PART I

Metallization Overview, Concerns and Diffusion Barriers

ELECTRICAL PROPERTIES AND SCHOTTKY BARRIERS OF METAL-SEMICONDUCTOR INTERFACES

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ABSTRACT

The electrical properties of metal/Si(100) and metal/Ge(100) interfaces formed by the deposition of metal on both n-type and p-type Si(100) and Ge(100) have been studied in the temperature range 77-295 K with the use of current- and capacitance-voltage techniques. Compound formation is found to have very little or no effect on the Schottky-barrier height and its temperature dependence. For silicon, the barrier height and its temperature dependence are found to be affected by the metal. For germanium, on the other hand, the barrier height and its temperature dependence are unaffected by the metal. The temperature dependence of the Si and Ge barrier heights is found to deviate from the predictions of recent models of Schottky-barrier formation based on the suggestion of Fermi-level pinning in the center of the semiconductor indirect band gap.

I. INTRODUCTION

Almost all theoretical models of Schottky-barrier formation at metal-semiconductor interfaces have been based on the original suggestion of Bardeen[1], that the Fermi level at the interface is pinned by states in the semiconductor band gap. The nature of these states is clearly one of the key issues in establishing a microscopic understanding of the barrier height. Recently, new models[2] have been proposed based on the suggestion of Fermi-level pinning in the center of the semiconductor indirect band gap by states intrinsic to the interface. In these models the effect of the metal has been neglected and the barrier height has been related to the semiconductor band-structure properties (i.e., indirect band gaps and spin-orbit splittings). Other models[3] of barrier formation have been proposed based on pinning by states associated with defects in the semiconductor. However, these defect models, which are commonly used to describe pinning on surfaces with submonolayer metal coverages, still provoke much controversy[4]. In an attempt to shed light on the nature of the states responsible for Fermi-level pinning, we have measured the dependence of the barrier height on temperature for metal(silicide)-silicon and metal(germanide)-germanium systems with a wide range in metal electronegativity in the temperature range 77-295 K using current-voltage (I-V) and capacitance-voltage (C-V) techniques. In this paper, we present and discuss the results of these measurements in terms of models of barrier formation based on pinning in midgap.

II. ELECTRICAL PROPERTIES

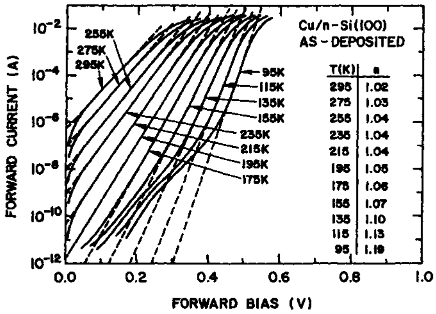
A. n-Type Si(100)

The forward I-V characteristics plotted in Fig. 1 as a function of temperature show examples of the results obtained for Cu[5] on lightly doped ($10^{14} - 10^{15} cm^{-3}$) n-type and p-type Si(100). The samples display a good ideality factor which, however, increases slowly as the temperature is lowered, reaching a value of 1.19 at 95 K. This temperature dependence of the ideality factor is found to have the form $n = 1 + (T_o / T)$, where T_o is a constant, independent of temperature. Figure 2 shows nkT/q plotted against kT/q. It is evident that the data can be fitted to a straight line parallel to the unity slope line. The value of T_o for these samples is found to be 20 K. Moreover, the dependence of $\ell n\ (J_o/T^2)$, where J_o is the saturation current density at zero applied voltage, on 1/T is found to be nonlinear in the temperature range measured; however, if $\ell n(J_o/T^2)$ is plotted against $1/nT = 1/(T + T_o)$, a straight line is obtained with a slope giving a barrier-height value at 0 K of 0.65 eV, as shown in Fig. 3, in very good agreement with the 0-K value reported by Arizumi and Hirose[6] for Cu on n-type Si(111). This shows that the saturation current density J_o can be described by

$$J_o = A^*T^2 \exp[-q\Phi_{Bn}/k(T + T_o)] \quad (1)$$

where A^* is the effective Richardson constant and Φ_{Bn} is the n-type barrier height. Similar results have also been found for Ti-Si[7] and W-Si[8] Schottky barriers formed on lightly doped n-type Si(100) and by other authors for Schottky barriers formed on lightly doped n-type GaAs[9] and n-type InP[10]. The temperature variation of the barrier height calculated using Eq.(1) is shown in Fig. 4 by the solid circles. The solid line shows the temperature variation of the barrier height calculated on the assumption that it is entirely due to the temperature dependence of the indirect band gap in Si with the barrier-height value at 235 K as a reference. It is clear from these data that the barrier height decreases with increasing temperature with a coefficient almost equal to that of the indirect band gap in Si. It is also to be noted that the barrier-height value calculated using Eq.(1) at 295 K is in very good agreement with that reported by Thanailakis[11] for Cu on n-type Si(111) using photoelectric measurements.

