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Swift heavy ion irradiation-induced defects and electrical characteristics of Au/n-Si Schottky structure

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Abstract
The formation and evolution of defects induced by 100 MeV Si^{7+} ion irradiation in the Au/n-Si (1 0 0) Schottky barrier structure were studied and correlated with the electrical characteristics of the structure. The Schottky barrier decreases to 0.67 ± 0.01 eV after irradiation at a fluence of 1×10^{11} ions cm^{-2} and remains immune to further irradiation up to a fluence of 1×10^{12} ions cm^{-2}. A combination of *in situ* deep level transient spectroscopy and current–voltage measurements of Au/n-Si diodes demonstrates that 100 MeV silicon ion irradiation introduces a hydrogen related defect complex, which has a major influence on the Schottky barrier height and the leakage current in the irradiated structure.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Swift heavy ion (SHI) irradiation is used in the controlled reduction of the minority carrier's lifetime in silicon power devices, the formation of deep buried layers and the introduction of controlled amount of defects in semiconductors [1–3]. These increasing interests in ion beams motivate the studies of modifications induced by SHI irradiation of semiconductors. The metal–semiconductor (MS) structure is one of the important research tools in the characterization of semiconductors. Moreover, MS structure-based devices have been of considerable interest due to their widespread application in terahertz meta-material devices, microwave FETs, RF detectors and solar cells [4]. In some fields, such as development of particle detectors, it is really important to correlate the influence of ion irradiation on the material properties with the modification of electrical characteristics. It is found that SHI (projectile heavy ions having a velocity comparable to the Bohr velocity of electron) irradiation of silicon Schottky diodes results in saturated values of the barrier height and other parameters after a critical ion fluence [5, 6]. It is well established that ion irradiation into semiconductors causes structural damage, which in turn results in electrically active defects. These electrically active defects produced in Si can result in pinning of the Fermi level to a dominant deep level [7, 8]. There are numerous studies on the defects produced by low energy ion implantation in silicon [9–16], but defects induced by irradiation using high energy heavy ion are not studied extensively. The important difference in the SHI irradiation case with respect to low energy ion implantation is the high electronic energy loss due to inelastic collisions of SHI in materials, which are initially two to three orders of magnitude larger than the nuclear energy loss due to elastic collisions. This high electronic energy loss produces a strong ionization of the target atoms all along the trajectory. In the case of SHI, the range of ions is a few tens of micrometres and the ions go deep into the substrate after modifying the interface unlike the case of low energy implantation where the ions get implanted close to the interface. This work is an attempt to systematically study the role of this high electronic energy loss in the evolution of defects and correlate them with the the electrical characteristics of the material. In particular, *in situ* deep level transient spectroscopy (DLTS) allowed us to monitor the evolution of irradiation-induced defects as a function of irradiation fluence. Since the electrical characteristics of the MS structure depend on interface properties, generally there are small variations in diodes fabricated on the same wafer. The effect of ion

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irradiation depends on the virgin or pristine state of the diode. Therefore, to study the true effect of ion irradiation as a function of the ion fluence, it is necessary that fluence dependent studies should be carried out *in situ* on the same sample at various ion fluences. In this study, *in situ* DLTS and current–voltage (I–V) characterization of an SHI irradiated Au/n-Si (1 0 0) Schottky barrier diode was carried out on the single diode keeping all other physical conditions such as ion flux, temperature and vacuum environment identical. The results of the detailed investigation of *in situ* electrical characterization at various irradiation fluences ranging from 5×10^9 to 1×10^{12} ions cm^{-2} are presented here.

