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# Determination of the laterally homogeneous barrier height of palladium Schottky barrier diodes on n-Ge (1 1 1)

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ABSTRACT

We have studied the experimental linear relationship between barrier heights and ideality factors for palladium (Pd) on bulk-grown (1 1 1) Sb-doped n-type germanium (Ge) metal-semiconductor structures with a doping density of about $2.5\times10^{15}$ cm$^{-3}$. The Pd Schottky contacts were fabricated by vacuum resistive evaporation. The electrical analysis of the contacts was investigated by means of current–voltage (*I–V*) and capacitance–voltage (*C–V*) measurements at a temperature of 296 K. The effective barrier heights from *I–V* characteristics varied from 0.492 to 0.550 eV, the ideality factor *n* varied from 1.140 to 1.950, and from reverse bias capacitance–voltage ($C^{-2}$–$V$) characteristics the barrier height varied from 0.427 to 0.509 eV. The lateral homogenous barrier height value of 0.558 eV for the contacts was obtained from the linear relationship between experimental barrier heights and ideality factors. Furthermore the experimental barrier height distribution obtained from *I–V* and ($C^{-2}-V$) characteristics were fitted by Gaussian distribution function, and their mean values were found to be 0.529 and 0.463 eV, respectively.

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## 1. Introduction

Metal-semiconductor (MS) interfaces are an essential part of virtually all semiconductor electronic and optoelectronic devices [1]. The MS structures are important research tools in the characterization of new semiconductor materials [2]. Schottky barriers formed by MS contacts have been widely studied in the past 60 years [1,3,4], for their basic physical properties and technological applications to electronic devices [5]. The electronic properties of the MS contacts are characterized by their barrier height (BH). The mechanisms that determine the BH are still not fully understood [3,6–8]. It is only in the past two decades that an inhomogeneous contact has been considered as an explanation for a voltage-dependent BH [1,3,9]. The BH is likely to be a function of the interface atomic structure, and the atomic inhomogeneities at MS interface, which are caused by grain boundaries, multiple phases, facets, defects, a mixture of different phases, etc. [9–12]. It has also been suggested by Song et al. [13] that the barrier inhomogeneities can occur as a result of inhomogeneities in the interfacial oxide layer composition, nonuniformity of the interfacial charges and interfacial oxide layer thickness. The presence of barrier inhomogeneities may greatly influence the current across the MS contact [13]. Tung [12] and Sullivan et al. 14 assumed lateral variations of BH to model imperfect Schottky structures, and they depicted larger ideality factors and smaller effective BHs when

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they increased the inhomogeneity of barriers. The experimental effective BHs and ideality factors obtained from the *I–V* and *C–V* characteristics differ from diode to diode even if they are identically prepared [12,14–17]. This has been attributed to interfacial patches, i.e. small regions with lower BH than the junction's main BH [1,14].

Although studies have been performed to investigate the relationship between the effective BHs and ideality factors of the metal/Si Schottky diodes [5,18–21], nothing much has been reported on the relationship between effective BHs and ideality factors from forward bias *I–V* and reverse bias *C–V* characteristics of the metals/Ge Schottky diodes. Due to shrinking of the advanced Si-based complementary metal-oxide-semiconductor (CMOS) device feature size, it is becoming increasingly difficult to further improve Si-based CMOS performance with traditional device scaling, and new materials and device structures to relax the physical limitation in device scaling are now required. Germanium (Ge) has been regarded as the replacement for Si as the channel material in the future high-speed CMOS technology, because it offers two times higher intrinsic electron mobility and four times higher intrinsic hole mobility than Si [22]. Optimal implementation of germanium technology will require an understanding of metal–germanium interactions from both metallurgical and electronic standpoints.

