



# Variation of Schottky barrier height induced by dopant segregation monitored by contact resistivity measurements



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## ABSTRACT

Change of contact resistivity ( $\rho_c$ ) is monitored for evaluation of Schottky barrier height (SBH) variation induced by dopant segregation (DS). This method is particularly advantageous for metal–semiconductor contacts of small SBH, as it neither requires low-temperature measurement needed in current–voltage characterization of Schottky diodes nor is affected by reverse leakage current often troubling capacitance–voltage characterization. With PtSi contact to both n- and p-type diffusion regions, and the use of opposite or alike dopants implant into pre-formed PtSi films followed by drive-in anneal at different temperatures to induce DS at PtSi/Si interface, the formation of interfacial dipole is confirmed as the responsible cause for modification of effective SBHs thus the increase or decrease of  $\rho_c$ . A tentative explanation for the change of contact resistivity based on interfacial dipole theory is provided in this work. Influences and interplay of interfacial dipole and space charge on effective SBH are also discussed.

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## 1. Introduction

Using a single metal silicide as metallic source/drain for both p- and n-type MOSFETs has been extensively studied as a probable solution to effectively reducing parasitic source/drain resistance in the MOSFETs of the 22-nm CMOS technology node and beyond [1–8]. This approach has been shown viable with the assistance of dopant segregation (DS) leading to considerable modification of effective Schottky barrier heights (SBHs) to electrons and holes towards desired values, which gives rise to either improved device performance or the reduction of specific contact resistivity ( $\rho_c$ ) [9–12]. For DS, dopants can be introduced [10,11] either prior to silicide formation in the so-called silicidation induced dopant segregation, SIDS, or into the pre-formed silicide film in the so-called silicide as diffusion source, SADS. During the course of studying the effects of DS on SBHs, it is usual to adopt either capacitance–voltage (C–V) measurements or current–voltage (I–V) characteristics to extract the SBHs on Schottky diodes with the silicide as the contacting electrode. However, large reverse leakage current occurs when the SBH is below 0.6 eV defeating the credibility and accuracy of extraction with C–V method. Low-temperature I–V

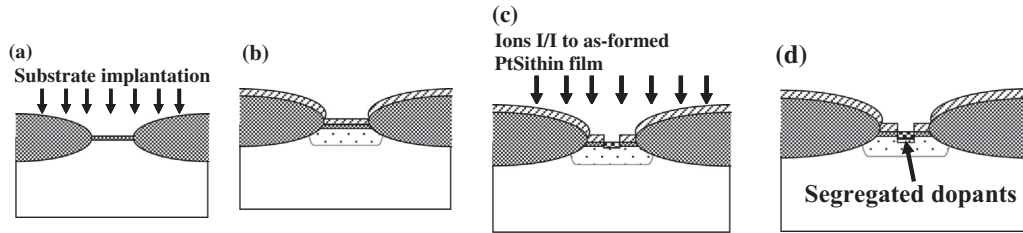
measurements are often necessary in order to reliably access low SBHs [9]. In the present work, an alternative approach on the basis of measurements of forward current at room temperature is introduced. This method relies on characterizing specific contact resistivity by monitoring its variation with DS. We will show that the use of this method leads to confirmation of the formation of an interfacial dipole as the dominating mechanism responsible for the modification of effective SBH induced by DS.

## 2. Test device and experimental procedure

The key process steps are schematically summarized in Fig. 1. Cross-bridge Kelvin resistors (CBKR) of a range of different contact dimensions were designed for contact resistivity extraction. SADS was chosen for DS, because of its ease of process control [10,11] as compared to SIDS. Both p- and n-type Si (100) wafers were used to allow for studies of both conduction polarities. Device isolation was realized using LOCOS process with an 800-nm thick SiO<sub>2</sub> to define the diffusion regions. High concentration doping in the diffusion regions was achieved by ion implantation of boron (B) at 50 keV and phosphorus (P) at 140 keV, both at a dose of  $1 \times 10^{16} \text{ cm}^{-2}$ , into the n- and p-type substrate, respectively, followed by an extensive anneal at 1000 °C for 8 h in N<sub>2</sub> ambient. According to numerical simulations using ISE TCAD [13], a 2-μm deep, uniform junction would be formed with a surface concentration of  $7 \times 10^{19} \text{ cm}^{-3}$  for both p- and n-type of diffusion

