Temperature-dependent barrier characteristics of swift heavy ion irradiated Au/*n*-Si Schottky structure

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The electrical behavior of Au/*n*-Si(100) structure, irradiated with 120 MeV $^{107}Ag^{8+}$, has been investigated in a wide temperature range (50–300 K). The forward bias current-voltage (*I*-*V*) and reverse bias capacitance-voltage (*C*-*V*) measurements have been used to extract the diode parameters. The variations in various parameters of the irradiated Schottky structure have been systematically studied as a function of temperature. It is found that the flatband barrier height is almost independent of the change in temperature. The ionized-donor concentration decreases while the ideality factor increases with decreasing temperatures. The behavior of Schottky parameters is explained by taking into account the role of the swift heavy ion irradiation induced defects at metal-semiconductor junction. The results are interpreted on the basis of recent models of Fermi level pinning. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2388855]

I. INTRODUCTION

The increasing interest of the heavy ion beams in processing technologies motivate a thrust in studies of defects induced by irradiations of swift heavy ions in semiconductors.[1–3] Metal-semiconductor (MS) structure is one of the important research tools in the characterization of semiconductor materials and fabrication of these structures plays a crucial role in construction of some useful devices in technology.[4] Formation of the potential barrier in a metal semiconductor junction is of prime interest in the current research. The position of the Fermi level within the semiconductor band gap determines the height of this potential barrier. In general, the exact position of the Fermi level depends on the properties of the interface. At an ideal, defect-free interface the barrier height is determined by the charge neutrality level of the metal induced gap states (MIGS).[5,6] These states originate from the tails of the metal wave functions into the semiconductor. These states are predominantly donorlike close to the valence band maximum while they are predominantly acceptorlike close to the conduction band minimum. The crossover between both types is known as the charge neutrality level. Alignment of this level with the Fermi level of the metals is required for the charge neutrality and therefore it determines the Schottkybarrier height (SBH). Any chemical reaction or imperfections at the interface is not considered in this model. In addition to the MIGS, defects can exist at the MS interface. The electrical characteristics of Schottky contacts are very sensitive to the defects at the MS interface. Swift heavy ion (SHI) irradiation is one of the mechanisms able to modify the barrier characteristics of MS interface.[7] When a swift heavy ion passes through the semiconductor it produces various types of defects. These defects give rise to additional discrete levels in the band gap (possibly deep levels) and the Fermi level is pinned to one of these levels, possibly quite far from the charge neutrality level.

As varying the temperature is the easiest way of varying the band gap in the semiconductor, the investigation of temperature dependence of SBH is very helpful to understand the problem of Fermi level pinning in a certain MS contact. When the Fermi level is pinned to the charge neutrality level, the temperature dependence of the barrier height is controlled by the temperature dependence of the band gap, the direct gap as well as indirect gap.[8,9] However, if the Fermi level is pinned by defects their ionization entropy would govern the temperature dependence of the barrier height.[10] Since the temperature dependence of the band gap is much larger than that of the ionization entropy, measurements evolution allow one to distinguish between both pinning mechanisms. Although some authors[11–13] considered the origin of the Fermi level pinning such as contamination in the interface and deep impurity level, such type of defects are never identified in silicon. The temperature dependence of the SBH in the Au/*n*-Si contacts is almost identical to that of the band gap in silicon.[14] But in our case of irradiated Au/*n*-Si, SBH is found almost independent of temperature.

In the present work, we have investigated the barrier height of irradiated Au/*n*-Si Schottky diode and its temperature dependence. The results are interpreted using recent models of Schottky barrier formation and Fermi level pinning. The role played by the SHI irradiation-induced interface defects in this process is discussed.

II. EXPERIMENT

The Schottky diodes were fabricated by using *n*-type Si (100) both side polished sample of resistivity 0.5 Ω cm. The samples were carefully cleaned chemically in trichloroethylene (TCE), acetone, and methanol. The samples were then deoxidized in a 2% HF solution and rinsed in de-ionized water of resistivity 15 MΩ for 30 s. To make Ohmic contacts aluminum was deposited by thermal evaporation method in high vacuum chamber followed by a temperature treatment at 525 °C for 25 min in argon gas environment. Schottky contacts were created by deposition of Au on the sample

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having Ohmic contact by thermal resistive heating technique in an ultrahigh vacuum chamber. A 100 nm Au layer was deposited through a stainless steel mask having contact diameter of 2 mm at a base pressure of 10^{-8} mbars region. The thickness of the metal layer was monitored with quartz crystal thickness monitor.