Some reports have indicated that metal-oxide-semiconductor field effect transistors (MOSFETs) can be replaced by Schottky barrier (SB) MOSFETs for sub-100 nm application [23,24]. Palladium is an interesting material to adjust SB heights because it has work function closer to the valence band of Ge layer [24]. Studies have also shown that Ni/n-Ge and Pd/n-Ge Schottky contacts offer the lowest sheet resistance [25], and remain stable over a wide temperature range during anneals [25,26]. Therefore, Ni and Pd are good candidates for contact metallization in Ge metal-oxide semiconductor devices. Chawanda et al. [27] have experimentally investigated the relationship between the effective BHs and ideality factors of Ni/n-Ge Schottky contact. The Schottky barrier height of the Pd/n-Ge Schottky contact has been reported to be in the range of 0.380–0.577 eV [24,28]. In this study, Pd Schottky diodes on n-Ge (1 1 1), (24 diodes) were fabricated under experimentally identical conditions in order to investigate the relationship between the effective BHs and ideality factors obtained from the forward bias *I–V* and reverse bias *C–V* characteristics of the Pd/n-Ge (1 1 1) Schottky diodes. The homogeneous BH value for the Pd Schottky contacts was obtained from the linear relationship between the experimental effective BHs and ideality factors. The essence of this homogeneous BH is that, it depicts the real meaningful value characteristic of the MS systems [19], which should be used to develop theories of physical mechanisms determining these BHs of Schottky contacts [29].

## 2. Experimental procedure

We used bulk-grown, (1 1 1)-oriented, n-type Ge doped with antimony (Sb) to a density of about $2.5\times10^{15}$ cm$^{-3}$ and is supplied by Umicore. Before metallization, the samples were first degreased and subsequently etched in a mixture of $H_2O_2$(30%): $H_2O$ (1:5) for 1 min. Immediately after cleaning, the samples were inserted into a vacuum chamber where AuSb (0.6% Sb), 100 nm thick, was deposited by resistive evaporation on their back surfaces as ohmic contacts. The samples were then annealed at 350 °C in Ar for 10 min to minimize the contact resistivity of the ohmic contacts [30]. Before Schottky contact deposition, the samples were again chemically cleaned as described above. Pd Schottky contacts were deposited by vacuum resistive evaporation through a mechanical mask. The contacts were $(0.60\pm0.05)$ mm in diameter and 30 nm thick. Thickness of the contacts was measured during deposition using an INFICON XTC 751-001-G1 crystal thickness monitor. After the contact fabrication, the samples were characterized by *I–V* and *C–V* measurements at room temperature.

## 3. Results and discussion

The barrier heights of the contacts were calculated from *I–V* characteristics, which were analyzed by the thermionic emission model given by the following equation [3,4]:

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

where $I_0$ is the saturation current determined by

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

where $A^*$ is the effective Richardson constant, $A$ is the diode area, $T$ the measurement temperature, $k$ the Boltzmann constant, $q$ is the electron charge, $\Phi_B$ is the zero bias effective Schottky barrier height (SBH) obtained from the extrapolation of $I_0$ in the semi-log forward bias ln *I–V* characteristics according to [3,4]:

$$\Phi_B=\frac{kT}{q}\ln\left(\frac{A^{*}AT^2}{I_0}\right) \quad (3)$$

and $n$ the ideality factor, which is a measure of conformity of the diode to pure thermionic emission. The values of $n$ are calculated from the slopes of the linear regions of the semi-log forward bias *I–V* characteristics (since the effect of series resistance in these linear regions is not significant [20]) according to [3,4]:

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

which is equal to 1 for an ideal diode and usually has a value greater than unity.

We fabricated 24 dots (Schottky barrier diodes) for the Pd/n-Ge (1 1 1) SBDs on the same n-type semiconductor substrate by evaporation of Pd as Schottky contact. Fig. 1 shows the room temperature experimental forward and reverse bias *I–V* characteristics of selected five Pd/n-Ge (1 1 1) Schottky barrier diodes (SBDs). The *I–V* effective BHs for the diodes varied from 0.492 to 0.550 eV, and the ideality factor ranged from 1.140 to 1.950. As can be seen, the experimental effective BHs and ideality factors from the *I–V* characteristics can differ from diode to diode even if they were identically prepared on the same sample.

