Electrical Properties of n⁻-p Amorphous-Crystalline Silicon Heterojunctions

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We have measured C-V characteristics and temperature dependence of J-V characteristics of undoped a-Si:H heterojunctions formed on p-type c-Si substrates with different resistivities. It has been found out that an abrupt heterojunction model is valid for a-Si:H/p c-Si heterojunctions, and the electron affinity of a-Si:H has been estimated as 3.93 \pm 0.07 eV from C-V characteristics. The forward current of all the junctions studied shows voltage and temperature dependence expressed as exp(- $\Delta E_{af}/kT$) x exp(AV), where ΔE_{af} and A are constants independent of voltage and temperature. The reverse current is proportional to exp(- $\Delta E_{af}/kT$) x (V_D-V)^{1/2}, where ΔE_{af} is constant independent of voltage.

§1. Introduction

Studies of heterojunctions hased on hydrogenated amorphous silicon (a-Si:H) are important from the viewpoints of understanding the fundamental device physics of a-Si:H as well as their applications to various devices. Moreover, in order to elucidate the nature of amorphousamorphous junctions, amorphous-crystalline heterojunctions should be interpreted as a necessary first step. In this paper, we present a systematic study of undoped (n-type) a-Si:H/p-type crystalline silicon (p c-Si) heterojunctions. One of the purposes of this paper is to establish an energy band diagram of a-Si:H/c-Si heterojunctions, and the other is to elucidate the current transport mechanism of our heterojunctions.

§2. Experimental

Undoped a-Si:H films were deposited by the glow discharge decomposition (GD) of pure SiH₄ on p c-Si (0.1-0.15, 1-2 and 5-10 Ω cm), p⁺ c-Si (0.005-0.01 Ω cm) and n⁺ c-Si (<0.02 Ω cm) substrates heated at 250 °C. Prior to a-Si:H deposition, silicon wafers were soaked in a solution of HF to remove SiO₂ and then rinsed in distilled water. A flow rate of 5 SCCM and a gas pressure of 50 mTorr were maintained during the deposition. Magnesium (Mg) was subsequently evaporated on an area of 0.785 mm² of the a-Si:H films in a vacuum of 7x10⁻⁷ Torr, forming an ohmic contact with undoped a-Si:H.¹ Table 1 summarizes Mg/undoped a-Si:H/p c-Si diodes used in the present work, where the film thickness L of a-Si:H, the resistivity ρ and the density of

Table 1. Various data of materials and diodes used in the present work. Experimental results obtained from C-V characteristics are also listed.

sample	p c-Si			undoped a-Si:H					
number	ρ (Ωcm)	N _A (cm ⁻³)	δ ₁ * (eV)	L (µm)	δ ₂ ** (eV)	***	v _D (v)	N _I (cm ⁻³)	X _a (eV)
1	5-10	2.0×10 ¹⁵	0.22	1.16	0.72	с	0.31	6.2×10 ¹⁵	4.00
2	1-2	9.0x10 ¹⁵	0.18	0.80	0.76	с	0.51	3.6×10 ¹⁵	3.80
3	1-2	9.0×10 ¹⁵	0.18	2.19	0.72	с	0.37	2.8×10 ¹⁵	3.98
4	0.005-0.01	-	0	1.02	0.72	с	-	-	-
5	0.1-0.15	1.8×10 ¹⁷	0.10	1.02	0.72	c	-	-	-
6	1-2	9.0×10 ¹⁵	0.18	1.02	0.72	с	0.42	3.9×10 ¹⁵	3.93
7	5-10	2.0×10 ¹⁵	0.22	1.02	0.72	c	0.38	4.0×10 ¹⁵	3.93
8	1-2	9.0×10 ¹⁵	0.18	1.76	0.84	I	0.37	1.6x10 ¹⁵	3.86
9	5-10	2.0×10 ¹⁵	0.22	1.78	0.84	I	0.20	1.8×10 ¹⁵	3.99

* $\delta_1 = kTln(N_V/N_A)$, $N_V = 1.02 \times 10^{19} \text{ cm}^{-3}$.

** δ_2 : the thermal activation energy of conductivity in dark.

*** C: capacitively-coupled GD reaction chamber, I: inductively-coupled GD reaction chamber.

acceptor impurities N_A of p c-Si are listed. N_A was determined by C-V measurements on Mg/p c-Si Schottky barrier diodes. The C-V characteristics of these diodes were measured at 100 kHz. The current-density vs. voltage (J-V) characteristics were measured as a function of temperature in the range between 297 and 374 K in N₂ atmosphere. Any hysteresis effect was not observed in J-V characteristics when the diodes were heated up and cooled down cyclically.

§3. Results and Discussion

3-1. Capacitance-voltage Characteristics of undoped a-Si:H/p c-Si structure

C-V characteristics of the diodes were measured at 100 kHz. This frequency is higher enough to be able to neglect a dielectric relaxation process in undoped a-Si:H (around 109 $\Omega_{\rm Cm}$ in resistivity),²⁾ by which one can get information on the depletion layer extending in the p c-Si side regardless of that of the a-Si:H side. In fact, the capacitance of the diodes using p⁺ c-Si instead of p c-Si (1-2, 5-10 $\,\Omega\,{\rm cm})$ measured at 100 kHz showed a constant value independent of applied voltage, coinciding with that of the capacitance determined only by the film dimension of a-Si:H, i.e.,

 $C = \frac{\varepsilon_0 \varepsilon_{s2}}{L} , \qquad ----- (1)$

where ε_{0} is the free space permittivity, ε_{s2} the dielectric constant of a-Si:H, and L the thickness of a-Si:H measured by Talystep. It clearly indicates that the measuring frequency is higher



Fig. 1.

than the reciprocal of the dielectric relaxation time of undoped a-Si:H²⁾, and besides, the depletion layer is negligibly thin in the p⁺ c-Si side.

