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Temperature dependent transport characterization of iron on n-type (111) $Si_{0.65}Ge_{0.35}$ Schottky diodes

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Temperature dependent transport characterization of Fe/n-$Si_{0.65}Ge_{0.35}$ Schottky diodes are investigated using current-voltage measurements between 60 K and 280 K. As temperature is decreased, ideality factor increased and apparent barrier height decreased. Following this trend, charge carriers transport through Metal-Semiconductor (MS) interface changes from Thermionic Emission (TE) to Thermionic Field emission (TFE) over barrier height. In addition, evidence is presented about lateral barrier height inhomogeneity at MS contact. Barrier height ϕ_{B0} vs (1/2 kT) plots show double Gaussian distributions (GD) each with its mean barrier height and standard deviation. Modified Richardson plots obtained using this double GD lead to Richardson constant (A^*) and ϕ_{B0} in good agreement with theoretical values for $Si_{1-x}Ge_x$. Interface states density is also strongly temperature dependent indicating some temperature driven restructuring and reordering taking place at MS interface.

1. Introduction

For many decades, Schottky barrier diodes (SBDs) have been experimentally investigated to find suitable materials, devices, fabrication technologies and applications [1,2]. Metal-semiconductor (MS) structures have found many uses in microwave applications, detectors and solar cells [1–4]. Performance and reliability of Schottky contact is radically determined by interface between deposited metal and semiconductor surface. For over two decades, $Si_{1-x}Ge_x$ has gained considerable scientific interest because of its potential use in opto-electronics and high-speed electronic devices, and its compatibility with current silicon technology [5,6]. Its band gap can be engineered by varying Germanium concentration, thus allowing fabrication of many devices, such as heterojunction bipolar transistor (HBT), modulation-doped field effect transistor (MODFET), and infrared detectors [3–6]. Analysis of current-voltage (I–V) characteristics of Schottky barriers on the basis of thermionic emission (TE) reveals an abnormal increase of barrier height (BH) and decrease of ideality factor with increasing temperature [1–10]. Furthermore, ideality factor has been found to increase with increasing carrier concentration, while BH calculated from (I–V) measurements decreased with increasing doping level [1]. Analysis of current-voltage (I–V) characteristics of SBDs at room temperature doesn't give detailed information about conduction mechanisms and nature of barrier at metal/semiconductor interface [12–15]. Temperature dependence of forward I–V characteristics allows identification of different conduction mechanisms across metal/$Si_{1-x}Ge_x$ interface and to study different effects, such as barrier inhomogeneities and surface states density, which affect carrier transport at metal/$Si_{1-x}Ge_x$ Schottky barrier diodes.

Bibliographical review has shown that only few experimental investigations have been made on electrical properties and conduction mechanisms of metal/$Si_{1-x}Ge_x$ Schottky barrier devices. Mamor et al. [16] has used I–V-T characteristics to study He-ion irradiated Pd/n-$Si_{0.90}Ge_{0.10}$ Schottky contacts. They observed a strong temperature dependence of BH and ideality factor, and related this behavior to the presence of defects created by He-ion irradiation that induced a variation in number of free carriers at surface of $Si_{0.90}Ge_{0.10}$ epilayers. Janardhanam et al. [17] have reported on temperature dependence of electrical characteristics and reverse leakage conduction mechanism in Pt/n-type $Si_{0.85}Ge_{0.15}$ Schottky contacts on n-Si(100) substrates. They found that barrier height, ideality factor and series resistance were temperature dependent, with barrier height increasing and ideality factor decreasing when temperature is increased. Saha et al. [18] studied

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the effect of temperature annealing (300–900 °C) on interface states of Ni-Silicide/p-$Si_{0.75}Ge_{0.25}$ on p-Si(100), and observed that barrier height, obtained by I–V and C-V measurements, was temperature annealing dependent, and energy distribution of interface states density determine by C-V method decrease with increasing states energy from valence band edge.

In previous work we have investigated Fe/n-$Si_{0.65}Ge_{0.35}$ and Pt/n-$Si_{0.65}Ge_{0.35}$ Schottky diodes at room temperature and found that Fe/n-$Si_{0.65}Ge_{0.35}$ present anomalous characteristics compared with Pt/n-$Si_{0.65}Ge_{0.35}$ (ideality factor; series resistance; Density of interface states). Electrical characteristics of Fe/n-$Si_{0.65}Ge_{0.35}$ are closer to the MIS structure than to the MS structure. For this raison we investigated the mechanism transports in such structure. Low temperature is usually advised for this investigation.

