schottky barriers: greater-than-unity ideality factor, the soft reverse characteristics, and the dependence of barrier height on the technique of measurement [17]. Werner and Güttler [20] have concluded that there is a direct influence of the interface crystallography on both the barrier height and its temperature dependence from the analysis of epitaxial $NiSi_2$/Si Schottky contacts. The existence of small local regions (patches) with a different barrier height was evidenced experimentally by using ballistic electron emission microscopy (BEEM) [37–39]. To describe the barrier inhomogeneties various types of distribution function have been used [40–48]. Horvath [41] analyzed the effect of the metal, semiconductor and interface parameters on the SBH in order to determine whether the lateral distribution of the barrier height obeys a normal and the lognormal law. He found that the fluctuations of some parameters result in a normal lateral distribution, while the fluctuations of the others yield a lognormal lateral distribution of the SBH. Simulation performed to see the effect of inhomogeneity in BHs favours the existence of Gaussian distribution of BHs in real Schottky diodes. Chand [42] revealed the discrepancies observed in the analytical results based on a Gaussian distribution model of barrier inhomogeneties. The influence of the distribution parameters and the temperature on the apparent barrier height and ideality factor was analyzed by Dobrocka and Osvald [46].

As mentioned above, it is clearly important to understand the physical origin of the non-ideal behaviors so that it can be controlled in future device applications. These homogeneous barrier heights rather than effective barrier heights of individual contacts or mean values should be used to discuss theories on the physical mechanisms that determine the barrier heights metal–semiconductor contacts. Provided the semiconductor substrate is well characterized, then the homogeneous SBH may be obtained from the I–V characteristic of even one contact as reported in Ref. [26]. Some investigations demonstrated that the experimentally observed dependence of the effective barrier heights and ideality factors of real metal–semiconductor contacts can be explained by lateral inhomogeneities of the BH [26–30]. As indicated in [16–22], the SBH is likely to be a function of the interface atomic structure, and the atomic inhomogeneities at the MS interface caused by grain boundaries, multiple phases, facets, defects, a mixture of different phases etc. The correlation between effective SBHs and ideality factors may be approximated by a linear relationship. That is, the SBHs become smaller as the ideality factors increase [26,27]. This finding was attributed to patchy of interfaces, i.e., lateral inhomogeneities of the SBH [26–30,36].

We attempted to study the electrical properties of the Sn/p-Si Schottky barrier diodes (SBDs) (30 diodes) fabricated under experimentally identical conditions. The aim of this paper is to confirm the experimental and theoretical results reported with respect to the laterally inhomegeneous distribution of barrier heights by some researcher [16–21].

2. Experimental procedure

We used p-type Si wafers with (100) orientation and 5–10 Ω cm resistivity. The wafer was chemically cleaned using the RCA cleaning procedure (i.e., a 10 min boil in $NH_4 + H_2O_2 + 6H_2O$ followed by a 10 min boil in $HCl + H_2O_2 + 6H_2O$). Before ohmic contact formed on the p-type Si substrate, the samples were dipped in dilute $HF{:}H_2O$ (1:10) for about 30 s to remove any native-thin-oxide layer on the surface, finally the wafer was rinsed with de-ionized water (purity up to 18.2 MΩ cm). Then Si wafer was inserted into the deposition chamber immediately after cleaning. The ohmic contact was made by evaporating Al on the back of the substrate, followed by a temperature treatment at 570 °C for 3 min in N_2 atmosphere. Sn films were evaporated onto the other surface of the sample to form circular Schottky contacts with 1 mm diameter. Evaporated film thickness was monitored using a quartz oscillator and the metal films had a thickness of 500 Å. All metallic surfaces were cleaned by acetone and methanol before processes. All evaporation processes were carried out in a vacuum coating unit at about 10^{-6} Torr. The I–V measurements of the diodes were performed using an HP 4140B Picoammeter/Voltage source at room temperature and in the dark.

