Thermal stability of ohmic contacts between Ti and Se-passivated *n*-type Si(001)

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The thermal stability of the interface between Ti and Se-passivated *n*-type Si(001) is investigated. As-deposited Ti contacts show ohmic characteristics. After annealing at temperatures from 200 °C to 480 °C in air, the Se-passivated samples are much more resistant to Schottky transition as compared to the bare samples. The bare samples turn to Schottky below 300 °C, whereas the passivated samples are ohmic all the way to 400 °C. A difference of over 100 °C is observed between the two types of samples. Schottky barrier heights are determined using capacitance–voltage and activation–energy methods. The bare samples reach a maximum barrier height of 0.39 eV as determined by activation–energy measurements, while the passivated samples maximize at 0.19 eV. We deduce that a monolayer of Se suppresses silicidation between Ti and Si by eliminating dangling bonds on Si(001). © 2004 American Institute of Physics. [DOI: 10.1063/1.1687047]

I. INTRODUCTION

Surface atoms on Si(001), due to the absence of lattice atoms above them, have to undergo reconstruction in an ultrahigh vacuum to minimize surface energy. Figure 1(a) shows the atomic structure of clean Si(001) in a vacuum. Each surface atom has a dangling bond and shares a dimer bond with its neighboring surface atom. When a metal is deposited on Si, these dangling bonds give rise to interface states within the energy band gap of Si. The interface Fermi energy is often pinned by these interface states, making the Schottky barrier height independent of the metal work function. The concept of valence mending, proposed by Kaxiras,¹ eliminates dangling bonds on semiconductor surfaces. Group-VI elements like S and Se are found to be good candidates for the passivation of Si(001) because of their comparable bond lengths to Si. Since they are divalent, they can fit between two surface Si atoms, thus terminating the dangling bonds and relaxing the dimer bonds and strained back bonds on Si(001). This surface structure is often referred to as (1×1) reconstruction, as shown in Fig. 1(b).

When Ti is deposited on *n*-type Si, the interface has an ideal Schottky barrier height of 0.04 eV. Here, the ideal barrier height is defined as the difference between Ti work function and Si electron affinity.² The reported Schottky barrier height in literature for this interface is 0.5 eV.³ The discrepancy is attributed to the presence of interface states, which pin the interface Fermi energy. We reported the ohmic behavior of the interface between Ti and Se-passivated *n*-type

Si(001).⁴ The ohmic nature was explained as a result of the negative or nearly negative Schottky barrier due to the elimination of interface states, as illustrated in Fig. 2(b). As a comparison, conventional ohmic contacts in today's Si devices, as shown in Fig. 2(a), employ a heavily doped Si surface. Electrons have to tunnel through the thinned Schottky barrier, which introduces a significant resistance. In this article, we present a detailed study on the thermal stability of the interface between Ti and Se-passivated *n*-type Si(001). Ti contacts on Se-passivated Si(001) are annealed from 200 °C to 480 °C and characterized by current–voltage (*I*–*V*) capacitance–voltage (*C*–*V*), and activation–energy measurements. Comparisons are made with Ti contacts on bare Si(001) annealed at the same temperatures. This study provides insight into the transition from ohmic to Schottky upon annealing for the two Ti/Si interfaces.

II. EXPERIMENT

Si(001) wafers with Sb doping of low 10¹⁵ cm^{−3} were used for the experiments. One set of wafers was Se passivated while the other had no Se passivation. The wafers were

FIG. 1. Atomic structures of (a) the reconstructed Si(001):2×1 surface and (b) the Se-passivated Si(001):1×1 surface.

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FIG. 2. Band diagrams for (a) conventional ohmic contacts and (b) a negative Schottky barrier for low-resistance ohmic contacts.

cleaned with 2% HF for 30 s and were immediately loaded into the molecular-beam epitaxy chamber. A Si buffer layer of 500 Å was grown with residual Sb doping of 10^{14} cm^{-3} at 600 °C and then annealed at 800 °C. This buffer layer ensured a perfect crystal structure on the Si(001) surface. For Se passivation, the wafer temperature was 300 °C and the Se source temperature was 224 °C. The passivation time was 60 s and the resulting Se-passivated Si(001) surface gave a sharp (1×1) reconstruction in reflection high-energy electron diffraction. A Ti layer of 500 Å was deposited in an electron-beam evaporator. A standard lift-off process was used to fabricate Ti circular dots of 100, 150, 200, and 300 μm in diameter. Mg was deposited on the back side of the wafers for back ohmic contact.⁵

III. RESULTS AND DISCUSSION

A. Current–voltage characterization

Figure 3 shows the current–voltage (I – V) behavior of Ti contacts on Se-passivated and bare n -type Si(001). Both types of samples show ohmic behavior with the bare samples showing a slightly higher resistance. The Se doping in these wafers is low (10^{15} cm^{-3}), hence Fig. 2(b) represents the band diagram at these interfaces. Electrons moving from Ti to Si encounter a minuscule energy hump that does not show up in the I – V data, leading to perfectly ohmic characteristic. To explore the thermal stability, Ti contacts on Se-passivated and bare Si(001) are annealed from 200 °C to 480 °C for 30 s on a hot plate and then characterized by I – V measurements. To quantify the extent of Schottky transition, the rectification ratio, i.e., the ratio of the forward current and reverse current ($R=I_f/I_r$), for the passivated and bare

FIG. 3. I – V characteristics of as-deposited Ti contacts on Se-passivated and bare Si(001).