Hence, it is of technological importance to analyze and understand the current transport mechanisms of Metal/$Si_{1-x}Ge_x$ structures at low temperatures. It is believed to offer a better understanding of the nature of the barrier formed at metal–semiconductor interface, which in turn can give insight into various aspects of conduction mechanisms. Although Metal/$Si_{1-x}Ge_x$ Schottky contact is of great importance in $Si_{1-x}Ge_x$ device technology, details are currently not available regarding current transport mechanisms and other properties of Fe/n-$Si_{1-x}Ge_x$ over a wide range of temperatures. Iron (Fe) has been used because of its good physical characteristics. Present work seeks to physically understand the origin of barrier inhomogeneity and to comprehend current transport characteristics of Fe/n-$Si_{1-x}Ge_x$ Schottky diodes in 60–280 K temperature range. The study investigates I–V-T characteristics of Fe/n-$Si_{0.65}Ge_{0.35}$ SBD under a wide range of low temperatures.

2. Experimental detail

Fabrication of Fe/n-$Si_{1-x}Ge_x$ (x = 35%) Schottky diodes used molecular beam epitaxy (MBE) growth, at a substrate temperature of 550 °C, of n-type (111) oriented $Si_{0.65}Ge_{0.35}$ films Antimony doped ($N_D = 3–4 \times 10^{15} cm^{-3}$). Films thickness was 2 µm on 350 µm thick (111) crystal orientated Si substrats having ≅0.7 Ω.cm resistivity. Immediately after surface cleaning, high purity (99.999%) circular Iron (Fe) contact, 1.3 mm in diameter and ~0.2 µm of thickness were thermally evaporated onto $Si_{1-x}Ge_x$ wafer. High vacuum metal evaporation system had a pressure of about 10^{-6} Torr. Low resistivity ohmic back metal contact was obtained with Al metallization of wafer back-side. More experimental detail on samples can be found in previous paper [19]. Fig. 1 shows schematic diagram of Fe/n-$Si_{0.65}Ge_{0.35}$ Schottky barrier devices.

Low-temperature I–V characteristics were obtained in temperature range 60–280 K using an automated setup including an Agilent precision semiconductor parameters analyzer (4156C) and a cryostat with Lakeshore 336 temperature controller. Carrier concentration of epitaxial layer, 3×10^{15} cm^{-3}, was determined using reverse-bias C-V characteristics at 1 MHz with an Agilent LCR meter (4980 A).

3. Results and discussion

3.1. Current–voltage- temperature (I–V–T) characteristics

Forward and reverse current-voltage (I–V) characteristics of Fe/n-$Si_{0.65}Ge_{0.35}$ Schottky contacts in temperature range 60–280 K are shown in Fig. 2. Current (I) through a Schottky barrier diode (SBD) at a forward bias (V) according to thermionic emission (TE) theory is given by Refs. [20,21].

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

where I_S is saturation current derived from forward-bias semi-logarithmic lnI vs V plots and can be written as

$$I_S = AA^*T^2 exp\left(\frac{-q\phi_{B0}}{kT}\right), \quad (2)$$

where A is diode area, V is applied voltage, q is electronic charge, k is Boltzmann's constant, T is absolute temperature in Kelvin, n is ideality factor and A^* is effective Richardson's constant (110 A/cm^{2}K^2 for n-type $Si_{1-x}Ge_x$ ($x \le 0.85$)). The value of n is calculated from slope of linear region of forward-bias lnI vs V plots and can be written from (1) as

$$n = \frac{q}{kT}\left(\frac{dV}{dln(I)}\right). \quad (3)$$

Ideality factor (n) is introduced to take into account deviation of experimental I–V data from ideal thermionic emission model and should be n = 1 for an ideal contact. Zero-bias barrier height ϕ_{B0} is determined from extrapolation of I_S in semi-log forward-bias lnI vs V characteristics as

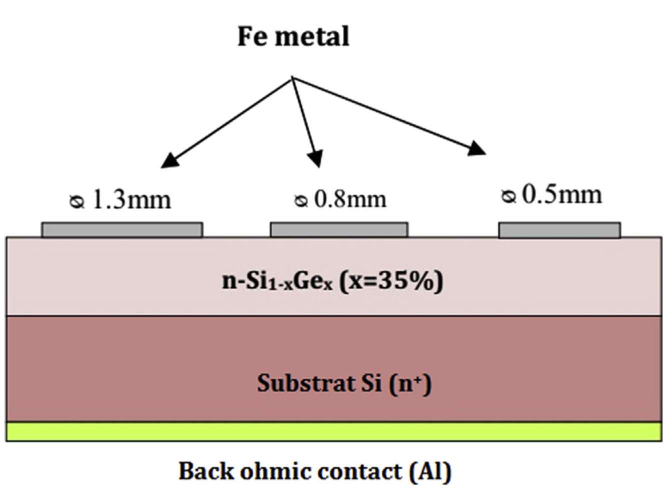

Fig. 1. Schematic diagram of Fe/n-$Si_{0.65}Ge_{0.35}$ Schottky barrier diodes.