In Fig. 5 we show the temperature variation of the barrier height calculated using Eq.(1) (open triangles) for W[8] on n-type Si(100). The barrier-height values obtained from C-V measurements are also shown in Fig. 5 by the solid circles. The solid line again shows the temperature variation of the barrier height calculated on the assumption that it is entirely due to the dependence of the indirect band gap in Si on temperature with the barrier-height value at 215 K as a reference. It is clear that the barrier-height values calculated using Eq.(1) are in very good agreement with those derived from C-V measurements, and that the change in the n-type barrier height with temperature is again almost equal to the change in the Si indirect band gap. This is consistent with the results of Crowell et al.[12] and of Duboz et al.[13] for Au and $CoSi_2$ on n-type Si(111).



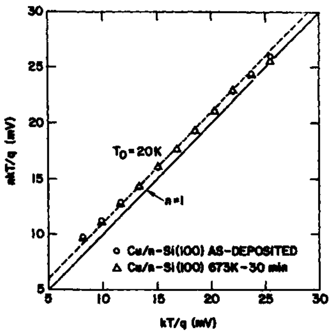
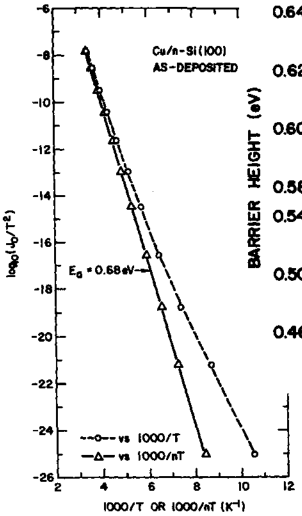


Fig. 1. Forward I-V characteristics of Cu on n-type Si(100) as a function of temperature for samples in the as-deposited state. Junction area is $3.974 \times 10^{-4} cm^2$.

Fig. 2. Temperature dependence of the ideality factor for n-type samples in the as-deposited state (open circles) and after annealing at 673 K for 30 min (open triangles).



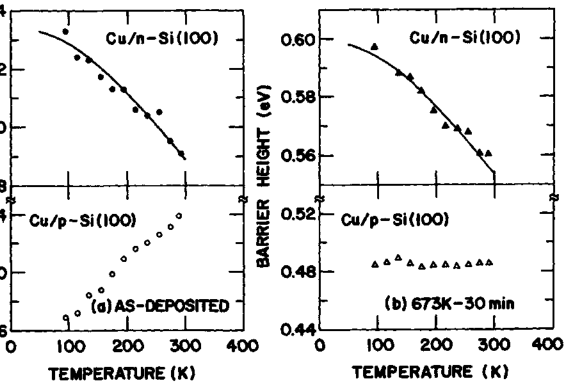


Fig. 3. Temperature dependence of forward current measured at zero applied voltage for n-type samples in the as-deposited state.

Fig. 4. Correlation of the Si indirect band gap change (solid line) and the barrier height variation with temperature for Cu on n-type (solid circles and triangles) and p-type (open circles and triangles) Si(100).

Two models have been proposed to explain the inclusion of the ideality factor in Eq.(1); the interface state model[14,15] and a doped interface model[15]. The former describes the interface in terms of a localized energy distribution of interface states, and the latter is a more macroscopic description in which the conversion of the n-type semiconductor near the interface to p-type results in a distribution of dopants which creates a voltage dependent potential energy maximum inside the semiconductor. Our results rule out the doped interface model, since in all the metal-Si(100) systems studied the n-type Si is found to retain its type of conduction after metal deposition[16]. It is likely that the T_0 anomaly observed here is related to a particular energy distribution of interface states resulting in a charge that causes an increase in the barrier height with forward voltage and a decrease with reverse voltage[15].