2. Experimental details

The sample used in this study was an Au/n-Si (1 0 0) Schottky barrier diode. The Schottky diodes were fabricated by using a Czochralski n-type Si (1 0 0) having both sides mirror polished and a resistivity of 1–10 Ω cm^{-1}. After standard cleaning, the oxide was removed by an HF dip and subsequently Al was deposited on the cleaned backside surface by the thermal evaporation method in a high vacuum chamber followed by temperature treatment at 525 °C for 25 min in the argon gas environment to make a low resistivity Ohmic contact. Schottky contacts were created by the deposition of Au on the sample by the electron beam heating technique in an ultra-high vacuum chamber. A 100 nm Au layer was deposited through a stainless steel mask having a contact diameter of 2 mm at a base pressure of $\sim 10^{-8}$ mbar. Ion irradiation was performed at room temperature by a 100 MeV $^{28}Si^{7+}$ ion beam using the 15UD Pelletron accelerator [17] facility at the Inter-University Accelerator Centre, New Delhi. The irradiation fluence was varied from 5×10^9 to 1×10^{12} ions cm^{-2}. During irradiation the beam current was 4.0 nA to avoid sample heating. A Boonton 7200 capacitance meter based computer controlled DLTS system was used for this study. Five DLTS spectra with rate windows between 115 and 2310 s^{-1} were simultaneously recorded during one single temperature scan from 80 to 300 K after each irradiation fluence. During measurements the ion beam was stopped in the beam line using a Faraday cup. The current–voltage (I–V) measurements were carried out with a programmable Keithley 2400 source meter. All measurements were carried out at various stages of irradiation in the experimental chamber maintained at a vacuum of $\sim 10^{-7}$ mbar.

3. Results

3.1. Current–voltage characterization

The current–voltage characteristics for the unirradiated and irradiated Au/n-Si Schottky diodes up to an ion fluence of 1×10^{12} ions cm^{-2} are shown in figure 1. In the case of a moderately doped semiconductor, thermionic emission is the dominant current transport mechanism across the barrier at room temperature. According to thermionic emission theory [18], the current I across the barrier under the application of a bias V is given by the expression

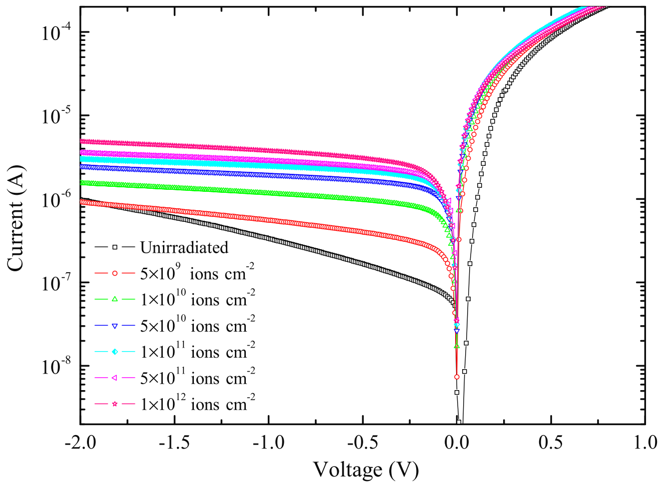

Figure 1. Experimental current–voltage characteristics of the Au/n-Si (1 0 0) Schottky barrier diode at different irradiation fluences.

$$I = AA^*T^2 \exp\left(\frac{-q\Phi_B}{kT}\right)\left[\exp\left(\frac{q(V - IR_s)}{nkT}\right) - 1\right]. \quad (1)$$

Here A is the diode area, A^* is Richardson's constant (120 A cm^{-2} K^{-2} for n-Si), Φ_B is the apparent barrier height, n is the ideality factor, R_s is the diode series resistance and other symbols have their usual meaning. From a fit of the linear region of the forward bias semilogarithmic I–V curve (where $V > 3kT/q$ and the series resistance is negligible) the values of the ideality factor and the Schottky barrier height were determined.

For the unirradiated diode the barrier height was 0.80 eV. The ideality factor for the as-prepared diode was 1.1. After irradiation at a fluence of 5×10^9 ions cm^{-2}, the barrier height decreases to a value of 0.72 eV without any significant change in the ideality factor. Thereafter, the barrier height decreases further till it reaches a value of 0.67 eV with an ideality factor of 1.23 for the irradiation fluence of 1×10^{11} ions cm^{-2}. Beyond this ion fluence, the Schottky barrier height remains immune to further irradiation up to the highest irradiation fluence used. The variation of the barrier height as a function of the irradiation fluence is shown in figure 2. This behaviour is quite in good agreement with that found in our previous work for Au/n-Si Schottky diodes [5, 6]. The ideality factor increases from a value of 1.10 to 1.25 after ion irradiation at a fluence of 1×10^{11} ions cm^{-2}.