In Schottky diodes, the depletion layer capacitance, $C$ can be expressed as [3]

$$C^{-2}=2(V_0-V)/q\varepsilon_sA^2N_D \quad (5)$$

where $A$ is the area of the diode, $V_0$ is obtained from the intercept of $C^{-2}$ with the voltage axis, $\varepsilon_s$ is the dielectric constant of the semiconductor, $N_D$ is the donor concentration of n-type semiconductor substrate. From Eq. (5), the values of $N_D$ can be determined from the slope of the $C^{-2}-V$ plot. Fig. 2 shows the room temperature reverse bias $C^{-2}-V$ characteristics for selected five samples of the Pd/n-Ge (1 0 0) Schottky diodes (24 dots) at 1 MHz. The value of the *BH* $\Phi_B(C-V)$can be obtained

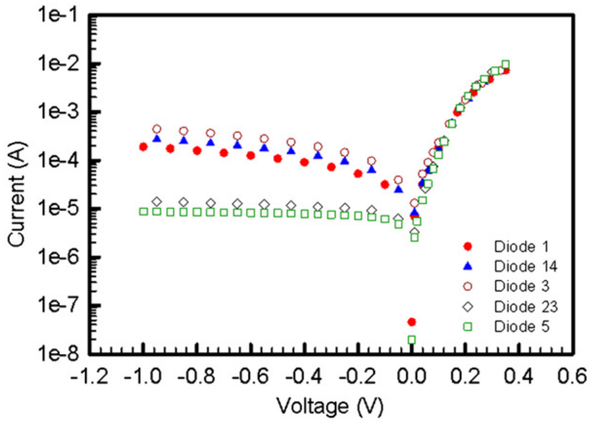


**Fig. 1.** The plot of the forward and reverse bias current–voltage (*I–V*) characteristics for selected five samples Pd/n-Ge (1 1 1) Schottky diodes at room temperature.

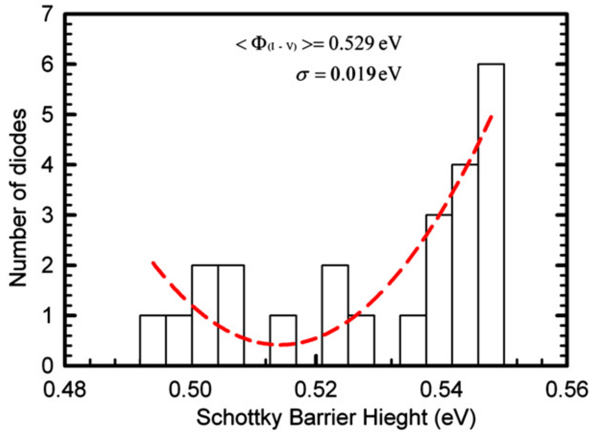


**Fig. 3.** Distribution of barrier heights from the forward bias *I–V* characteristics of the Pd/n-Ge (1 1 1) Schottky diodes at room temperature.

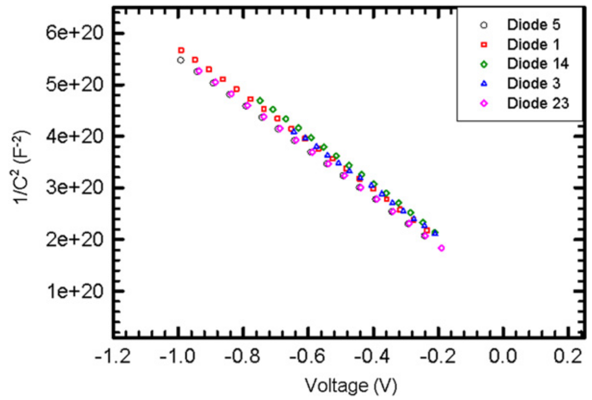


**Fig. 2.** Reverse bias $C^{-2}$–V characteristics for selected five samples Pd/n-Ge (1 1 1) Schottky diodes at frequency 1 MHz and room temperature.