The irradiation was performed by 120 MeV $^{107}Ag^{8+}$ ion beam using the 15UD Pelletron accelerator facility at Inter-University Accelerator Centre, New Delhi.[15] The irradiation fluence was 5×10^{11} ions cm^{-2}. The current-voltage (I-V) measurements were carried out with a programmable Keithly 2400 source meter at varying temperature from 300 to 50 K. The capacitance-voltage (C-V) measurements were carried out at 1 MHz by using Boonton 7200 capacitance meter. Cooling was performed with a close cycle He refrigerator. The temperature was controlled by a stabilization loop consisting of a temperature diode, a heating resistance, and a Lakeshore temperature controller, which regulates the temperature to a preset value. The variation of temperature was better than ±0.5 K during each temperature point of measurement. All measurements were carried out in a vacuum of 10^{-3} mbar region.

III. EXPERIMENTAL RESULTS AND DISCUSSION

A. Capacitance-voltage characteristics

The experimental C-V characteristics have been analyzed using the Schottky-Mott equation,[16]

$$C = \frac{\varepsilon_S A}{W} = \sqrt{\frac{q\varepsilon_S N_D A^2}{2(V_{\mathrm{bi}} - V - V_T)}}, \tag{1}$$

where ε_S the dielectric constant of the semiconductor, A is the area of the Schottky contact, W is the depletion width, N_D is the concentration of ionized donor atoms, V_{bi} is the built-in potential, V_T ($=kT/q$) is the thermal voltage, and V is the applied reverse bias. Using Eq. (1) the value of N_D may be written as

$$N_D = \frac{2}{q\varepsilon_S A^2}\left[\frac{-1}{(d(1/C^2)/dV)}\right]. \tag{2}$$

Hence from the slope of $1/C^2$ vs V curve the value of ionized dopant concentration N_D or free carrier concentration can be obtained. The SBH Φ_B (C-V) is related to the built-in voltage V_{bi} by the following equation:

$$\Phi_B(C-V) = V_{\mathrm{bi}} + \frac{kT}{q}\ln\left(\frac{N_C}{N_D}\right), \tag{3}$$

with

$$N_C = 2\frac{(2m^* kT)^{3/2}}{h^3}, \tag{4}$$

where N_C is the effective density of states in Si conduction band and N_D is the donor concentration. $m^* = 1.08 m_0$ is the effective mass of electrons in Si and m_0 is the rest mass of electron.[4] From the intercept of the $1/C^2$ vs V curve on the voltage axis, the value of V_{bi} is calculated.

Figure 1 shows the $1/C^2$ vs V characteristics of irradiated Au/n-Si Schottky diode at different temperature. The

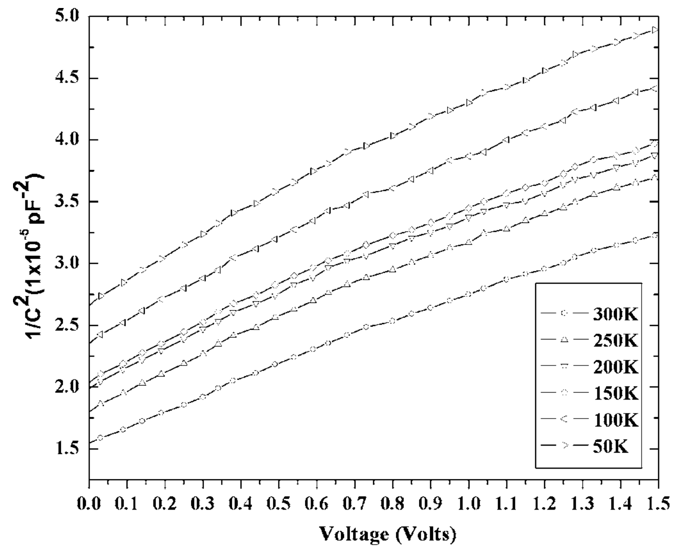

FIG. 1. Reverse bias capacitance-voltage characteristics of irradiated Au/n-Si(100) Schottky barrier diode at different temperatures.

capacitance decreases as a function of temperature. At room temperature the value of capacitance at zero bias was 255 pF while at a temperature 50 K its value becomes 195 pF. From the experimental $1/C^2$ vs V curve, the values of donor concentration N_D and SBH Φ_B (C-V) have been determined. The donor concentration at room temperature was 1.27×10^{15} cm^{-3}. It then decreased with decrease in temperature and at a temperature 50 K its value came down to 1.07×10^{15} cm^{-3}. The value of SBH for irradiated diode at 300 K was 0.86 eV and then it increases with decreasing temperature. At a temperature 50 K, the value of SBH increases to 0.90 eV. The variation of SBH with temperature has been shown in Fig. 2.