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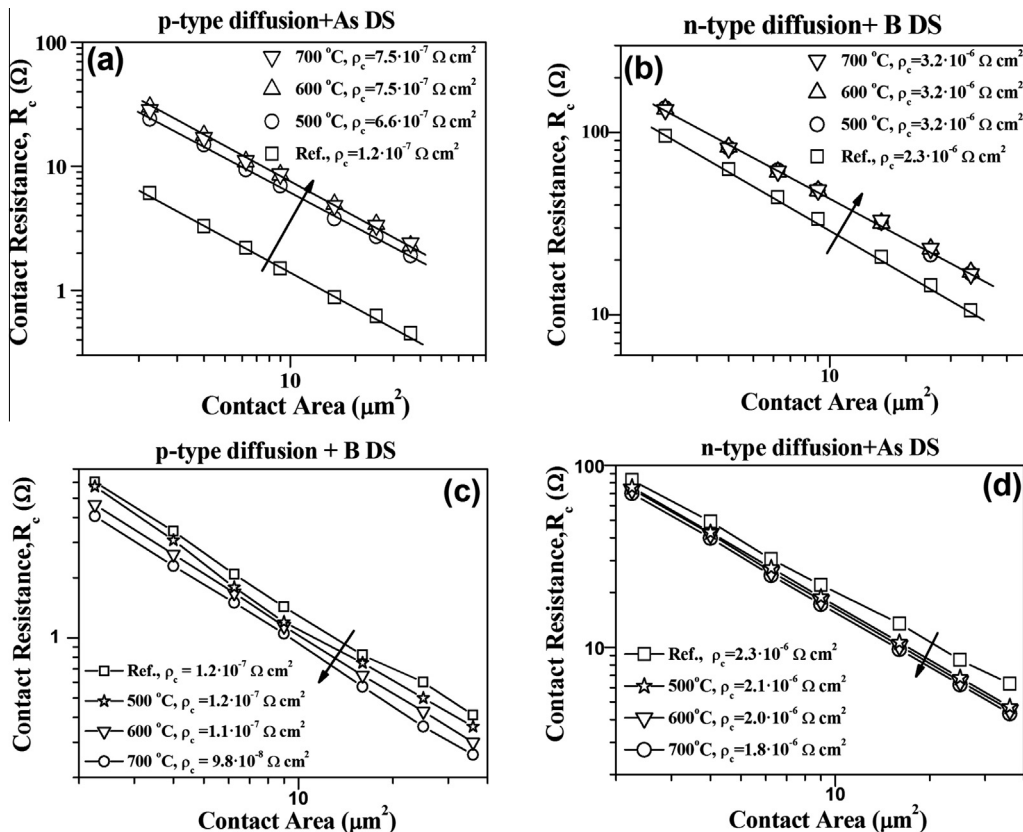
**Fig. 1.** Schematic process flow for fabrication of CBKRs. (a) LOCOS followed by ion implantation of P or B, both at  $1 \times 10^{16} \text{ cm}^{-2}$  to form the diffusion regions in substrates of the opposite conduction polarity, (b) Diffusion and activation of P and B, followed by deposition of  $\text{Si}_3\text{N}_4/\text{SiO}_2$  layer stack, (c) Self-aligned formation of PtSi followed by ion implantation of As or B to the PtSi films on both n- and p-type diffusion layers, respectively, both to  $1 \times 10^{15} \text{ cm}^{-2}$ . (d) Drive-in anneal to induce DS at the PtSi/Si interface.