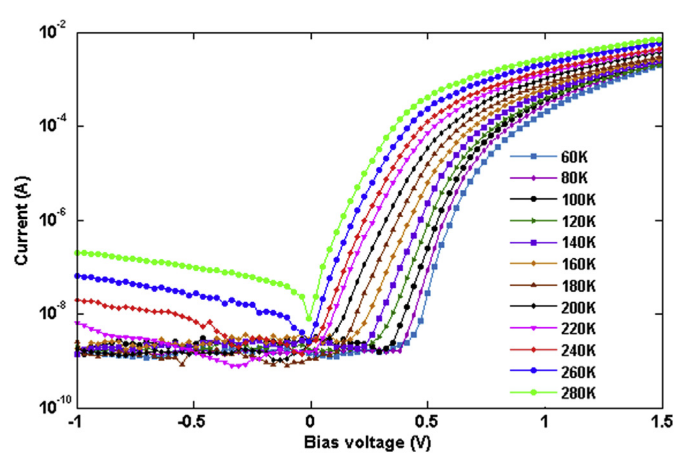

Fig. 2. Current-voltage (I–V) characteristics of Fe/n-$Si_{0.65}Ge_{0.35}$ Schottky contact in the temperature range of 60–280 K.

$$\phi_{B0} = \frac{kT}{q} ln\left(\frac{AA^*T^2}{I_S}\right). \tag{4}$$

Values of extracted barrier height and ideality factor for various values of temperature from 60 K to 280 K are determined from intercepts and slope of forward-bias lnI vs V plots at each temperature using Eq (3) and Eq (4). Estimated values of n and ϕ_{B0} for Fe/n-$Si_{0.65}Ge_{0.35}$ Schottky diodes range from 5.8 to 0.236 eV (at 60 K) and 1.85 to 0.684 eV (at 280 K), respectively. Such temperature dependence of apparent Schottky barrier height and ideality factor is shown in Fig. 3a. It can be seen from Fig. 3a that ϕ_{B0} decreases while n increases with decreasing temperature. Obtained experimental values of I_S, n and Φ_{B0} for the Fe/n-$Si_{0.65}Ge_{0.35}$ SBD for Ln(I) versus V plots at each temperature are tabulated in Table 1.

This behavior is possibly caused by structural defects in semiconductor, inhomogeneous doping, interface roughness and/or interfacial reactions. Other possible effects are thickness and stoichiometry inhomogeneities, non-uniformity in interfacial charges distribution and/or the presence of a thin insulating layer between metal and semiconductor [3,22,23]. Since current transport across metal/semiconductor (MS) interface is a temperature activated process, electrons at low temperatures can overcome lower Schottky barrier heights (SBHs) and dominant current flow is through regions of lower SBHs. As temperature increases, more electrons have sufficient energy to surmount higher SBHs. Therefore, dominant barrier height increases with temperature and current transport will be dominated by current flowing through patches of lower SBHs [10]. Since in high voltage region Ln(I)-V slope deviates from linearity, Fe/n-$Si_{0.35}Ge_{0.65}$ SBD series resistance profile was obtained from I–V data by replacing voltage by (V–IR_S) in Eq. (1). Fig. 3 b shows such series resistance profile as a function of temperature. R_S values change exponentially with temperature and decrease from 456 Ω to 107 Ω in 60–280 K temperature range. Such expected behavior is related to an increase in $Si_{1-x}Ge_x$ conductivity with temperature [11].

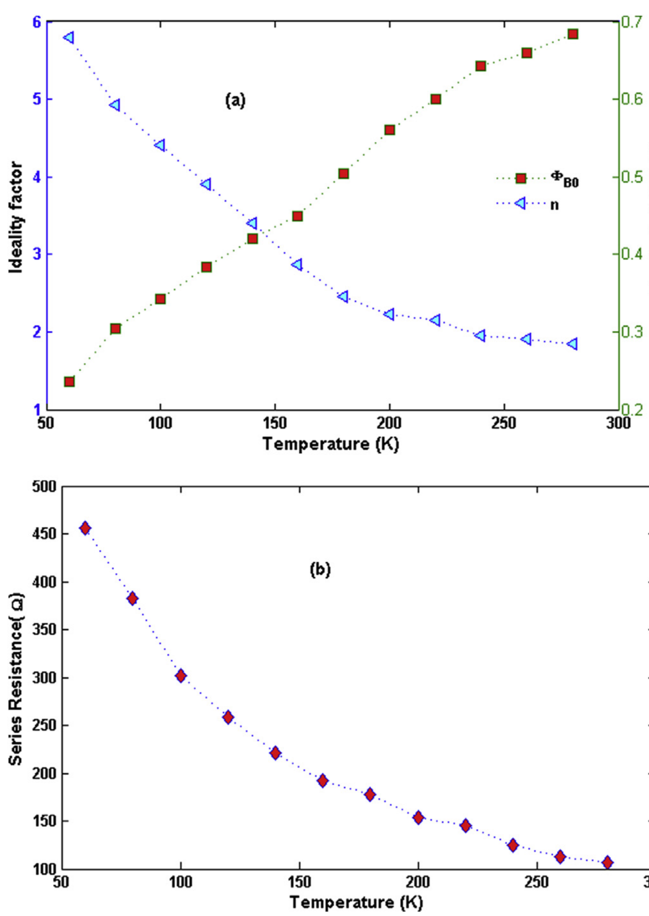

Fig. 3. Temperature dependence plot of (a) barrier height and ideality factor, (b) series resistance (R_S) in 60–280 K range.