To understand the observed modification in the C-V characteristics, it is important to analyze the implication of high-energy ion irradiation at the MS interface. It is well

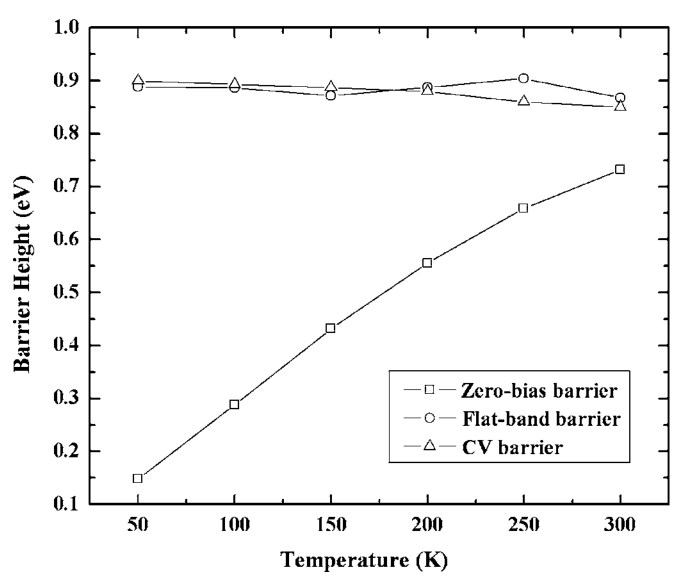

FIG. 2. Temperature dependence of the zero-bias barrier height, flatband barrier height, and C-V barrier height for the irradiated Au/n-Si(100) Schottky barrier diode.

known that when a SHI penetrates a solid target, it transfers its energy to the solid through two mechanisms: (1) electronic energy loss S_e due to inelastic collision causing excitation and ionization of the atoms of the target, and (2) nuclear energy loss S_n due to elastic collision causing displacements of the atoms from their regular lattice sites.[17,18] The elastic collision creates defects in semiconductor material such as vacancies, interstitials, and combination/agglomeration of these defects leading to the formation of complex and stable defect structures.[19,20] These defects have associated deep levels present inside the band gap of silicon and they act as traps for the free carriers resulting in reduction of their concentration. The swift-ion irradiation of silicon produces traps levels at $E_C-0.23$ eV, and $E_C-0.43$ eV, which belong to vacancies and their combinations[21,22] while the energy levels at $E_C-0.62$ eV and $E_C-0.86$ eV belong to interstitial point defects and clusters.[23–27] The decrease in capacitance of the Schottky diode implies a widening in the semiconductor depletion width. Since the charge neutrality condition at the interface should be satisfied, widening of the depletion width results from a reduction of the ionized donor concentration. This is confirmed from the C-V measurements. One of the mechanisms causing a decrease in the net ionized donor concentration is the existence of negatively charged deep defect centers as has been shown by many authors using Deep Level Transient Spectroscopy (DLTS) measurements. The presence of these levels causes a drop in the capacitance at lower temperature. This behavior is due to a freeze out of electrons on the deep centers in the band gap and causes a strong increase in the series resistance of the diode, which makes the measured capacitance to appear smaller. Presence of these centers causes the compensation of the positive shallow donors in the depletion region so that the effective net ionized-donor concentration is decreased. The donor compensation results in widening of the depletion width so that the charge-neutrality condition is maintained at the MS interface. As can be seen from Eq. (1) the increase in the depletion width results in decrease in Schottky diode capacitance.