regions. After deposition of a  $\text{Si}_3\text{N}_4/\text{SiO}_2$  layer stack, square contact windows of various dimensions were defined. By stripping the  $\text{Si}_3\text{N}_4/\text{SiO}_2$  layer stack in the contact windows, a 20-nm-thick platinum layer was deposited by means of electron-beam evaporation. A two-step rapid-thermal-processing (RTP) was employed to achieve self-aligned silicidation of the diffusion regions; first at  $500^\circ\text{C}$  for 30 s in  $\text{N}_2$  atmosphere to form PtSi, and then at  $600^\circ\text{C}$  for 60 s in  $\text{O}_2$  atmosphere in order to form a protective  $\text{SiO}_2$  layer for subsequent aqua regia etching [14]. Ion implantation of arsenic (As) at 12 keV or B at 2 keV to a  $1 \times 10^{15} \text{ cm}^{-2}$  dose, into the pre-formed 40 nm-thick PtSi films on both p- and n-type of diffusion regions was performed. Monte Carlo simulations showed that the implanted ions should be mainly confined in the PtSi films and the shallow implantation would yield a concentration at the PtSi/Si interface below  $1 \times 10^{15} \text{ cm}^{-3}$ . Dopant drive-in anneal was then carried out between 500 and  $700^\circ\text{C}$  for 30 s in a RTP chamber and  $\text{N}_2$  ambient. To monitor dopant activation or deactivation in the

substrate, identical drive-in anneal was performed for control wafers without As or B implantation into the PtSi films. The metal contact and leads, composed of a TiW/Al layer stack deposited by magnetron sputtering, was defined by deposition and subsequent dry etching. The fabrication process ended with forming gas annealing (FGA) in  $\text{N}_2:\text{H}_2$  (1:3) ambient at  $400^\circ\text{C}$  for 30 min. Four-point probe measurements on the CBKR structures were performed using Agilent 4156A parameter analyzer.

### 3. Results and discussion

The measured CBKR values are shown in Fig. 2, (a) for p-type diffusion region with arsenic DS, (b) for n-type diffusion region with boron DS, (c) for p-type diffusion region with boron DS, and (d) for n-type diffusion region with arsenic DS. The extracted  $\rho_c$  data are summarized in Table 1. As can be seen, two major observations are made. First, DS on the diffusion region of opposite



**Fig. 2.** Measured data for CBKRs on (a) p-type diffusion region with As DS, (b) n-type diffusion region with B DS, (c) p-type diffusion region with B DS, and (d) n-type diffusion region with As DS.

**Table 1**

Results of  $\rho_c$  (in  $\Omega\text{cm}^2$ ) extracted using the CBKR (Fig. 2) after different drive-in anneals for DS at PtSi/Si interface.

Drive-in temperature ( $^{\circ}\text{C}$ )	Arsenic DS		Boron DS	
	p-Type diffusion	n-Type diffusion	p-Type diffusion	n-Type diffusion
Reference	$1.2 \times 10^{-7}$	$2.3 \times 10^{-6}$	$1.2 \times 10^{-7}$	$2.3 \times 10^{-6}$
500	$6.6 \times 10^{-7}$	$2.1 \times 10^{-6}$	$1.2 \times 10^{-7}$	$3.2 \times 10^{-6}$
600	$7.5 \times 10^{-7}$	$2.0 \times 10^{-6}$	$1.1 \times 10^{-7}$	$3.2 \times 10^{-6}$
700	$7.5 \times 10^{-7}$	$1.8 \times 10^{-6}$	$9.8 \times 10^{-8}$	$3.2 \times 10^{-6}$