3.2. Effect of thermionic field emission (TFE)

Usually current-voltage (I–V) characteristics of Fe/n-$Si_{0.65}Ge_{0.35}$ SBDs are analyzed based on TE model. Observed ideality factors are greater than unity for our sample, implying that pure TE model is inappropriate to explain current-voltage (I–V) characteristics. Mechanisms such as tunneling and generation–recombination must be considered to explain observed variation of ideality factor and zero-bias barrier height. If current transport is controlled by thermionic field emission (TFE) theory, the relation between current and voltage can be expressed as [24].

$$I = I_s exp\left(\frac{V}{E_0}\right) \tag{5a}$$

$$E_0 = E_{00} coth\left(\frac{qE_{00}}{kT}\right) = \frac{nkT}{q} \tag{5b}$$

where E_{00} is characteristic energy, which is related to transmission probability of carrier through barrier and given as

$$E_{00} = \frac{h}{4\pi}\left(\frac{N_D}{m_e\varepsilon_s}\right)^{1/2} = 18.5\times10^{-15}\left(\frac{N_D}{m_r\varepsilon_r}\right)^{1/2} \tag{6}$$

In the case of Fe/n-$Si_{0.65}Ge_{0.35}$ Schottky diodes, with $N_D = 3\times10^{15}$ cm^{-3}, $m_e = 0.92m_0$, and $\varepsilon_s = 12.9\varepsilon_0$, E_{00} value turns out to be 9.2 meV. According to transport theory, TFE dominates only when $E_{00} \approx kT$ and the value of E_{00} calculated using Eq. (6) is almost equal to the value of kT at 110 K. Barrier height lowering, $\Delta\phi_{TFE}$, due to TFE can be determined from Ref. [20].

$$\Delta\phi_{TFE} = \left(\frac{3}{2}E_{00}\right)^{2/3}(V_d)^{1/3} \tag{7}$$

where V_d is built in potential. For a built in potential of 0.59 V and a value of E_{00} of 9.2 meV, calculated barrier height lowering is 49 meV. This cannot account for the presently observed lowering of barrier height. Fig. 4 shows a plot of E_0 versus kT/q where E_0 is determined from Eq. (5b). A data linear fit results in a y-intercept that gives an E_0 value of 6.8 meV. This linear fit is good enough down to a 120 K temperature and deviates below that temperature. This experimentally deduced E_0 value of 6.8 meV is less than theoretically calculated value of 9.2 meV. For temperatures around 80 K, characteristic energy is high and conduction mechanism is TFE dominating.

Values of 1/n were theoretically calculated using the following equation [21]:

$$\frac{1}{n} = \frac{kT(1-\beta)}{qE_0} \tag{8}$$

where β indicates bias dependence of barrier height. Experimentally observed values of 1/n were superimposed on theoretically generated 1/n versus 1000/T plots in Fig. 5, to estimate characteristic energy. This plot provides a good check to know whether conduction mechanism is TFE or TE. By analyzing the experimental

Table 1
Electrical parameters extracted from I–V-T of Fe/n-$Si_{0.65}Ge_{0.35}$.

Temperature T (K)	Saturation current I_S (A)	Barrier height ϕ_{B0} (eV)	Ideality factor (n)	Series resistance R_S (Ω)
60	5.23×10^{-17}	0.236	5.80	456
80	8.47×10^{-16}	0.304	4.92	382
100	2.11×10^{-14}	0.342	4.40	302
120	2.50×10^{-13}	0.384	3.90	258
140	2.62×10^{-12}	0.420	3.40	221
160	2.23×10^{-11}	0.450	2.87	192
180	9.41×10^{-11}	0.504	2.45	178
200	3.25×10^{-10}	0.560	2.23	154
220	6.87×10^{-10}	0.600	2.15	145
240	2.16×10^{-09}	0.643	1.95	125
260	6.88×10^{-09}	0.660	1.90	113
280	3.60×10^{-08}	0.684	1.85	107

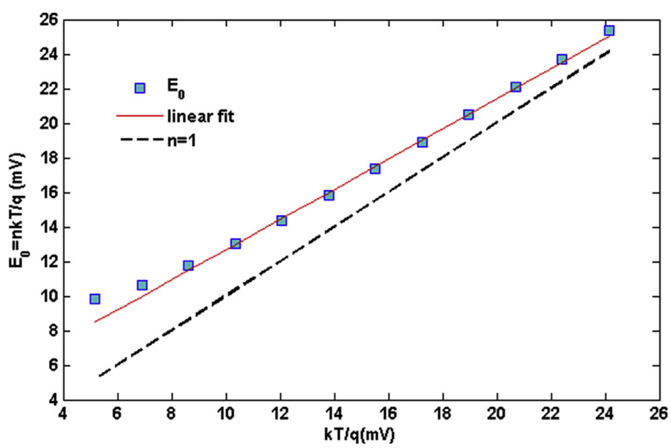

Fig. 4. Plot of E_0 vs kT/q using Eq. (5b) assuming TFE conduction.