B. Current-voltage characteristics

The metal-semiconductor contacts usually exhibit nonideal current-voltage characteristics. The experimental data is fitted by the thermionic emission equation, which is given by[4,16]

$$I = I_0 \exp\left(\frac{qV}{nkT}\right)\left[1-\exp\left(-\frac{qV}{kT}\right)\right], \tag{5}$$

where I_0 is the saturation current and n is the ideality factor. The ideality factor n is introduced to take into account the deviation of the experimental I-V data from the ideal thermionic model and its value should be one for an ideal contact. This deviation arises from the presence of surface charges and image force effects. The saturation current I_0 is given by

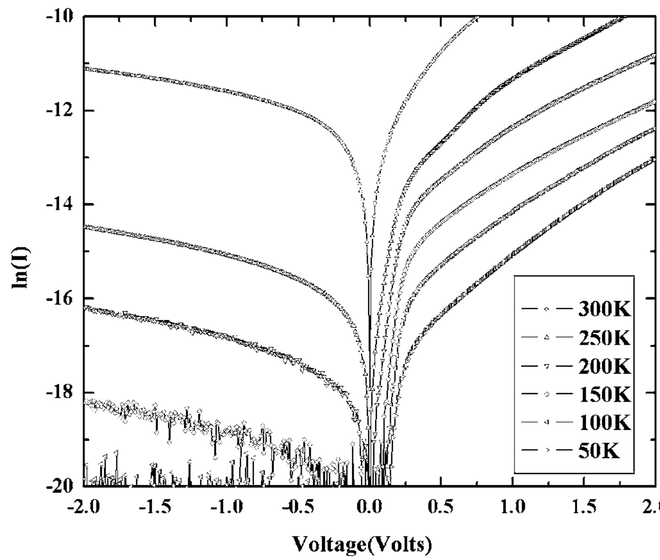

FIG. 3. Temperature dependent $\ln I$ vs V characteristics of irradiated Au/n-Si(100) Schottky barrier diode.

$$I_0 = AA^*T^2 \exp\left(-\frac{q\Phi_{B0}}{kT}\right), \tag{6}$$

where A^*, A, and Φ_{B0} represents the Richardson constant, the contact area, and zero-bias Schottky barrier height, respectively. The other symbols in the above equations have their usual meaning. From the slope of $\ln(I)$ vs V curve, the value of ideality factor is calculated using the relation

$$n = \frac{q}{kT}\left(\frac{dV}{d\ln(I)}\right). \tag{7}$$

The I_0 is determined from the intercept of $\ln(I)$ vs V curve on the y axis. The value of zero-bias SBH is evaluated at each temperature putting this value of I_0 in equation,

$$\Phi_{B0} = \frac{kT}{q}\ln\left(\frac{AA^*T^2}{I_0}\right). \tag{8}$$

Figure 3. shows the $\ln(I)$ vs V characteristics of Au/n-Si diode at different temperatures. The values of ideality factor n and zero-bias barrier height Φ_{B0} of the diode were calculated and are plotted as a function of temperature in Fig. 4. The ideality factor n exhibits an increasing trend with decreasing temperature, whereas the zero-bias barrier height decreases with decreasing temperature. Usually, the forward bias $\ln(I)$ vs V characteristics are linear at low forward bias voltages, but deviate considerably from linearity due to the effect of series resistance, the interfacial layer, and the interface states when the applied voltage is sufficiently large. The series resistance is significantly in downward curvature of forward bias I-V characteristics, but the other two parameters are significant in both the linear and nonlinear regions of I-V characteristics. The lower the interface state density and series resistance, the greater the range over which $ln(I)$-V curve yields at straight line.[28] As the linear range of the forward I-V plots is reduced, the accuracy of the determination of n and Φ_{B0} becomes poorer. The barrier height of a Schottky barrier depends on the electric field across the contact and consequently on the applied bias voltage. Therefore,

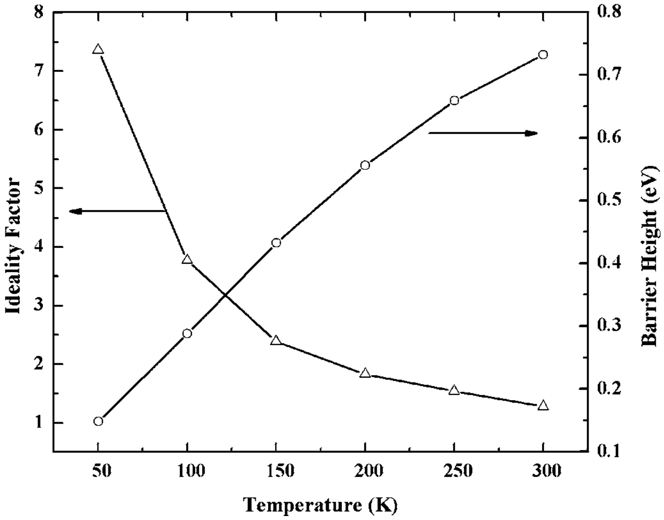

FIG. 4. Temperature dependence of the ideality factor and zero bias barrier height for the irradiated Au/n-Si(100) Schottky barrier diodes in the temperature range of 50–300 K.