3. Results and discussion

The current I across the metal–semiconductor interface under the application of the bias voltage V according to the thermionic emission theory is given by [8,9]

$$I = I_o \exp\left(\frac{qV}{nkT}\right)\left[1 - \exp\left(-\frac{qV}{kT}\right)\right] \tag{1}$$

where I_o is the saturation current determined by

$$I_o = AA^*T^2 \exp\left(-\frac{q\Phi_b^{eff}}{kT}\right) \tag{2}$$

where A is the geometrical area of the diode, A^* is the effective Richardson constant and equals $32\ \mathrm{A\,cm^{-2}\,K^{-2}}$ for p-type Si semiconductor, T is the absolute temperature, k is Boltzmann constant, q is the electron charge, Φ_b^{eff} is the effective barrier height obtained from the extrapolation of I_o in the semi-log forward bias ln I–V characteristics according to [8,9]

$$q\Phi_b^{eff} = kT \ln\left(\frac{A^*AT^2}{I_o}\right) \tag{3}$$

and n is the ideality factor. In this equation n is a dimensionless parameter introduced to account for the departures from thermionic emission theory (ideally $n = 1$). The values of n are calculated from the slope of the linear regions of the forward I–V characteristics according to [8,9]

$$n = \frac{q}{kT}\frac{dV}{d(\ln I)}. \tag{4}$$

Fig. 1 shows the experimentally semilog reverse and forward bias current-voltage characteristics of one of the H-terminated Sn/p-Si (100) Schottky barrier diodes (SBDs) at the room temperature. We fabricated 30 Schottky barrier diodes for the Sn/p-Si(100) SBDs on the same p-type semiconductor substrate. The effective barrier height and ideality factor values were obtained from individual I–V characteristics. The effective barrier heights (EBHs) Φ_b^{eff} for the diodes varied from 0.729 to 0.749 eV, and the ideality factor n ranged from 1.083 to 1.119. It is shown from these results that the parameters of SBDs vary from diode to diode even if they are identically prepared. However, the effective barrier height and ideality factor values for ideal diodes that are identically prepared should be equal to each other. Due to the large range of the diode parameters obtained, it is a common method to take averages.

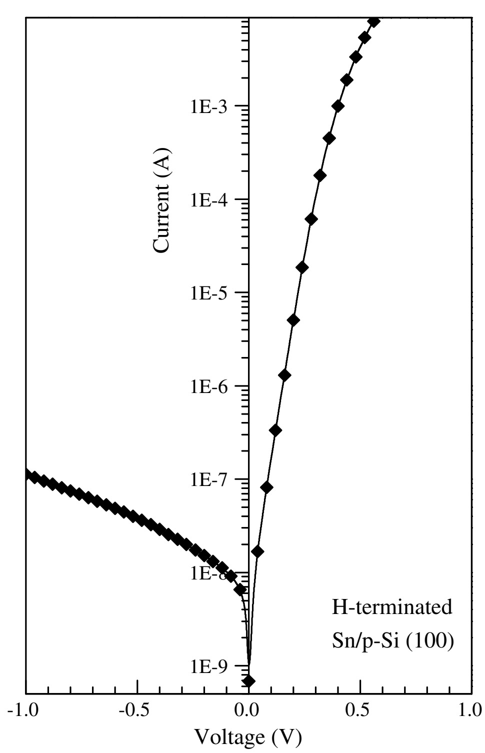

Fig. 1. The experimental semilog forward and reverse bias current versus voltage characteristics of one of the 30 Sn/p-Si Schottky barrier diodes at room temperature.

Figs. 2a and b show the histograms of the effective barrier heights and ideality factors for as many as 30 Sn/p-Si(100) SBDs. Gaussian distribution function was used to obtain good fits to the histograms. The statistical analysis of the ideality factor yields an average value of 1.099 ± 0.009. The ideality factor determined by the image-force effect should be close to 1.01 or 1.02 [10]. It is seen that the fabricated diodes have ideality factors that are larger than the value determined by the image-force effect alone. Explanations for this deviation of the ideality factor from unity ranged from assumptions of generation-recombination current in the space-charge region [8–10] to interface dielectric layers or field emission or thermionic field emission [49–51]. As can be seen from Fig. 2b, two Gaussian distributions are necessary to obtain a good fit for the data of the Sn/p-Si SBDs. In the literature, the existence of two Gaussians was already proven for GaAs Schottky diodes [52]. The first one given a mean barrier height values of 0.739 eV with a standard deviation of 30 meV and the second one a mean barrier height values of 0.733 eV with a standard deviation of 10 meV. The standart deviation (σ) is a measure of the barrier homogeneity. The lower value of σ corresponds to a more homogenous barrier height. Only recently, it has been shown that an ideality factor in excess of unity is consistent with the existence of SBH inhomogeneity [16–40]. Tung et al. [19] have confirmed the theoretically predicted dependence of the ideality on SHH inhomogeneity through numerical simulations. The high values of n can be attributed to the presence of a wide distribution of low-SBH patches [19].