It can be seen from Fig. 1 that an excess current region of the forward characteristics becomes much more pronounced at low voltages as the temperature is lowered below 175 K. This excess current exhibits a small temperature dependence, suggesting that it is likely caused by high electric field effects near the edges of the junctions[17]. However, this excess current appears to have little effect on the temperature dependence of the ideality factor at higher forward voltages where thermionic emission dominates, since if the effect is large, then T_0 would be expected to be temperature dependent, i.e., to increase at low temperatures[17]. This is clearly not the case here, as shown in Fig. 2.

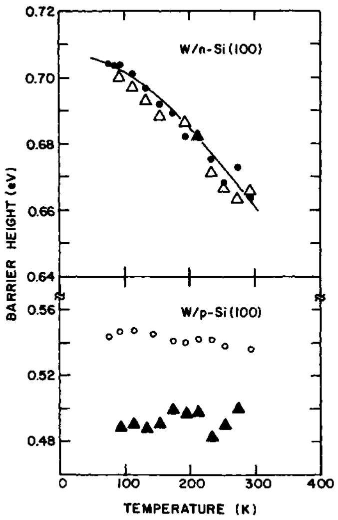


Fig. 5. Correlation of the Si indirect band gap change (solid line) and the barrier height variation with temperature for W on n-type and p-type Si(100). Open and solid triangles: barrier-height values determined from I-V measurements using Eq.(1) (see text). Solid and open circles: barrier-height values determined from C-V measurements.

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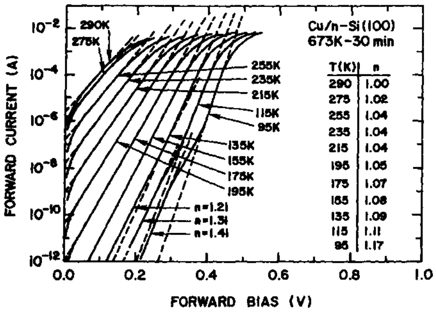
In Fig. 6 we show examples of the forward I-V characteristics obtained after annealing the Cu/n-type Si(100) samples at 673 K for 30 min. The samples display a good ideality factor which again increases slowly with decreasing temperature, reaching a value of 1.17 at 95 K. Again, this temperature dependence of the ideality factor is found to have the form $n = 1 + (T_o / T)$, with T_o having a value of 20 K(Fig. 2). Moreover, the dependence of $\ell n(J_o/T^2)$ on 1/T is again not linear, whereas the dependence of $\ell n(J_o/T^2)$ on 1/nT is linear in the temperature range measured with a slope giving a barrier- height value at 0 K of 0.62 eV, as shown in Fig. 7. The temperature variation of the barrier height calculated using Eq.(1) is shown in Fig. 4 by the solid triangles. The solid line again shows the temperature variation of the barrier height calculated on the assumption that it is entirely due to the temperature dependence of the indirect band gag in Si. It is clear that in these samples the barrier height also decreases with increasing temperature with a coefficient almost equal to the temperature coefficient of the indirect band gap in Si.

X-ray photoemission-spectroscopy measurements[18] on Cu-Si(100) samples with 1000Å Cu showed that an annealing at 473 K for 30 min is sufficient to cause the Cu film to fully react with Si to form a metal-rich Cu-Si compound with stoichiometry close to Cu_3Si. The results in Fig. 4 then indicate that silicide formation has very little or no effect on the barrier height and its temperature dependence.



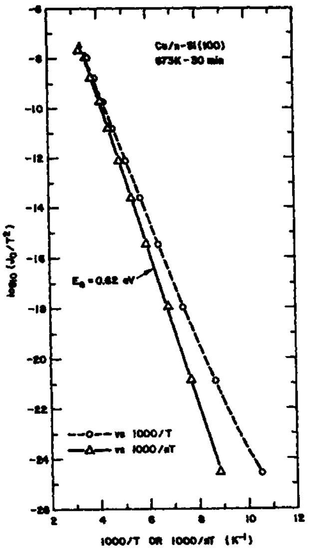


Fig. 6. Forward I-V characteristics of Cu on n-type Si(100) as a function of temperature for samples annealed at 673 K for 30 min.

Fig. 7. Temperature dependence of forward current measured at zero applied voltage for n-type samples annealed at 673 K for 30 min.