it is necessary to specify standard field conditions. The electric field in the semiconductor is zero under flat-band conditions and thus the semiconductor band is flat, which eliminates the effect of tunneling and image force lowering from affecting the I-V characteristics. The barrier height obtained under the flatband conditions is called flatband barrier height. Flat-band barrier height is the real barrier height which should be used when comparing experiments with theory.[29,30] In order to obtain the flatband barrier height, the analysis of Wagner *et al.*[29] and Chin *et al.*[30] have been followed. The flatband barrier height is given by

$$\Phi_{\mathrm{Bf}} = n\Phi_{B0}(IV) - (n-1)\frac{kT}{q}\ln\left(\frac{N_C}{N_D}\right), \tag{9}$$

where N_C and N_D both are functions of temperature. The experimental carrier concentration N_D depending on the temperature is calculated from the reverse bias $1/C^2$ vs V plot in Fig. 1. The values of N_C and N_D are 2.8×10^{19} and 1.21×10^{15} cm^{-3} at 300 K, which become 1.91×10^{18} and 1.08×10^{15} cm^{-3} at 50 K, respectively. The flatband barrier height is calculated from zero-bias I-V barrier heights and corresponding ideality factor at each temperature. Figure 2 shows the variation of the flatband barrier height Φ_{Bf} as a function of the temperature. The flatband barrier height is invariably larger than the zero-bias barrier height at low temperature. From Fig. 2 we can see that the flatband barrier height is essentially the same as the barrier height determined by the capacitance-voltage (C-V) method. Flatband barrier height measurements are in good agreement between the values of barrier height were obtained from both methods over a wide temperature range. The temperature dependence of the flatband barrier height in the range of 50–300 K can be expressed as

$$\Phi_{\mathrm{Bf}}(T) = \Phi_{\mathrm{Bf}}(T=0\ \mathrm{K}) + \alpha T, \tag{10}$$

where Φ_{Bf} (T=0 K) is the flatband barrier height extrapolated to zero temperature and α is temperature coefficient of the barrier height. The fit of Eq. (10) to the data shown in Fig. 2 gives $\alpha = -7.4\times10^{-6}$ eV K^{-1} and Φ_{Bf} (T=0 K) =0.88 eV, respectively. This low value of temperature coefficient implies that the Fermi level is pinned by interface defects or imperfections at the MS interface. If defects caused the Fermi level pinning, the temperature change of the barrier would reflect the temperature motion of the defect relative to the appropriate band edge, i.e., their ionization entropy. Revva *et al.*[10] reported that if the Fermi level is pinned by the defects, the barrier height of a n-type semiconductor changes weakly with temperature because their ionization entropy changes only weakly with temperature. This explains our result for the irradiated Schottky contact. Earlier studies[21–27] on the irradiation of Si reported that the divacancy, impurity-vacancy combinations, and interstitial defect cluster are the radiation induced defect centers in silicon. The irradiation of Si gives rise to a trap level at 0.27 ± 0.02 eV above the valence band maximum due to interstitial point defect clusters.[23–27] Pinning of the Fermi level at this energy results in a barrier height of 0.85 ± 0.02 eV in close agreement with the barrier height measured for irradiated Au/n-Si Schottky diodes. In conclusion, the defects at the interface (deep levels) are responsible for the weak temperature dependence of the barrier height for Au/n-Si (100) contacts.

IV. CONCLUSION

In this work, the C-V and I-V measurements have been made in the temperature range of 50–300 K to investigate the barrier characteristics of the irradiated Au/n-Si(100) Schottky barrier diode. The I-V characteristics of the irradiated Au/n-Si(100) Schottky barrier diode have been investigated taking into account thermionic emission theory. The ideality factor and zero-bias barrier height are found to be strong functions of temperature while the flatband barrier height is almost independent of the temperature. The negligible temperature dependence of the flatband barrier height suggests that the interface defects produced by the SHI irradiation are responsible for the pinning of the Fermi level because their ionization entropy is only weakly dependent on the temperature. It is found that the barrier height obtained by I-V measurements are in close agreement with the barrier height found by C-V measurements at 1 MHz.

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