The interface between the metal and semiconductor is not atomically flat but rough, with the result of spatial fluctuations of the potential and SBH. Apart from the roughness of the interface due to thickness modulations of metal as well as atomic steps, dislocations and grain boundaries in the metal, these potential fluctuations may also originate from numerous structural defects, stacking faults and a mixture of different metallic phases with different SBHs, doping inhomogeneity and undesirable reaction products at metal–semiconductor interface, dopant clustering [16–22].

The Schottky barrier height of an epitaxial $NiSi_2$ layer grown on Si(100) is shown to depend critically on the morphology of the interface [17]. Single-crystal, uniform,

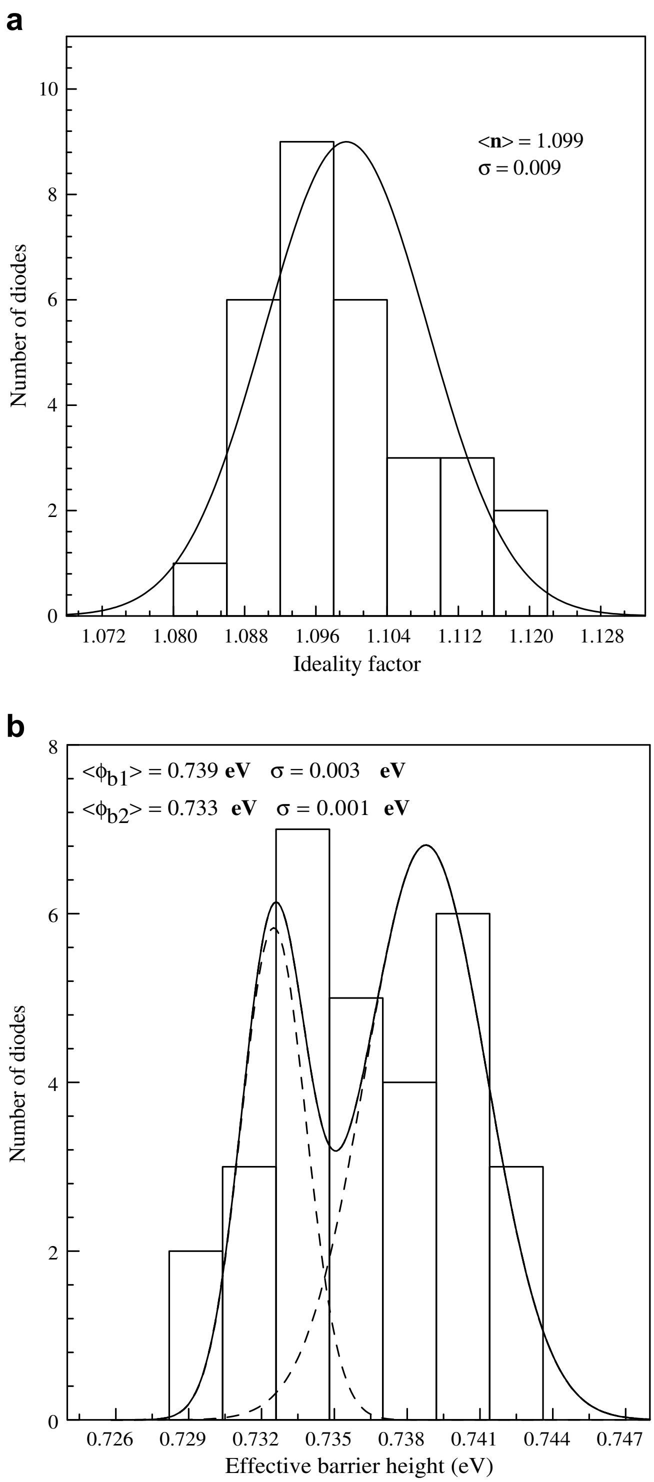

Fig. 2. The histograms of effective barrier heights and ideality factors obtained from the forward bias current–voltage characteristics of the Sn/p-Si Schottky barrier diodes at room temperature. (a) The Gaussian fits yields $n = 1.099$ and $\sigma = 0.009$ for the ideality factors. (b) The fit for the Sn/p-Si SBDs contains two Gaussian distributions with $\Phi_{b1} = 0.739$ eV and $\sigma_1 = 0.003$ eV; $\Phi_{b2} = 0.733$ eV and $\sigma_2 = 0.001$ eV.

planar $NiSi_2$/Si (100) layers have a much lower (n-type) SBH than that of interfaces which are made up inclined $\langle 111 \rangle$ facets. Interfaces with both planar $\langle 100 \rangle$ sections and inclined $\langle 111 \rangle$ sections exhibit electrical behavior expected of a spatially inhomogeneous SBH. Tung et al. [17] suggested that the physics controlling Schottky barrier formation depends on the spatially local metal-semiconductor interface atomic structure.