The leakage current (measured at −2 V) remained almost unchanged with respect to the as-prepared sample after low fluence ion irradiation and increased at higher fluences. The leakage current increases from a value of 9.8×10^{-7} A for the unirradiated diode to 4.9×10^{-6} A after irradiation at a fluence of 1×10^{12} ions cm^{-2}. The increase in the value of the leakage current is associated with irradiation-induced defects. Earlier [5, 6], the decrease in the barrier height, the increase in the ideality factor and the leakage current were explained in terms of an increase in the interface state density due to defects at the interface.

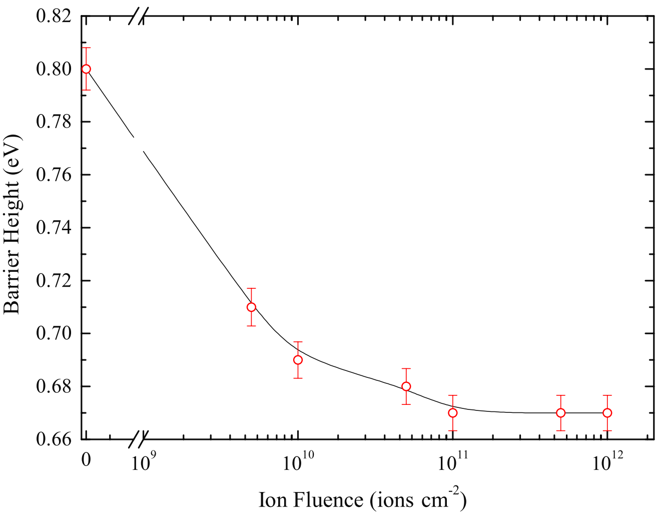

Figure 2. Irradiation fluence dependence of the Schottky barrier height for the Au/n-Si (1 0 0) Schottky barrier diode.

3.2. DLTS characterization

In order to develop a better understanding of the influence of defects on the electrical characteristics, the creation and evolution of irradiation-induced defects in the Au/n-Si (1 0 0) structure were monitored by means of the DLTS technique. DLTS is a high frequency capacitance transient method useful for observing deep level defects in semiconductor devices [19]. The DLTS spectrum is a plot of difference in the capacitance (δC) versus temperature (T). The time constant (τ) for the capacitance transient, activation energy ($E_c - E_T$) and capture cross-section (σ) of the deep level are related as [20]

$$\tau T^2 = \frac{\exp\left[(E_c - E_T)/kT\right]}{\gamma\sigma}, \qquad (2)$$

where γ is the material coefficient and is defined as

$$\gamma = \frac{16\pi m_e^* k^2}{gh^3}, \qquad (3)$$

where m_e^* is the electron effective mass, h is Plank's constant and g is the degeneracy factor. The γ value for n-Si is $1.07 \times 10^{21}\,\mathrm{cm^{-2}\,s^{-1}\,K^{-2}}$. The slope of the Arrhenius plot $\ln(\tau T^2)$ versus $(1000/T)$ yields the activation energy of the defects, and the intercept on the y axis $\ln[(1/\sigma\gamma)]$ gives the capture cross section (σ). The trap concentration (N_T) can be determined by knowing the peak height (δC_{max}) in the DLTS spectrum.