FIG. 4. Rectification ratio (I_f/I_r at $V=\pm 1 \text{ V}$) as a function of annealing temperature for bare and Se-passivated samples.

samples is calculated at $V_f=1 \text{ V}$ and $V_r=-1 \text{ V}$. As plotted in Fig. 4, the rectification ratio for the passivated samples remains close to unity till 400 °C. In other words, Ti contacts on Se-passivated n -type Si(001) are ohmic all the way to 400 °C. On the other hand, the bare samples start to show Schottky behavior from 300 °C. In some samples (data not shown) the transition occurs at 225 °C or 250 °C. At 350 °C, the bare samples have a rectification ratio of 50, whereas the passivated samples reach a maximum rectification ratio of 22 at 480 °C. Thus, a difference of more than 130 °C is observed between the two types of samples.

The I – V relationship at different annealing temperatures is plotted for the passivated samples in Fig. 5(a) and bare samples in Fig. 5(b). Comparing the two plots, we find that

FIG. 5. I – V characteristics of (a) Se-passivated samples and (b) bare samples annealed at different temperatures.

FIG. 6. $1/C^2$ vs V plot for bare and Se-passivated samples annealed at (a) 450 °C and (b) 480 °C.

the reverse current of the passivated samples at 350 °C is two orders of magnitude higher than that of the bare samples at the same temperature. A smaller reverse current indicates a more extensive transition to Schottky. Similar distinctions are observed for 400 °C, 1.4 mA versus 57 μ A, and 450 °C, 185 μ A versus 30 μ A, at $V_r = -2$ V. It is suggested that Se passivation hinders silicidation at the interface by making the Si(001) surface chemically less reactive.

B. Capacitance–voltage characterization

For a Schottky contact, a plot of $1/C^2$ versus V yields a straight line provided a constant doping level in the semiconductor.⁶ The Schottky barrier height Φ_{Bn} can be determined from the intercept on the voltage axis, V_i , as

FIG. 7. Barrier height, determined from C – V measurements, vs annealing temperature for bare and Se-passivated samples.

FIG. 8. Activation–energy plot for (a) Se-passivated samples and (b) bare samples annealed at different temperatures.

$$\Phi_{Bn} = V_i + V_n + \frac{kT}{q} - \Delta\Phi, \quad (1)$$

where V_n is the depth of the Fermi energy below the conduction band and $\Delta\Phi$ is the Schottky barrier lowering given by

$$\Delta\Phi = \frac{q}{\epsilon_{Si}} \sqrt{\frac{n_1 a}{4\pi}}, \quad (2)$$

where n_1 is the doping level in the buffer layer and a is the thickness of the buffer layer. Our samples have a maximum $n_1 a$ product of 4×10^{12} cm^{−2}, giving a maximum Schottky barrier lowering of 0.087 eV.

C – V measurements are performed on bare and passivated samples annealed at various temperatures. Since the

FIG. 9. Barrier height, determined from activation–energy measurements, vs annealing temperature for bare and Se-passivated samples.

passivated samples behave ohmic at and below 400 °C, $C-V$ data are obtained only for samples annealed at 450 °C and 480 °C, as shown in Figs. 6(a) and 6(b), respectively. The passivated samples always show lower barrier heights as compared to the bare samples at the same annealing temperature. Figure 7 is a plot of barrier height versus annealing temperature for the bare and passivated samples. The bare samples reach a stable barrier height at 350 °C, whereas the passivated samples reach the same barrier height at 480 °C. Again, we observe a difference of 130 °C between the two types of samples.

C. Activation–energy measurement

In a plot of $\ln(I/T^2)$ versus $1/T$, the slope gives the Schottky barrier height

$$\text{slope} = - \frac{q(\Phi_{Bn} - V_f)}{k} \quad (3)$$

where V_f is the forward bias. Both the passivated and bare samples are cooled from 23 °C to –70 °C and $I-V$ measurements are performed at interval of 10 °C. Figures 8(a) and 8(b) are the activation–energy plots for the passivated and bare samples at different annealing temperatures, which give the barrier heights. Figure 9 plots the barrier height versus annealing temperature. Although the numbers are different, the general trend agrees with $C-V$ measurements in Fig. 7. The bare samples reach a stable barrier height at 325 °C, and a maximum barrier height of 0.39 eV at 480 °C. The latter probably represents complete silicidation at the interface between Ti and Si. The passivated samples give lower barrier heights as compared to the bare samples at all annealing temperatures, with a maximum barrier height of 0.19 eV.

IV. CONCLUSION

When Ti is deposited on Se-passivated n -type Si(001), the interface shows ohmic behavior. Chemically, Se passivation reduces the reactivity of the Si(001) surface, hindering silicidation between Ti and Si upon annealing. Electrically, the interface between Ti and Se-passivated Si(001) is less prone to Schottky transition as compared to the Ti/bare–Si interface. We observe a difference of about 130 °C in Schottky transition temperature between the two interfaces. Barrier height measurements by the activation–energy and $C-V$ methods show that the interface between Ti and Se-passivated n -type Si(001) has lower barrier heights at all annealing temperatures as compared to the Ti/bare–Si interface. The passivated samples reach a maximum barrier height of 0.19 eV, whereas the bare samples show 0.39 eV at 480 °C.

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