The barrier heights of Ag/n-Si(111)-7×7 and -1×1 contacts were determined from their current–voltage and capacitance–voltage characteristics [53]. Least-squares fits to the data give zero-bias barrier heights of 0.70 and 0.74 eV with Ag/n-Si(111)-7×7 and -1×1 contacts, respectively, for an ideality of 1.01 which is obtained for only image-force-lowering of the barrier. The lower barrier heights of the 7×7 – reconstructed with respect to unreconstructed 1×1 interfaces are explained by the stacking fault in one of the triangular subunits of the 7×7 unit mesh. Stacking faults in bulk silicon are electrically neutral but are associated with electric dipoles, as reported in Ref. [53]. In 7×7 reconstructed metal/Si(111) contacts the fault-induced dipoles are oriented in such a way that the respective barrier heights are lower than at unfaulted 1×1 interfaces [53].

Ideally, the reverse current should saturate according to thermionic emission theory [8–10]. However, in practice and as shown in Fig. 1 this is rarely the case. Lack of saturation (soft) is partly due to imaging force effect which results in a voltage-dependent barrier height and an additional SBH lowering mechanism which is linear in the electric field, though to arise from interface states [54]. In addition, the soft reverse characteristics are attributed to the existence of barrier height non-uniformities [19]. As pointed out by Tung [19], for inhomogeneous MS contacts, the reverse current may be dominated by the current which flows through the low-SBH patches, which is controlled by the potential at the saddle point. Increasing reverse bias drops the potential at the saddle point, hence the reverse current increases with increasing reverse bias and does not saturate.

The homogeneous barrier heights rather than effective barrier heights of individual contacts or mean values should be used to discuss theories on the physical mechanisms that determine the barrier heights of metal–semiconductor contacts [26]. The laterally homogeneous barrier heights were computed from the observed linear correlation between effective barrier heights and ideality factors that are determined from current–voltage characteristics of metal–semiconductor contact using the method of Schmitsdorf et al. [26].

Fig. 3 shows a plot of the effective barrier heights of the same 30 diodes as a function of the respective ideality factors. As can be seen from Fig. 3, there is a linear relationship between experimental effective barrier heights and ideality factors of SBDs. This shows that the BHS decreases as the ideality factor increases. This finding may be attributed to lateral inhomogeneities of the EBHs in SBDs [26]. The straight line in Fig. 3 is a least-square fit to the experimental data. From Fig. 3, the laterally homogeneous barrier height value was found to be

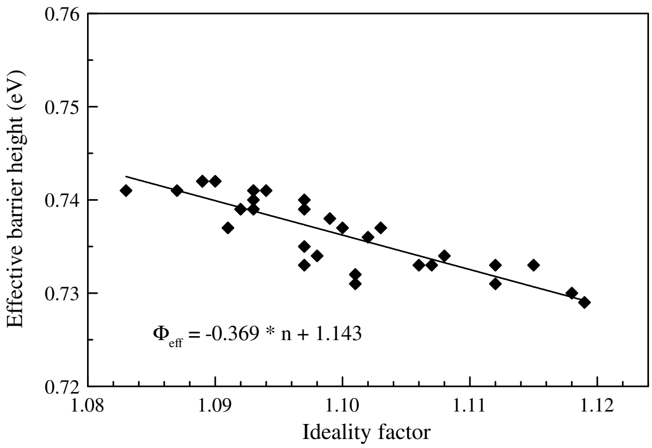

Fig. 3. The effective barrier heights versus ideality factors of the same 30 Sn/p-Si Schottky barrier diodes at room temperature.

0.770 eV for the H-terminated Sn/p-Si(1 0 0) SBDs by extrapolation of Φ_b^{eff} versus n plots to an ideality of 1.01 which is obtained for only image-force-lowering of the barrier. Thus, the homogeneous and the mean effective barrier heights of the Sn/p-Si(1 0 0) SBDs differ by $\Phi_{bp}^{hom} - \langle \Phi_{bp1} \rangle =$ 31 meV and $\Phi_{bp}^{hom} - \langle \Phi_{bp2} \rangle = 37$ meV. These differences can be explained by the pinch-off theory for a more physical picture of the patches [10,19]. As pointed out by Tung [19]; when the SBH varies locally at a metal–semiconductor interface, the potential also varies from region to region. Tung [19] has treated a system of discrete regions or patches low barrier embedded in a higher uniform barrier. The nanometer-sized patches are taken to be small relative to the size of the depletion region such that the interaction of the patch with the surrounding depletion region causes a pinch-off or saddle point in the potential away from the interface. Then, the mean effective barrier heights are expected to be correlated with the ideality factor and to be smaller than homogeneous barrier heights.