Figure 3 shows the DLTS spectra of an unirradiated Au/n-Si (1 0 0) Schottky diode and after irradiation at fluences of 5×10^9, 1×10^{10}, 1×10^{11} and 1×10^{12} ions cm^{-2}. The Arrhenius plot for the unirradiated Au/n-Si diode is shown in figure 4. There are two dominant DLTS peaks E_1 ($E_c - 0.23$ eV) and E_2 ($E_c - 0.40$ eV) in an unirradiated sample, which are identified as the doubly negative divacancy, $V_2(=/-)$, and the singly negative divacancy, $V_2(-/0)$, respectively [21–24]. A new level E_3 at $E_c - 0.32$ eV is generated during SHI irradiation after a fluence of 5×10^9 ions cm^{-2}. Interestingly, it is found that the height

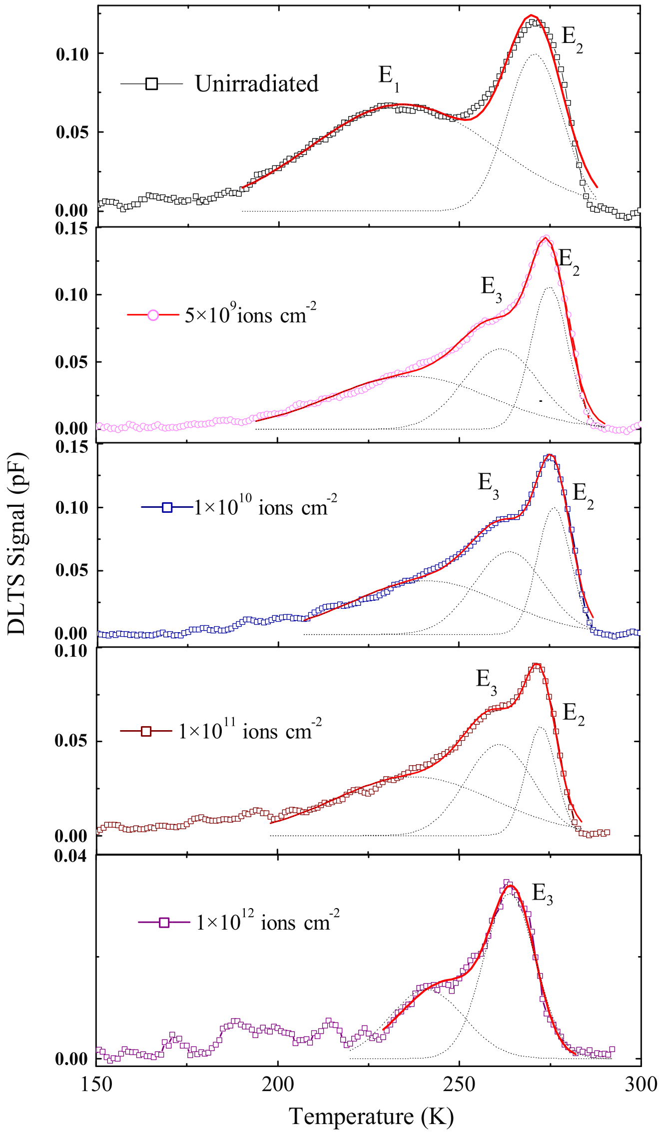

Figure 3. DLTS spectra of unirradiated and irradiated Au/n-Si (1 0 0) Schottky barrier diodes at different ion irradiation fluences.

of the DLTS peak of the E_3 level remains almost unchanged with increasing irradiation fluence, while after a fluence of 1×10^{10} ions cm^{-2} the peak height of E_2 starts decreasing for further irradiation fluences and this level disappears at higher irradiation fluences.

4. Discussion

Now the implication of high-energy ion transport through the Au/n-Si Schottky diode is necessary to understand to realize the observed behaviour. When the 100 MeV $^{28}Si^{7+}$ ion passes through the MS interface, it loses energy by two nearly independent processes: (1) elastic collisions of the ion with the target atoms known as nuclear energy loss (S_n) and (2) inelastic collisions of the highly charged projectile ion with the atomic electrons of the materials known as electronic energy loss (S_e). In our case, electronic energy loss is the dominant energy loss process at the interface and S_n dominates only at the end of the ion range as shown in figure 5. All energy

