Schottky Barrier Height Dependence on the Metal Work Function for p-type Si Schottky Diodes

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We investigated Schottky barrier diodes of 9 metals (Mn, Cd, Al, Bi, Pb, Sn, Sb, Fe, and Ni) having different metal work functions to p-type Si using current-voltage characteristics. Most Schottky contacts show good characteristics with an ideality factor range from 1.057 to 1.831. Based on our measurements for p-type Si, the barrier heights and metal work functions show a linear relationship of current-voltage characteristics at room temperature with a slope ($S = \phi_b/\phi_m$) of 0.162, even though the Fermi level is partially pinned. From this linear dependency, the density of interface states was determined to be about $4.5 \cdot 10^{13}$ 1/eV per cm^2, and the average pinning position of the Fermi level as 0.661 eV below the conduction band.

Key words: Schottky Diodes; Barrier Height; Series Resistance; Work Function; Miedema Electronegativity.

1. Introduction

The investigation of rectifying metal-semiconductor contacts (Schottky diodes) is of current interest for most elemental and compound semiconductors. In general, Schottky barrier diodes (SBDs) are of interest as the least complex power device and are discussed as an alternative for p-n junctions [1 – 5]. They have very fast switching times with no reverse recovery current, because they work with only majority carriers [1, 2, 6, 7]. So, SBDs play an important role in the performance of semiconductor devices for various electronics and optoelectronic applications. In recent years, Si Schottky diodes have received much attention due to their maximum potential for heigh power devices in novel band engineered heterostructure devices [8 – 11].

For a better understanding of the electrical properties of any semiconductor material it is important to know its contact behaviour with several other substance. Thus, the formation of Schottky barriers (SBs) at metal-semiconductor interfaces has been a subject of debate for decades. Schottky and Mott [12, 13] proposed a model, called the Schottky-Mott model, that the SB height (ϕ_b) equals to the difference between the work function of the metal (ϕ_m) and the electron affinity of the semiconductor (χ_s). Then, a linear dependence should exist between the ϕ_b and the ϕ_m. Corresponding to this, SB heights of various elemental metals, including Au, Ti, Pt, Ni, Cr, have been reported [14 – 16]. In these reports it has been found that the SB heights change with ϕ_m but do not scale proportionally with ϕ_m within experimental scattering. In addition, generally in covalent semiconductors, such as GaAs, the Fermi level is pinned by surface states, so that the barrier height hardly depends on the ϕ_m [17]. On the other hand, Guo et al. [18] reported that the SB height of *n*-GaN is independent of ϕ_m. In some studies [19 – 22] it has been found that the SB height is almost independent of the surface orientation of the substrate, preparation of the surface and type of the metal being used. Furthemore, it has been shown that the SB height is restricted to within the 0.4 – 0.7 eV for p-type Si, independent of contact metal. These low SB heights have detrimental effects on the realizability, performance and reliability of devices such as metal-semiconductor field-effect transistors and metal-semiconductor-metal integrated photodetectors [23]. Although for a given semiconductor the SB heights generally increase when ϕ_m of the metal in contact becomes larger, the simple Schottky-Mott model is not confirmed by the experimental data. Barden [24] attributed this discrepancy to the presence of interface states. We have studied the electrical and interfaces properties of metal/p-Si Schottky diodes as functions of the metal work function by measuring *I-V* characteristics at room temperauture.

2. Experimental Method

Metal/p-type Schottky diodes were prepared, using mirror cleaned and polished p-type Si wafers with [100] orientation and 5 – 10 Ωcm resistivity. The wafer was chemically cleaned and the ohmic contact was made by evaporating Al on the back of the substrate, followed by a temperature treatment at 575 °C for 3 min in an N_2 atmosphere. The native oxide on the front surface of the substrate was removed in HF:H_2O (1:10) solution, and finally the wafer was rinsed in deionised water for 30 s.

For metal/p type Si Schottky structures, various contact metals, such as Mn, Cd, Al, Bi, Pb, Sn, Sb, Fe, and Ni with diameters of about 1 mm on the front surface of the wafer, were deposited by thermal evaporation. All evaporation processes were carried out with a turbo molecular pump at about 10^{-6} mbar.

The dark current-voltage (*I-V*) measurements were made using a Keitley 487 picoammeter/voltage source at room temperature.