It can be seen from Fig. 6 that a region of the forward characteristics with a high value of ideality factor (which increases with decreasing temperature) becomes evident at low voltages as the temperature is lowered below 155 K. A plot of $\ell n(J_o/T^2)$ obtained by extrapolating this low-voltage linear region of the forward characteristics to zero applied voltage, versus 1/T (not shown here) is found to be linear in the temperature range 95-135 K with a slope giving an activation energy of 0.26 eV. This low activation energy value is evidently associated with recombination which causes deviations from thermionic emission behavior at low voltages and low temperatures[19]. This excess thermally activated current, however, has essentially no effect the temperature dependence of the ideality factor at higher forward voltages and low temperatures, as shown in Fig. 2.

B. p-Type Si(100)

The forward I-V characteristics plotted in Fig. 8 as a function of temperature show examples of the results obtained for Cu[5] on lightly doped ($10^{14} - 10^{15} cm^{-3}$) p-type Si(100). The samples display a high ideality factor which, however, remains essentially unchanged in the temperature range 98-290 K. In contrast to the n-type samples, the data of nkT/q against kT/q can be fitted to a straight line passing through the origin with a slope equal to 1.23, as shown in Fig. 9. In addition, the dependence of $\ell n(J_o/T^2)$ on 1/T is now linear in the temperature range measured with a slope giving an activation energy of 0.43 eV, as shown in Fig. 10. This activation energy value is less than the barrier height for Cu on p-type Si(100) at 0 K (0.49 eV). These results indicate that in these samples the current is due to thermionic emission in combination with recombination. In fact, if the relation for thermionic emission [$J_o = A^*T^2 \exp(-q\Phi_{Bp}/kT)$] is used to calculate a barrier height, the barrier height is found to increase with increasing temperature, as shown in Fig. 4 by the open circles. This is due to the fact that deviations from thermionic emission behavior due to recombination become more pronounced as the temperature is lowered[19]. It is to be noted that the p-type barrier height is not expected to exhibit a temperature dependence, since almost all the change in the Si indirect band gap is reflected in the change of the n-type barrier height with temperature. For W[8] on p-type Si(100), on the other hand, where the current is due to thermionic emission, the barrier height determined from I-V and C-V measurements does not exhibit a temperature dependence, as shown in Fig. 5 by the solid triangles and the open circles.

It can be seen from Fig. 8 that an excess current region of the forward characteristics becomes evident at low voltages as the temperature is lowered below 195 K. A plot of $\ell n(J_F/T^2)$ at 0.2 V versus 1/T (not shown here) is found to be linear in the temperature range 98-155 K with a slope giving an activation energy of 0.14 eV. This low activation energy value is again associated with recombination which causes even more deviations from thermionic emission behavior at low voltages and low temperatures.

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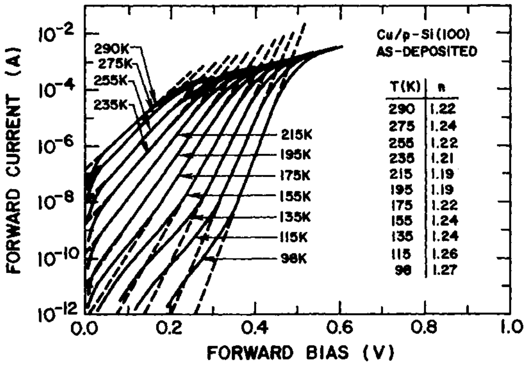

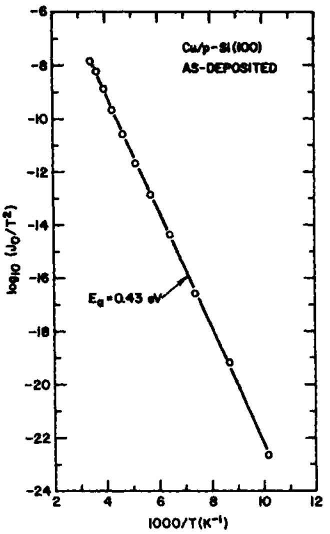

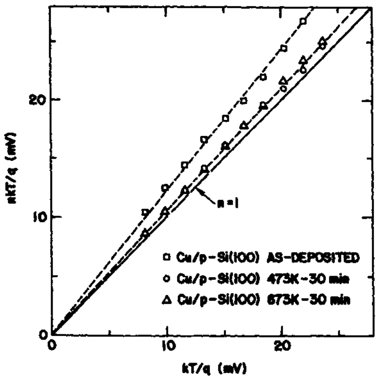

Fig. 8. Forward I-V characteristecs of Cu on p-type Si(100) as a function of temperature for samples in the as-deposited state. Junction area is 1.31×10^{-4}cm^2.