The most popular theories with regard to Schottky barrier formation involve Fermi level pinning by either defect states [55,56] or by states derived from the semiconductor [4]. The metal-induced-gap-states (MIGS) model represents the primary mechanism, which determines the barrier heights in ideal, i.e. intimate, abrupt and laterally homogeneous metal–semiconductor contacts [4]. The charge transfer across such interfaces is modelled by the electronegativities difference of the metal and semiconductor in the contact [27]. The MIGS line in the laterally homogeneous barrier heights versus electronegativity difference plot for p-type Si gives the following relation

$$\Phi_{bp} = 360 - S_x(X_m - X_s), \tag{5}$$

where X_m and X_s are the electronegativities of the metal and the semiconductor, respectively, and the value of 0.360 eV is the zero-charge-transfer barrier heights or the charge neutrality level of the MIGS with respect to the top of the valance band at the surface of the p-type Si semiconductor [57]. The electronegativity values of the Sn and semiconductor Si were taken as $X_m = 4.15$ eV and $X_s = 4.70$ eV [10], respectively. The slope parameter S_x is obtained as 0.101 from the electronic contribution ε_∞ of the static dielectric constant of the semiconductor [10]. Eq. (5) gives the BH values of about 0.412 eV for Sn/p-Si SBHs. The laterally homogeneous barrier height value obtained from Fig. 3 is larger than what is predicted by the MIGS plus electronegativity model. The observed difference in barrier heights may be attributed to secondary mechanisms like structure-related interfaces dipoles, interface structure, and interface defects, as pointed out in Ref. [27]. Silicon surfaces may be terminated with hydrogen by wet chemical etching [58–62]. A most simple case of extrinsic interface dipoles is the layer of hydrogen atoms at metal–semiconductor interfaces. The interface-dipole model was also successfully used in explaining the smaller BHs for metal contacts on H-terminated p-diamond surfaces with respect to what was found earlier with the metals on clean p-diamond surfaces [58]. Hydrogen layers induce extrinsic charge densities of positive and negative sign at silicon and diamond interfaces, respectively. Thus, hydrogen layers will increase and reduce the barrier heights in metal contacts on p-Si and diamond, respectively, in complete agreement with the experimental findings [58]. This different behavior was explained by oppositely oriented H–C and H–Si interface dipoles. The reason for this is that hydrogen is electropositive with regard to carbon but more electronegative than silicon. A layer of extrinsic interface dipoles may be described by an electric double layer. The corresponding variation of the barrier height due to extrinsic interface dipoles then equals the potential drop across the double layer [58].

4. Conclusions

Silicon is the most important semiconductor for semiconductor device technology, and the Si(1 0 0) surface is probably its most studied surface. We were attempted to study the electrical properties of the Sn/p-Si(1 0 0) Schottky barrier diodes (SBDs) (30 diodes) fabricated under experimentally identical conditions. The effective barrier height and ideality factor values were obtained using the thermionic emission theory from individual I–V characteristics of metal–semiconductor contacts. We have shown that both effective barrier heights and ideality factors varied from diode to diode even though they were identically prepared. The mean values of EBH of the H-terminated Sn/p-Si(1 0 0) SBDs found to be 0.739 and 0.733 eV by using two Gaussian distribution. Furthermore, the effective barrier height was observed to decrease linearly as a function of the ideality factor. This behavior is attributed to spatial variations of the barrier heights. The laterally homogeneous Schottky barrier height value of 0.770 eV for H-terminated Sn/p-Si(1 0 0) SBDs were obtained by extrapolation of the effective barrier heights versus their ideality factors plots to n_{if}. This value is higher than that of the clean Si(1 0 0) surface because the H atoms saturate the dangling bonds of the surface Si atoms. In conclusion, the increasing of barrier heights at metal/*p*-Si contacts by an interfacial hydrogen layer is explained by interface dipole which exists in addition to the MIGS continuum [58].

Acknowledgements

This work has been supported by the Scientific Research Project Unit of Erciyes University through Project No. FBT-07-20 EÜBAP. The English text has been kindly checked by Lecturer Fikret KARA from English Language and Literature Department, Erciyes University.

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