3. Results and Discussion

The *I-V* data were analyzed under the assumption that the dominant current transport mechanism is thermionic emission. According to this theory, the *I-V* relationship of a Schottky diode is given by [1, 2, 14, 25]

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

where q is the electronic charge, V the applied voltage and n is the ideality factor, which is given by

$$n = \frac{q}{kT}\left[\frac{\partial V}{\partial(\ln I)}\right]. \qquad (2)$$

In (1), I_S is the saturation current derived from the straight line intercept of $\ln I$ at $V = 0$, and is given by

$$I_S = AA^*T^2 \exp\left[\frac{-q\phi_b}{kT}\right], \qquad (3)$$

where A is the effective diod area and A^* the effective Richardson constant of 32 A/cm^{2}K^2 for p-Si [3, 14].

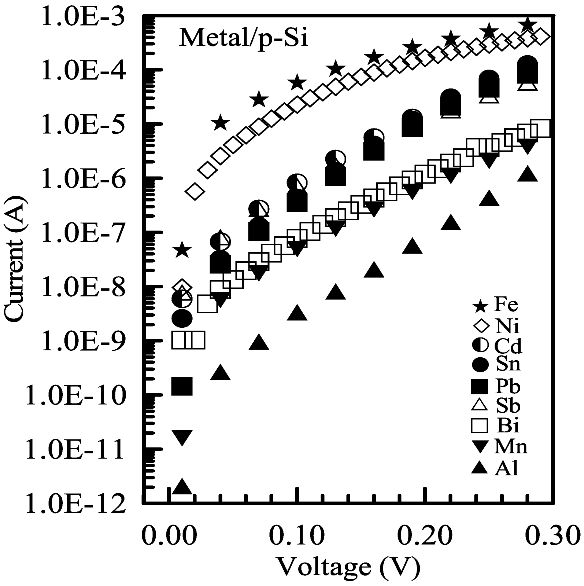

Fig. 1. Experimental forward current-voltage characteristics of various metal/p-Si Schottky diodes at room temperature.

The *I-V* characteristics of various metals/p-type Si samples under room temperature condition are shown in Figure 1. It is evident that the thermionic emission assumption is valid except in the high current region. On the basis of well-known thermionic emission theory, SB heights were calculated with the help of (3) from the *y*-axis intercepts of the semilogarithmic forward bias *I-V* plots, and the values of *n* were obtained using (2) in the linear region of these plots, indicating that the series resistance effect in the linear region is not important (Fig. 1). In this work, the SBHs for metals/p-type Si diodes ranged from 0.567 eV to 0.854 eV, and the ideality factor *n* from 1.057 to 1.831. It is well known that the *I-V* characteristics, however, are strongly affected by the ideality factor, series resistance, and leakage current. Hence, the SB heights obtained from *I-V* characteristics with an ideality factor larger than unity would be lower than the real values.

When a metal and a semiconductor are brought into contact, a potential barrier occurs at the interface which is found to exhibit rectifying properties. It is well known that the SB height ϕ_b is expressed by [20, 26, 27]

$$\phi_b = S(E_S - \phi_m) + (1-S)\phi_{cnl}, \qquad (4)$$

where ϕ_{cnl} is charge neutrality level, ϕ_m the work function of the metal, E_S the ionization energy of the electron that equals the sum of the electronegativity of the

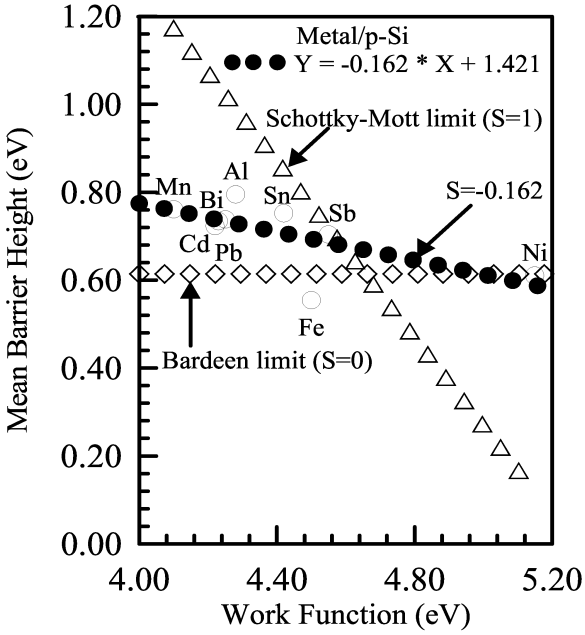

Fig. 2. The mean Schottky barrier height of various metal/p/Si schottky diodes as function of the metal work function.