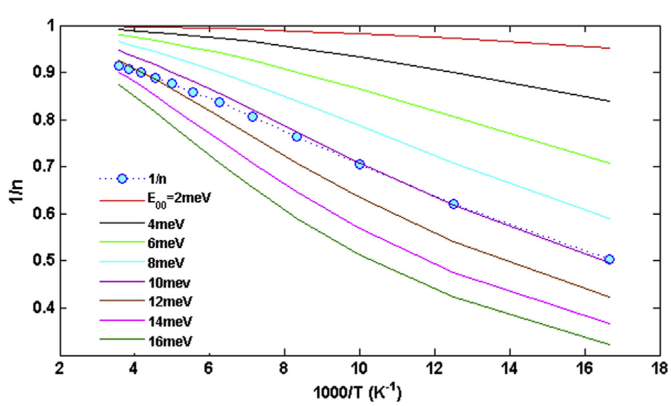

Fig. 5. 1/n vs 1000/T plots with E_{00} as parameter and generated using Eq. (8) with $\beta = 0$.

values, a characteristic energy E_{00} of 10 meV and β of 0.02 were obtained for a temperature range of 60–120 K. At high temperature, E_{00} is about 12 meV as observed on Fig. 5. Higher values of E_{00} confirm that at lower temperatures diode conduction mechanism is TFE dominated, while at higher temperatures it is TE-diffusion that dominates. A high characteristic energy has been related to several effects such as density of states and electric field present on semiconductor surface [24]. Electric field near semiconductor surface can be increased by mechanisms such as surface roughness, geometrical inhomogeneities due to crystal defects, and presence of thick interfacial insulating layer between deposited metal and semiconductor surface [24,25].

3.3. Barrier height inhomogeneities

Fig. 6 shows a plot of ideality factor versus barrier height for Fe/n-$Si_{0.65}Ge_{0.35}$ SBDs. This straight line plot indicates a linear relationship between experimental effective barrier height and ideality factor of Schottky diodes. Again, the decrease of ideality factor and increase of barrier height with increasing temperature shows a discontinuity at the Fe/n-$Si_{0.65}Ge_{0.35}$ interface. Similar results have been reported in the literature [26–28]. Fig. 6 shows two distinct linear regions that indicate lateral inhomogeneities in barrier heights. Extrapolating these straights lines for ideality factor $n = 1$ gives barrier heights values of 0.954 and 0.59 eV for linear fit 1 and linear fit 2, respectively.

To explain barrier height decrease with decreasing temperature, let consider a lateral Gaussian distribution of barrier height values over Schottky contact area with a mean barrier height, $\overline{\phi}_{B0}$ and standard deviation, σ_0. Standard deviation will measure barrier homogeneity. This Gaussian distribution [3,29,30] is expressed as

$$\phi_{ap} = \overline{\phi}_{B0}(T=0) - \frac{q\sigma_0^2}{2kT}, \tag{9}$$

where ϕ_{ap} is apparent barrier height measured experimentally. Temperature dependence of σ_0 is usually small and can be neglected. Variation of observed ideality factor with temperature in such model is given [3,31] as

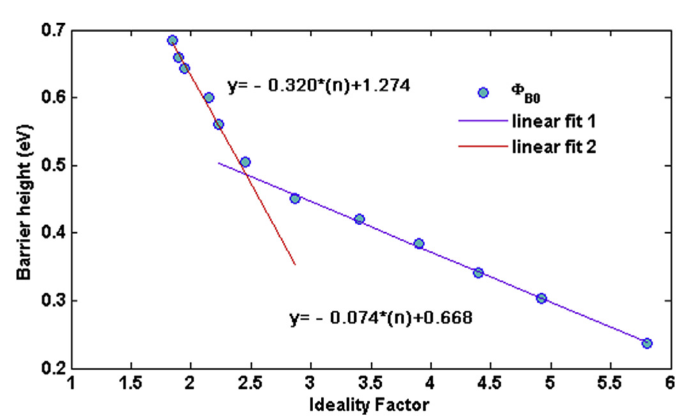

Fig. 6. Schottky barrier heights *vs* ideality factor plots of Fe/n-$Si_{0.65}Ge_{0.35}$SBDs in 60–280 K temperature range.