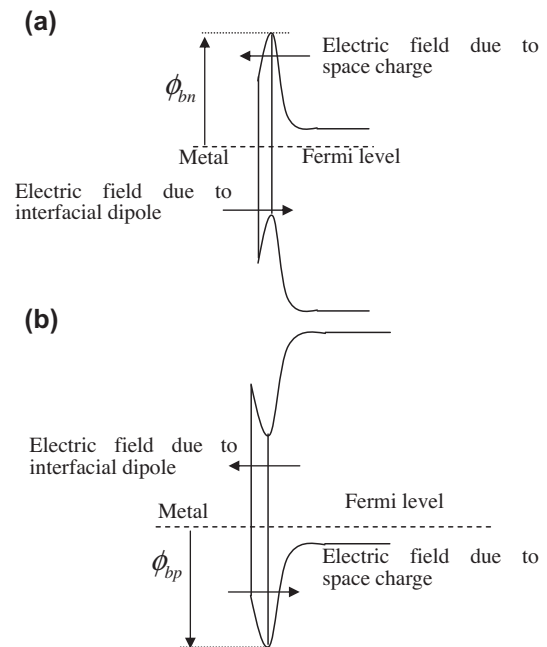
polarity, i.e., boron DS on n-type diffusion region and As DS on p-type diffusion region, leads to an increase in  $\rho_c$  for both systems with boron out-diffusion from PtSi on n-type diffusion region and arsenic out-diffusion from PtSi on p-type diffusion region, as shown in Fig. 2(a and b). On the other hand, DS on the diffusion region of alike polarity, i.e., boron DS on p-type diffusion region and As DS on n-type diffusion region, results in a decrease in  $\rho_c$  for both systems with dopant out-diffusion similarly as aforementioned, as shown in Fig. 2(c and d). Second, the increase or decrease in  $\rho_c$  is nearly temperature-dependent, since it tends to become saturated at high drive-in annealing temperatures slowly. Activation or Deactivation of substrate doping in the diffusion regions during low temperature processing, i.e., silicide formation and subsequent SADS for DS, can be ruled out as the cause for observed increase or decrease in  $\rho_c$ , since identical anneals as in Fig. 2 of reference samples without boron or arsenic implantation into the pre-formed PtSi films did not lead to conclusive changes in  $\rho_c$ .

The observed increase in  $\rho_c$  in Fig. 2(a and b) can be anticipated due to the use of dopants of opposite polarity to the substrate doping in diffusion regions. However, the saturation with the increase immediately rules out compensation doping of the diffusion regions near the PtSi/Si interface as responsible for the increase in  $\rho_c$ . More out-diffusion of dopants of opposite polarity should occur at higher drive-in annealing temperatures leading to more compensation doping (or even reverting the type of doping) in the interface region. Since this non-saturation behavior is absent in the experiment, the formation of an interfacial dipole that induces an increase in effective SBH is thus concluded as the cause responsible for the increase in  $\rho_c$ . This conclusion supports our earlier discussions in [10,11] where interaction of dopants with point defects and subsequent dopant diffusion are considered insignificant, and hence the formation of an interfacial dipole is more likely to be the cause for the modification of effective SBH. Similarly, the observed decrease in  $\rho_c$  in Fig. 2(c and d) should rather be ascribed to the formation of an interfacial dipole, instead of the use of dopants of alike polarity to the substrate doping in diffusion regions. There is little possibility that the additive doping in the interfacial region is able to result in a significant decrease in  $\rho_c$  at drive-in annealing temperature (500–700  $^{\circ}\text{C}$ ) [11]. Reducing  $\rho_c$  by means of DS has been also reported in [12] which also attribute the decrease in  $\rho_c$  to the formation of interfacial dipole.

For the observed increase in  $\rho_c$  in Fig. 2(a and b) using dopants of opposite polarity to the substrate doping in diffusion regions, a couple of differences are found between the two types of doping. First, a more significant increase in  $\rho_c$  is evident for the arsenic DS on the p-type diffusion region than for the boron DS on the n-type diffusion region. This difference is easily understood since the SBH of PtSi without DS lies close to the valance band with  $q\phi_{Bp} \approx 0.2$  eV and  $q\phi_{Bn} = 0.93$  eV [10,11]. Hence, more room is available for the reduction of  $q\phi_{Bn}$  than of  $q\phi_{Bp}$ . Second, calculations using the relationship  $\rho_c \propto \exp\left[\frac{4\sqrt{m^* \epsilon_s \phi_B}}{h\sqrt{N}}\right]$  as well as known physical parameters yielded the largest change of  $q\phi_{Bp}$  by 0.1 eV for the arsenic DS on the p-type diffusion region at 600–700  $^{\circ}\text{C}$ .