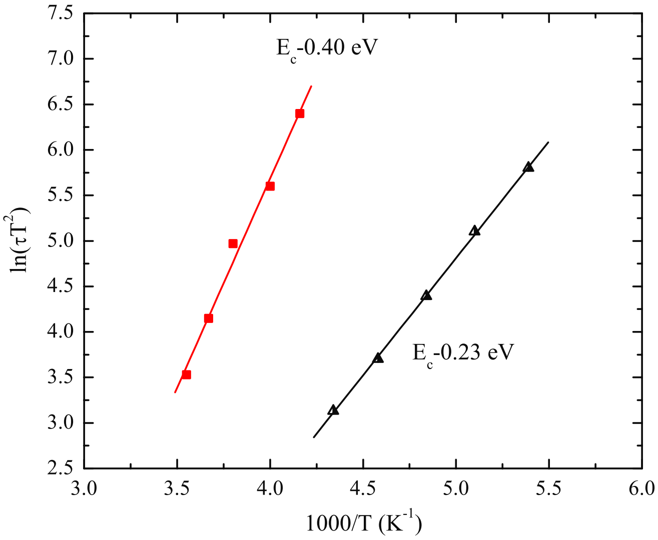

Figure 4. The Arrhenius plot for an unirradiated Au/n-Si (1 0 0) Schottky barrier diode.

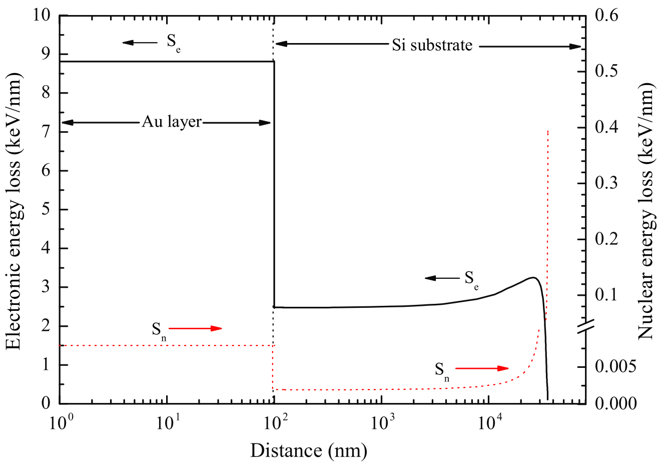

Figure 5. The nuclear and electronic energy losses of 100 MeV $^{28}Si^{7+}$ ions as a function of the distance inside the Au/n-Si (1 0 0) Schottky barrier diode.

loss calculations have been performed using the standard Monte Carlo simulation program [25] called SRIM-2006. It is well established that S_n causes the creation of defects such as vacancies, interstitials and combination/agglomeration of these defects leading to the formation of complex and stable defect structures [26], while S_e causes strong ionization of the target atoms along its trajectory. During their relaxation, the electronic excitation can produce several specific structural defects and phase transitions [27, 28]. The Au layer is not affected due to the strong screening of charges in metals. According to the widely used thermal spike model [29], rapid energy transfer through electron–phonon coupling makes the system abnormally excited and the region around the ion track gets suddenly heated to a very high temperature within a small time scale [30]. The temperature evolution of the ion track for 100 MeV Si^{7+} ions in silicon is above 800 K [31]. In this case 100 MeV Si^{7+} ions' irradiation produces a deep level at E_3 ($E_c - 0.32$ eV). This level has been reported previously after proton irradiation and is identified as a hydrogen related defect [11, 12, 15]. The ion irradiation produced defects are enhanced by hydrogen resulting in the formation of weak Si–H bonds at the defect sites, which is dissociated at around 150 °C. The released hydrogen atoms interact with the irradiation-induced defects to form electrically active centres [32]. In this case hydrogen was not deliberately introduced or implanted but experimentally it is found that the hydrogen content in crystalline silicon by far exceeds the estimated equilibrium concentration. It had been shown that during the annealing of the Si ion implanted silicon, the formation of the $E_c - 0.32$ eV level is associated with the annealing of the $E_c - 0.23$ eV level [12]. In this case the region around the ion pathway goes to a very high temperature than that required to release the hydrogen atoms. These hydrogen atoms interact with irradiation-induced defects to form electrically active centres. The level at $E_c - 0.32$ eV gets saturated with increasing ion fluence due to the fact that the concentration of hydrogen in silicon is limited, which results in saturation at higher irradiation fluences. This released hydrogen can also interact with divacancies V(−/0) to passivate the defects, which becomes electrically neutral and modifies the Schottky barrier height [33]. It is also established that despite impurities such as oxygen and carbon atoms being potential annihilation centres, apparently the localized disordered zones created by ion irradiation also act as sinks and annihilate diffusing point defects such as the divacancy centres [10]. Since the divacancies anneal out at higher fluences, so E_3 influences mainly the electrical characteristics and results in a saturated value of interface states' density at the interface.