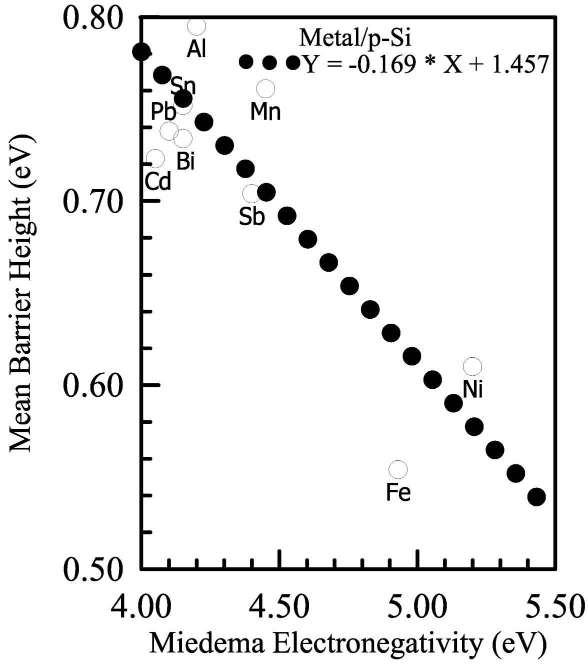

Fig. 3. The mean Schottky barrier height of various metal/p-Si Schottky diodes as function of the Miedema electronegativity.

semiconductor (χ_S) and its band gap (E_g). How ϕ_b depends on ϕ_m is usually expressed phenomenologically in terms of the interface index S defined by $S = \phi_b/\phi_m$, where $0 \leq S \leq 1$. The situation with $S = 1$ is called the Schottky limit, where the Fermi level is free from pinning. When S is 0, the SB height becomes constant and is independent of the metal work function. This situation of the strongest pinning is the Bardeen limit. The SB heights on most semiconductors are found to have a much weaker dependence on the metal work function. This phenomenon, known as Fermi level pinning, has stimulated much discussion and many models [28].

Figure 2 shows the SB heights as a function of the metal work funktion ϕ_m. It is seen that the SB heights depend on ϕ_m, giving an interface index S of about 0.162, and the Fermi level is partially pinned at room temperature. This indicates that the metal/p-Si Schottky contacts are weakly dependent on the ϕ_m of the contact in metal. The theoretically S parameter is 0.05 for Si [29]. It has been found that many Schottky diodes having large barrier heights show good characteristics with low ideality factors, the barrier height depending on ϕ_m without fermi-level pinning for all polytypes. Corresponding to this, linear relationship with slopes of about 0.2 to 0.7 are observed between the SB height and the ϕ_m [30]. The main difference between the S values has been explained by *I-V* measurements depending strongly on the homogenity of the interface [31]. On the other hand, since the practical interface index S has values between the Schottky and Bardeen limit, we can partially control the barrier height by changing the metal. In this study the minimum and maximum SB heights for metal/p-Si are 0.567 eV and 0.854 eV. Therefore, the SB heights can be controlled about maximum 0.287 eV. This value is 0.510 eV for Schottky contacts on *n*-InP [32].

From this linear dependency between SB height and ϕ_m, the density of interface states was calculated to be about $4.5 \cdot 10^{13}$ 1/eV per cm^2. It is well known that, if the density of interface states is large enough, the Fermi level becomes pinned at the neutral level. In this case, the SB height is independent, or only weakly dependent on the work function of the metal [33–36]. In this work, the neutrality level (the average pinning position of Fermi level) was determined as 0.661 eV below the conduction band. These values has been calculated as $6 \cdot 10^{13}$ 1/eV per cm^2 and 0.55 eV for p-GaAS [33].

In addition, the parameter S and the average pinning position of the Fermi level can be calculated by replacing the ϕ_m with electronegativities (X_m) [32, 35].

Figure 3 shows a plot of mean barrier heights against Miedema electronegativities. From this plot, it has been found that the charge neutrality level and S value calculated by using Miedema electronegativities are pinned about 0.614 eV below the conduction band and 0.169, respectively. We can say that as the Fermi level calculated by using ϕ_m and X_m is the same, the S values are very close to each other. In [36] these values have been found to be 0.17 and 0.04 eV for metal-and silicide-silicon contacts.

4. Conclusions

Schottky contacts on p-type Si were produced and characterized by the current-voltage (*I*-*V*) technique. The contacts exhibit nearly ideal thermionic emission characteristics. The Schottky barrier (SB) heights depend weakly on the work function of the contact metal, and the Fermi level is pinned at about 0.661 eV below the conduction band.

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