Similarly, the largest change of  $q\phi_{Bn}$  by 0.03 eV for the boron DS on the n-type diffusion region was calculated. These changes in SBHs are about 8 times smaller than those extracted using Schottky diodes made of PtSi formed on lightly doped substrates using C–V method [10,11]. This difference is attributed to the difference in the strength of electric field due to space charge that is determined by the doping concentration in the substrate. According to [15–18], the effective SBH is determined by the electric field at the metal–semiconductor interface. This electrical field comprises two major components, one due to interfacial dipole and one due to space charge. Compared to Schottky diodes without DS, additional electric fields due to interfacial dipole caused by B DS or As DS for Schottky diodes are shown in Fig. 3(a and b), respectively. Because of the opposite polarity of DS dopants to the substrate doping, the electric field originating from interfacial dipole is opposite to the electric field caused by the space charge in the diffusion region. For the lightly doped substrates ( $10^{15} \text{ cm}^{-3}$ ) used in the Schottky diodes [10,11], the maximum electric field produced by ionized dopants is around  $10^4$  V/cm. For the heavily doped diffusion regions ( $7 \times 10^{19} \text{ cm}^{-3}$ ) used in the present work, the corresponding electric field is above  $10^6$  V/cm. If the segregated dopants at the silicide/Si interface have a concentration of  $10^{12} \text{ cm}^{-2}$  which is about 0.1 at.% of a monolayer roughly corresponding to the bulk doping concentration of  $7 \times 10^{19} \text{ cm}^{-3}$ , the resulting electric field due to interfacial dipole is  $10^5$  V/cm. Therefore, the high electric field as a result of high doping concentration in the diffusion regions tends to shadow the effect of DS on the effective SBH. The same shadow effect of DS on the effective SBHs by the high doping concentration in the diffusion regions also applies to the observed decrease in  $\rho_c$  in Fig. 2(c and d), in which dopants of alike polarity to the substrate doping in diffusion regions are used. As a result, the decrease in  $\rho_c$  is not as large as expected if the changes in effective SBHs are identical to the extracted using Schottky diodes made of PtSi formed on lightly doped substrates using C–V method [10,11].

Heavy doping of the diffusion regions of the CBKR has been chosen in the present work in order to avoid current crowding effects and recourse to complex extraction procedure [19,20]. With



**Fig. 3.** Schematic presentation of the energy band structure in the vicinity of the PtSi/Si interface: (a) n-type diffusion region with B DS, (b) p-type diffusion region with As DS.

lightly doped diffusion regions, a further risk is large uncertainties as a result of extracting a small quantity out of large quantities. Although use of lightly doped diffusion regions would allow for a direct comparison with the diode results, the analysis above clearly demonstrates the validity of the contact resistivity method in assessing how the Schottky barrier could be modified by means of DS as well as in confirming the formation of interfacial dipole as the responsible mechanism for the modification.

#### 4. Conclusions

Monitoring contact resistivity has been shown as an alternative to commonly used I–V and C–V characterization of Schottky diodes for determination of SBH. This method is especially advantageous for contacts with small SBH, as it neither requires low-temperature measurement nor is affected by reverse leakage current. Through a systematic study of the variation of  $\rho_c$  of the PtSi/Si interface induced by DS, we have confirmed the formation of interfacial dipole as the cause responsible for the modification of SBH. Furthermore, the DS presents an effective way to reducing specific contact resistivity in the state-of-the-art devices.

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