According to Bardeen's Fermi level pinning model [34], if the interface density D_S is very high, the Schottky barrier height on an n-type semiconductor is given by

$$\Phi_{BB} = \left(\frac{E_g}{q} - \Phi_0\right) - \Delta\Phi \quad \text{(Bardeen limit)}, \tag{4}$$

where E_g is the band gap of the semiconductor, $q\Phi_0$ is the energy level coincident with the Fermi level before the MS contact was formed and $q\Delta\Phi$ is the lowering of the Schottky barrier due to the image force. It being of the order of 0.01 eV may be neglected. On the other hand, when D_S is zero, then the barrier height of a Schottky barrier diode on an n-type semiconductor is given by

$$\Phi_{BS} = \Phi_M - \chi - \Delta\Phi \quad \text{(Schottky limit)}, \tag{5}$$

where Φ_M is the work function of the metal and $q\chi$ is the electron affinity of the semiconductor. According to Sze (1981) [35] $q\Phi_0 = 0.30 \pm 0.36$ eV, and $q\chi = 4.05$ eV, $E_g = 1.12$ eV for Si at 300 K, and $q\Phi_M = 5.1$ eV for Au. Using these values, the estimated values of $q\Phi_{BB}$ and $q\Phi_{BS}$ are 0.82 ± 0.36 eV and 1.05 ± 0.36 eV, respectively. This means that when the interface state density D_S increases from the Schottky limit to the Bardeen limit, the barrier height should decrease. From the forward bias I–V characteristics for the unirradiated diode we have calculated the barrier height as 0.80 ± 0.01 eV. This implies that there is a finite density of interface states D_S existing at the Au/n-Si (1 0 0) interface for the unirradiated sample. This is confirmed by

DLTS measurements that there are finite concentrations of divacancies in unirradiated samples, which are the cause of interface states. High energy ion irradiation releases hydrogen in silicon, which produces deep level defect complexes ($E_c - 0.32$) and passivates the localized defects at the interface such as divacancies V(−/0). The barrier height decreases after irradiation, which correlates well with an increase in the interface states density due to deep level defects. These defects cause an increase in the defect-assisted tunnelling of free electrons, which results in an increase in the reverse leakage current. After a particular fluence the concentration of divacancies becomes very less compared with E_3, and E_3 becomes saturated due to a limited supply of hydrogen in silicon. The saturation in the defect concentration results in a saturated value of interface states' density, which leads to a saturated value of the barrier height with respect to the ion fluence.

5. Conclusion

We have studied the defects induced by SHI irradiation and their influence on the electrical characteristics in the Au/n-Si (1 0 0) Schottky structure by using combined *in situ* DLTS and current–voltage measurements. The Schottky barrier height decreases initially after ion irradiation and becomes immune after a critical ion fluence. We have demonstrated that a hydrogen related defect complex is formed after SHI irradiation. Due to the limited concentration of hydrogen in silicon, the concentration of this level saturates at a higher irradiation fluence. This defect complex has a strong influence on the electrical characteristics of the Au/n-Si Schottky diode and causes saturation in the barrier parameters at a higher fluence.

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