$$\left(\frac{1}{n_{ap}}-1\right)=-\rho_2+\frac{q\rho_3}{2kT}, \tag{10}$$

where n_{ap} is apparent ideality factor, ρ_2 is voltage coefficient of mean barrier height, and ρ_3 is voltage coefficient of standard deviation. Assuming a linear bias dependence of both mean barrier height, $\overline{\phi}_{B0}$ and square of standard deviation, σ_0^2, with coefficient ρ_2 and ρ_3 such as $\overline{\phi}_B$ (V) = $\overline{\phi}_{B0}$ + ρ_2V and σ_0^2(V) = σ_0^2 + ρ_3V, one can plot experimental ϕ_{ap} vs 1/2 kT and (n^{-1}-1) vs 1/2 kT, Figs. 7 and 8. Both plots show two straight lines instead of one single line with transition occurring at 140 K. These two different slopes at the lower and higher temperatures indicate two interface regions with different mean barrier heights. Two sets of σ_0 and $\overline{\phi}_{B0}$ values are obtained from slopes and intercepts of these straight lines. They are 0.124 V and 1.01eV in 160–280 K temperature range (distribution 1), and 0.054 V and 0.521 eV in 60–120 K temperature range (distribution 2), respectively. Chand and Kumar [31] have also attributed the existence of a double Gaussian barrier heights distribution at metal/semiconductor contacts to interface nature inhomogeneities that influence I–V characteristics, particularly at low temperatures. Hence, barrier height patched interface electrically influence I–V characteristics of Schottky diodes, particularly at low temperatures. Thus, I–V measurements at very low temperatures reveal interface nature and covered temperature range by each straight line suggests where corresponding distribution is effective [31].

Fig. 8 shows n_{ap} vs 1/2 kT plots with intercept and slope of straight lines used to evaluate voltage coefficients ρ2 and ρ3, respectively. Obtained ρ2 values are −0.202 eV in 140–280 K range (distribution 1) and 0.67 eV in 60–120 K range (distribution 2), whereas ρ3 values are −0.0154 eV in 140–280 K range (distribution 1) and −0.0017 eV in 60–120 K range (distribution 2). Such linear behavior also explains voltage deformation of Gaussian distribution of Schottky barrier heights. Evaluated ρ_3 value of distribution 1 is larger than that of distribution 2 indicating that distribution 1 has larger and relatively higher BH. This is also obvious from determined mean BH and standard deviation values of distributions 1 and 2. According to Reddy et al. [32], one may attribute distribution 2 at very low temperatures to some phase changes taking place on cooling below a certain temperature.

Barrier height is also accurately evaluated from Richardson's plot ln(I_s/T^2) vs q/kT, shown in Fig. 9, and obtained by rewriting equation (2) as

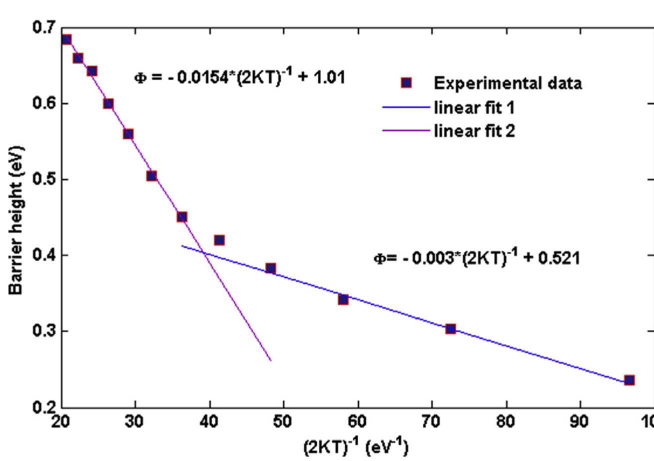

Fig. 7. Zero-bias apparent barrier height ($\phi_{B0\ (I-V)}$) vs q/2 kT plots for Fe/n-$Si_{0.65}Ge_{0.35}$ SBD (Double Gaussian model).

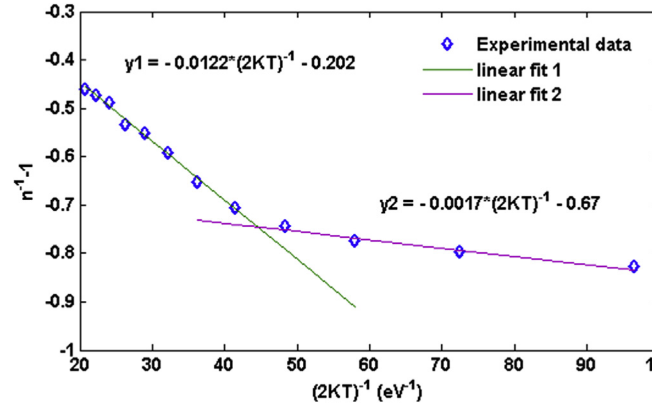

Fig. 8. Ideality factor (n^{-1}-1) vs q/2 kT plots for Fe/n-$Si_{0.65}Ge_{0.35}$SBDs (Double Gaussian model).