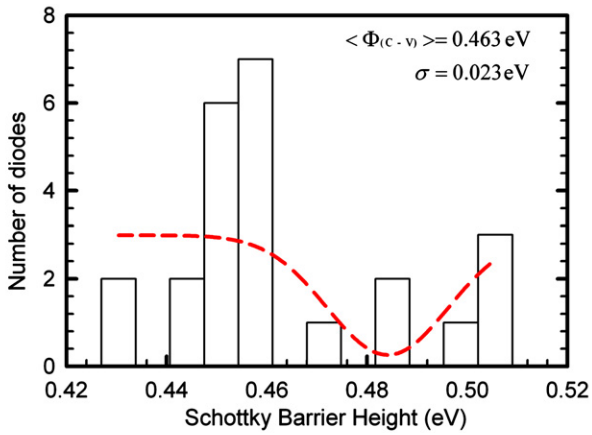


**Fig. 4.** Distribution of barrier heights from the reverse bias $C^{-2}$–V characteristics of the Pd/n-Ge (1 1 1) Schottky diodes at 1 MHz and room temperature.

from Fig. 2 as

$$\Phi_B(C-V) = V_D + E_F - \Delta\Phi_B \tag{6}$$

where $E_F$ is the energy difference between the bulk Fermi level and the conduction band edge, $V_D$ is the diffusion potential and $\Delta\Phi_B$ is the image-force barrier lowering and is given by [3,4]

$$\Delta\Phi_B = \left[\frac{qE_m}{4\pi\varepsilon_s\varepsilon_0}\right]^{1/2} \tag{7}$$

where $E_m$ is the maximum electric field and is given by

$$E_m = \left[\frac{2qN_DV_0}{\varepsilon_s\varepsilon_0}\right]^{1/2} \tag{8}$$

As shown in Fig. 2, for each diode, the $C^{-2}-V$ plots give straight lines. The capacitance–voltage BH for the Pd/n-Ge (1 1 1) Schottky structures varied from 0.427 to 0.509 eV. These results depict that the parameters of SBDs vary from diode to diode even if they are identically prepared.

Fig. 3 shows the histograms of BHs from the forward bias *I–V* plots of the Pd/n-Ge(1 1 1) MS structures and Fig. 4 shows the histogram of BHs from the reverse bias $C^{-2}-V$ plots of the same diodes. A Gaussian distribution function was used to obtain fits to the histograms. Considering the statistical distribution of SBHs obtained from *I–V* measurements (Fig. 3), the statistical analysis yielded a mean BH value of 0.529 eV with a standard deviation of 0.019 eV. In the distribution of the BHs from the reverse bias $C^{-2}-V$characteristics at 1 MHz (Fig. 4) the statistical analysis yielded a mean BH value of 0.463 eV with standard deviation of 0.022 eV. The difference between the mean SBH values obtained from $C^{-2}-V$and *I–V* is 0.066 eV. Due to the different nature of the *I–V* and *C–V* measurement techniques, BHs deduced from them are not always the same [19]. When the difference between $\Phi_B(I-V)$ and $\Phi_B(C-V)$approaches zero, it implies that the potential profiles approach a uniform barrier height [19]. Although, in general, BHs from *C–V* measurements are higher than BHs from *I–V* measurements, in our study we obtained *I–V* BHs that were higher than *C–V* BHs ($\overline{\Phi}_{(I-V)} = 0.529$ eV and $\overline{\Phi}_{(C-V)} = 0.463$ eV). Therefore, further studies are needed to clarify these results.

Fig. 5 shows the statistical distribution of ideality factors from the forward bias *I–V* characteristics. A Gaussian distribution function was used to obtain a fit to the histogram. The statistical analysis of the ideality factor yielded an average value of 1.414 with a standard deviation of 0.270. The fabricated diodes have ideality factors that are larger than 1.01, the value determined by the image-force effect alone [18]. The ideality factor determined by the image-force effect should be close to 1.01 or 1.02 [31]. Schottky contacts, ideality factor greater than 1.0 indicate that the transport properties are not well modeled by the thermionic emission alone although their contacts remain rectified [32]. Explanations for the deviation of the ideality factor from unity range is from assumptions of generation–recombination current in the space-charge region [3,4,18] to the interface dielectric layers or field emission [18] or thermionic field emission [33]. The high values of ideality factors are attributed to secondary mechanisms at the interface [7,17]. For example, interface defects may lead to lateral inhomogeneous