Fig. 9. Temperature dependence of the ideality factor for p-type samples in the as-deposited state (open squares) and after annealing at 473 K for 30 min (open cirles) and 673 K for 30 min (open triangles).

Fig. 10. Temperature dependence of forward current measured at zero applied voltage for p-type samples in the as-deposited state.

In Fig. 11 we show examples of the forward I-V characteristics obtained after annealing the Cu/p-type Si(100) samples at 473 K for 30 min. Results of the annealing at 673 K for 30 min are very similar. The samples display a good ideality factor which remains unchanged in the temperature range 95-290 K. Again, for these samples the data of nkT/q against kT/q can be fitted to a straight line passing through the origin with a slope now equal to 1.04 (Fig. 9). Moreover, the dependence of $\ell n(J_o/T^2)$ on 1/T is linear in the temperature range measured with slopes giving barrier-height values of 0.48 and 0.49 eV for the 473-K and 673-K annealed samples, respectively, as shown in Fig. 12. It is also clear from the open triangles shown in Fig. 4 that in these samples the barrier height calculated using the relation for thermionic emission does not exhibit a temperature dependence.

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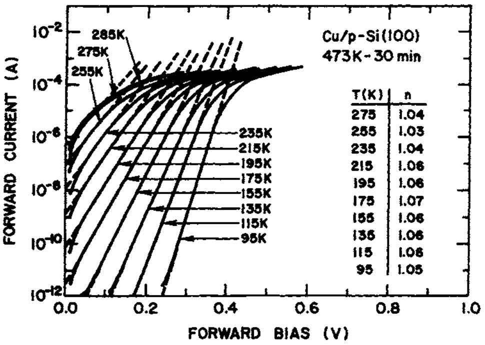

T(K)	n
275	1.04
255	1.03
235	1.04
215	1.06
195	1.06
175	1.07
155	1.06
135	1.06
115	1.06
95	1.05

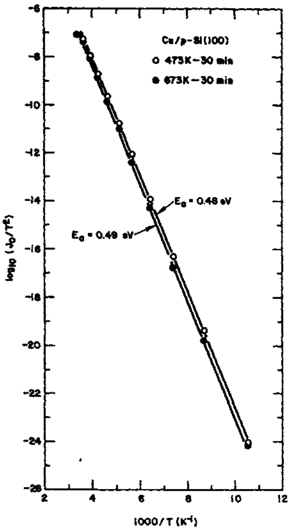

Fig. 11. Forward I-V characteristics of Cu on p-type Si(100) as a function of temperature for samples annealed at 473 K for 30 min.

Fig. 12. Temperature dependence of forward current measured at zero applied voltage for p-type samples annealed at 473 K for 30 min (open circles) and 673 K for 30 min (solid circles).

C. n-Type Ge(100)

The forward I-V characteristics plotted in Fig. 13 as a function of temperature show examples of the results obtained for Ti on n-type Ge(100). The samples display a good ideality factor which remains essentially unchanged with temperature. In addition, the dependence of $\ell n(J_o/T^2)$ on 1/T is linear in the temperature range measured with a slope giving a barrier-height value at 0 K of 0.60 eV, as shown in Fig. 14. The temperature variation of the barrier height calculated using the relation for thermionic emission $[J_o = A^*T^2 \exp(-q\Phi_{Bn}/kT)]$ is shown in Fig. 15 by the open circles. In Fig. 15 we also show the temperature variation of the barrier height obtained from C-V measurements for Cu on n-type Ge(100) (open triangles). The solid lines show the temperature variation of the barrier height calculated on the assumption that it is entirely due to the temperature dependence of the indirect band gap in Ge with the barrier-height value at 215 K as a reference. It is clear from these data that for both Cu and Ti the change in the n-type barrier height with temperature is almost equal to the change in the Ge indirect band gap. It is also to noted that for Cu, the barrier-height values at 295 K are in very good agreement with those reported by Thanailakis and Northrop[20] for Cu on Ge(111) using I-V and C-V measurements.