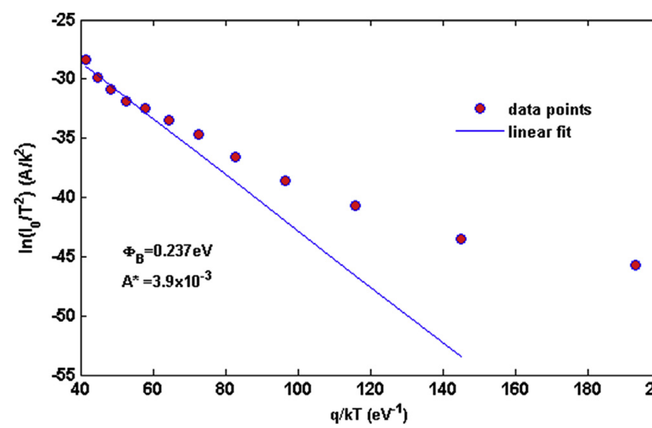

Fig. 9. Richardson's plot for Fe/n-$Si_{0.65}Ge_{0.35}$ SBDs.

$$ln\left(\frac{I_s}{T^2}\right)=ln(AA^*)-\frac{q\phi_B}{kT} \tag{11}$$

Intercept at q/kT = 0 gives ln(AA^*) value from which Richardson constant A^*can be evaluated. Richardson's plot slope gives barrier height value ϕ_{B0}.

From this plot linear fit, evaluated Richardson constant A^* is 3.9×10^{-3} $Acm^{-2}K^{-2}$ and barrier height ϕ_{B0} is 0.237 eV. Richardson constant is found to be much lower than theoretically expected value of 110 $Acm^{-2}K^{-2}$ for $Si_{1-x}Ge_x$ ($x \leq 0.85$). Equally, barrier height 0.237 eV value is also found to be much lower than that expected for metal-$Si_{1-x}Ge_x$ contact. This discrepancy in values is another proof of interface inhomogeneities at Schottky contact and non uniformity of Schottky barrier height over entire metal contact area.

These barrier height inhomogeneities are accounted for in modified Richardson's plot. Equation that takes care of Gaussian distribution of mean barrier height ϕ_{B0} with standard deviation σ_0^2 is given by

$$\ln\left(\frac{I_s}{T^2}\right)-\left(\frac{q^2\sigma_0^2}{2k^2T^2}\right)=ln(AA^*)-\frac{q\overline{\phi}_{B0}}{kT} \tag{12}$$

I_S/T^2 -($q^2\sigma_0^2/2k^2T^2$) values are calculated using σ_{01} = 0.124 V in 120–280 K temperature range (region I) and σ_{02} = 0.054 V in 60–120 K temperature range (region II), Fig. 10. The linear fits to the modified experimental data are delineating by solid lines in Fig. 10 which represent the true activation energy plots in respective temperature ranges. Slopes calculations give zero-bias mean

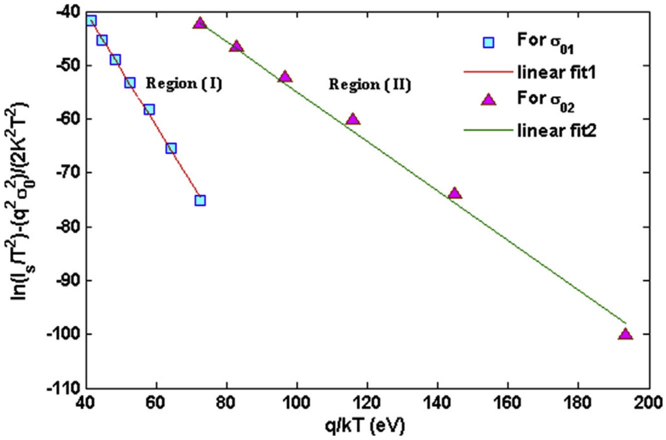

Fig. 10. Modified Richardson $\ln(I_S/T^2)$-$(q^2\sigma_0^2/2k^2T^2)$ vs q/kT plots of Fe/n-$Si_{0.65}Ge_{0.35}$ SBDs.

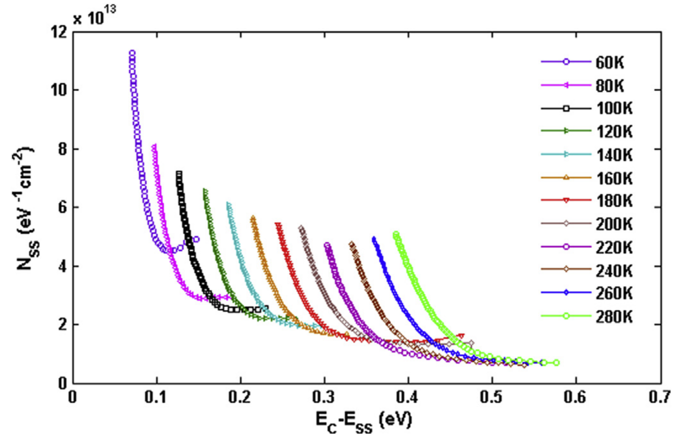

Fig. 11. N_{SS} as a function of E_C -E_{SS} for Fe/n-$Si_{0.65}Ge_{0.35}$ Schottky diodes at various temperatures.

barrier height ϕ_{B0} of 0.462 eV in region I and 1.06 eV in region II. From intercepts at ordinate, Richardson's constant A* is 113.77 A $cm^{-2}K^{-2}$ in region I and $8.28_{\times}10^4$ A.$cm^{-2}K^{-2}$ in region II. This Richardson coefficient value in region I is close to 110 A $cm^{-2}K^{-2}$ theoretical value adopted for n-type $Si_{1-x}Ge_x$ at room temperature [33]. In region II, modified A* value is 700 times higher than theoretical value and is explained in terms of barrier height variation with the temperature [40].