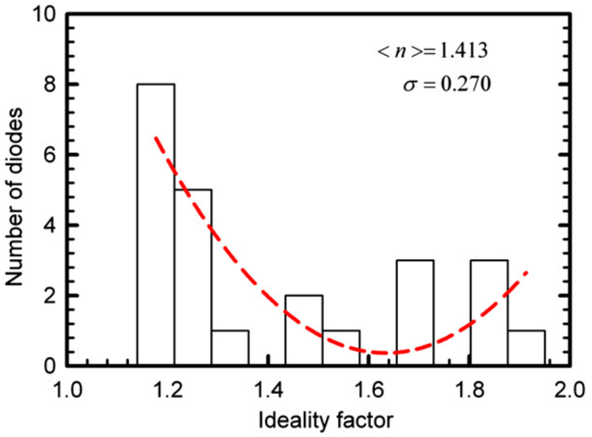


**Fig. 5.** Distribution of ideality factors from the forward bias *I–V* characteristics of the Pd/n-Ge (1 1 1) Schottky diodes at room temperature.

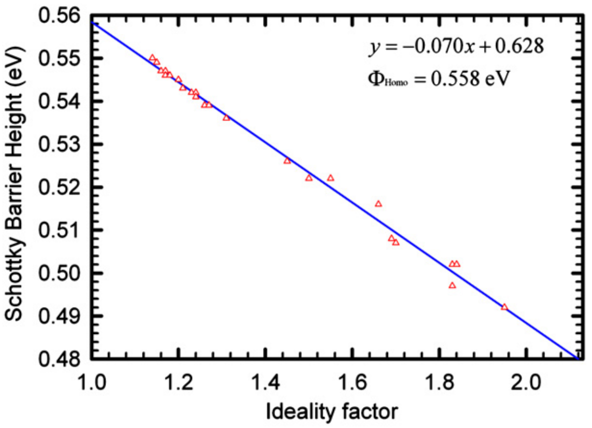


**Fig. 6.** Experimental Schottky barrier heights versus the ideality factors plot of the Pd/n-Ge (1 1 1) Schottky diodes for the barrier inhomogeneity model.

distribution of barrier heights at the interface resulting in the presence of wide distribution of low-SBH patches.

Fig. 6 shows a plot of the effective barrier heights as a function of the respective ideality factors. The straight line is the least squares fit to the experimental data. The BH decreases as the ideality factor increases. That is, there is a linear relationship between experimental effective BHs and ideality factors of Schottky contacts [34]. This may be attributed to lateral inhomogeneities of the effective BHs in Schottky barrier diodes [35]. Similar results have been reported in the literature [1,14]. It has been mentioned that higher ideality factors among identically prepared diodes were often found to accompany lower observed barrier heights [19]. Such behaviors of the ideality factor and BH can be explained by means of bias dependence of saddle-point potential of an inhomogeneous BH [1,14]. Since Gaudet et al. [25] has reported the formation of Pd germanide after 200 °C annealing, germanide formation is not expected in the as-deposited Pd/n-Ge Schottky contacts. Therefore, SBH inhomegenities in as-deposited Pd/n-Ge Schottky contacts could not be due to compound formation. Mönch [31] also proposed that the SBH inhomogeneities at interface may be due to defects induced during contact fabrication. These defects give rise to additional discrete levels in the band gap and the Fermi level is pinned to one of these levels, possibly quite far away from the charge neutrality level [5]. A lateral homogeneous barrier height value of 0.558 eV for the Pd/n-Ge (1 1 1) Schottky structures was obtained from the extrapolation of the plot to $n=1.0$. The homogeneous barrier heights rather than effective BHs of individual contacts or mean values should be used to discuss theories on the physical mechanisms that determine the BHs of MS contacts [29,35].

## 4. Summary

Pd Schottky diodes (24 dots) on n-Ge (1 1 1) were fabricated by resistive deposition under experimentally identical conditions. The BHs and ideality factor values were obtained from individual *I–V* characteristics of MS contacts. We have shown that both BHs and ideality factors varied from diode to diode even though they were identically fabricated. The laterally homogeneous BH value of 0.558 eV for the Schottky contacts was obtained from the linear relationship between *I–V* effective BHs and ideality factors that can be explained by lateral inhomogeneities. The statistical analysis yielded the mean effective SBH $=(0.529\pm0.019)$ eV, mean ideality factor $=1.413\pm0.270$ for these devices from *I–V* characteristics, and mean effective SBH $=(0.463\pm0.023)$ eV for these devices from *C–V* characteristics.

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