3.4. Determination of interface state density

Ideality factor is found to be greater than unit for high current injections [20] and at low temperatures as shown above. Interface states play an important role in conduction in metal/semiconductor rectifying devices [21]. Indeed, effective barrier height ϕ_e is assumed to be bias-dependent because of interface states and is given [34] as

$$\phi_e = \phi_{B0}^{I-V}\left(\frac{d\phi_e}{dV}\right) = \phi_{B0}^{I-V} + \beta V \tag{13}$$

where $\beta = 1-(1/n)$ is change in effective barrier height with bias voltage. For Fe/n-$Si_{0.35}Ge_{0.35}$ Schottky diodes having interface states in equilibrium with semiconductor, ideality factor becomes greater than unity [35] and is given as

$$n(V) = 1 + \frac{\delta}{\varepsilon_i}\left[\frac{\varepsilon_S}{W_D} + qN_{SS}\right] \tag{14}$$

where W_D is space charge region width, δ is thickness of interfacial layer, ε_i and ε_S are permittivities of interfacial layer and semiconductor and N_{SS} is density of interface states, respectively. Thus, from equation (14), interface density of states can be given as

$$N_{SS}(V) = \frac{1}{q}\left[\frac{\varepsilon_i}{\delta}(n(V) - 1) - \frac{\varepsilon_S}{W_D}\right] \tag{15}$$

In an n-type semiconductor, energy of interface states E_{SS} with respect to the bottom of semiconductor conduction band is given [35–37] as

$$E_C - E_{SS} = q(\phi_e - V) \tag{16}$$

Thus, using equations (15) and (16) and taking into account bias dependence of ideality factor n(V), interface states density in equilibrium with semiconductor is determined as a function of (E_C-E_{ss}), Fig. 11. From the figure, it can be seen that an exponential increase in interface states density exists from mid gap to bottom of conduction band. At low temperatures (60 K) interface state density (N_{SS}) varied from 11.1×10^{13} $eV^{-1}cm^{-2}$ to 4.38×10^{13} $eV^{-1}cm^{-2}$ when E_{ss} changed from 0.078 eV to 0.144 eV. At high temperatures (280 K), N_{SS} varied from $50.1 \times 10^{12} eV^{-1}cm^{-2}$ to 6.87×10^{12} $eV^{-1}cm^{-2}$ when E_{ss} changed 0.385 eV–0.593 eV. Such N_{SS} temperature dependence follows ideality factor temperature dependence and is due to lateral inhomogeneities of barrier height at metal-semiconductor interface [38]. Increasing barrier height with increasing temperature leads to an increase in (E_C-E_{SS}) energy (Eq. (16)) and this is clearly shown in the strong shift of state density distribution curves. Increase in N_{SS} with decreasing temperature is the result of thermal driven molecular rearrangement of metal-semiconductor interface [39].

4. Conclusion

Rectifying properties of Fe/n-$Si_{0.65}Ge_{0.35}$ (111) Schottky contacts are investigated at low temperatures from 60 K to 280 K using current-voltage measurements. Apparent barrier height ϕ_{B0} and ideality factor n are extracted and found to increase and decrease with increasing temperature, respectively. This behavior of Φ_{B0} and n with temperature was attributed to barrier inhomogeneities assuming Gaussian distribution at M/S interface. In Fe/n-$Si_{1-x}Ge_x$ (111) structures, Thermionic Field Emission (TFE) electronic transport is found to dominate at low temperatures in the range (60 K-120 K) while TE transport mechanism is dominant at greater temperatures. Relationship between ϕ_{B0} and n showed two linear regions that indicate a barrier height patched-like interface. Extrapolation of experimental barrier height and ideality factor plots for n = 1 gave barrier height mean values of 0.954 and 0.59 eV for region I and region II, respectively. Assuming Gaussian distribution in each region weighting coefficients, standard deviations, and mean barrier heights are calculated for each distribution. Richardson constant estimated in temperature range 140–280 K (113 A $cm^{-2}K^{-2}$) is in close agreement with theoretical value (110 A $cm^{-2}K^{-2}$). Calculated interface states density value (N_{SS}) ~ 10^{13} $eV^{-1}cm^{-2}$ is in the range found for Schottky diodes. N_{SS} was also found to decrease with increasing temperature. This behavior can be attributed to thermally driven restructuring and reordering taking place at interface.

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