Figure 1 shows C-V characteristics of the sample 6 (p c-Si:1-2 Ω cm). The capacitance level of a diode replaced by p^+ c-Si (sample 4) is also indicated in the figure by a broken line. Different from the conventional C-V theory, as shown in the figure, $1/C^2$ is not proportional to the applied voltage.

Since 100 kHz is much higher than the reciprocal of the dielectric relaxation time of undoped a-Si:H, the capacitance (C) measured at this frequency is approximately expressed by the relation,

$$C = \frac{\begin{array}{c} \varepsilon & \varepsilon \\ o & s \end{array}}{L + W_1} , \qquad ----- (2)$$

where W_1 is the width of the depletion region in p c-Si. From the abrupt heterojunction model 3) and Eq. (2),

$$W_{1}^{2} = \left(\frac{\overset{\varepsilon}{o}\overset{\varepsilon}{s}}{\overset{c}{s}} - L\right)^{2}$$
$$= \frac{2\overset{\varepsilon}{o}\overset{\varepsilon}{s}}{\overset{v}{s}} \frac{v_{D}}{v_{A}} (V_{D} - V) \qquad ---- (3)$$

is easily derived, where V is the applied bias voltage being supported in the depletion region, N_{A} the acceptor impurity density of p c-Si, $\ensuremath{\mathbb{N}_{\tau}}$ the effective density of localized gap states in a-Si:H, q the magnitude of electric charge, and V_D the diffusion voltage.

Figure 2 shows W_1^2 vs. $(V_D - V)$ relationship of sample 6, which was replotted from the data of



 $1/C^2$ -V characteristics of sample 6. Fig. 2. W_1^2 -V characteristics of sample 6.

Fig. 1. The data reveals quite a good linear relationship, indicating that the abrupt heterojunction model is applicable to the present system consisting of amorphous-crystalline heterolayer structure.

As is clear from Eq. (3), the magnitudes of N_I and V_D are graphically determined from the slope of the curve and the intercept on the horizontal axis in the figure, respectively, which are listed in Table 1. Thus obtained values of N_I almost coincide with those determined independently from the low-frequency C-V measurement⁴⁾ on the Au/undoped a-Si:H/n⁺ c-Si Schottky barrier diodes.

According to the abrupt heterojunction model, the electron affinity of undoped a-Si:H (χ_a) can be estimated from C-V data. Actually, experimental results obtained from several different samples give an identical value, $\chi_a = 3.93 \pm 0.07$ eV, as is clearly seen in the table.

Figure 3 shows the energy band diagram for each diode with different doping levels of p c-Si, sketched on the basis of the above results.

3-2. Current-voltage Characteristics

We consider the current transport mechanism on the basis of temperature dependence of J-V characteristics of Mg/undoped a-Si:H/p c-Si diodes, sample 4 ($\rho_{cryst.} = 0.005-0.01 \ \Omega cm$), 5 ($\rho_{cryst.} =$ 0.1-0.15 Ωcm), 6 ($\rho_{cryst.} = 1-2 \ \Omega cm$) and 7 ($\rho_{cryst.} =$ 5-10 Ωcm). Undoped a-Si:H films of 1.02 μm in thickness were deposited simultaneously on four different p c-Si substrates. Figure 4 shows J-V characteristics for different temperatures.

3-2-1 Forward J-V Characteristics

According to any of the diffusion model, the emission model and the recombination model, a relation between J and V is represented by

$$J_{\alpha} \exp(\frac{qV}{nkT})$$
 , ---- (4)

where k is the Boltzmann's constant, T the measuring temperature, and η the diode factor being independent of temperature.

As is clear from the results shown in Fig. 4, a slope of the forward-bias curve is kept almost constant for varying temperatures, which indicates that Eq. (4) dose not hold in the present system. Rather it suggests the transport phenomenon limited



Fig. 3. Energy band diagrams at crystalline-amorphous interface.



Fig. 4. J-V characteristics of sample 4 for different temperatures.

by tunneling, being described as

 $J=J_{O}\exp(AV)$, ----- (5)

where A is a temperature-independent constant. The data in Fig. 5 was analyzed using Eq. (5), resulting in the temperature dependence of the pre-exponential factor J_0 , as shown in Fig. 5. Namely, the relation

$$J_0 \propto \exp(-\frac{\Delta E_{af}}{kT}) \qquad ----- \qquad (6)$$

holds between J_0 and T, where ΔE_{af} takes values of 0.72, 0.80, 0.65 and 0.63 eV for samples 4, 5, 6 and 7, respectively, details of which will be published elsewhere.

3-2-2. Reverse J-V Characteristics

A saturated value of the reverse current is expected to be J_. However, as is clear from Fig. 4, the reverse current density exceeds the value of J_{0} , indicating that the reverse current (J_p) is limited by another transport mechanism. Furthermore, ΔE_{ar} of the reverse current at - 0.1 V is found to be 0.68, 0.70, 0.63 and 0.62 eV for the samples 4, 5, 6 and 7, respectively, which are different from ΔE_{af} for forward the bias characteristics.

Figure 6 shows the reverse current density plotted against $(V_{\rm p}-V)^{1/2}$ for the samples 4 and 5, using lower-resistivity p c-Si diodes the substrates. The values of $V_{\rm D}$ is taken from Fig. 3. As shown in the figure, the reverse current is proportional to $(V_{D}-V)^{1/2}$ for two samples. It is noted that this proportionality holds in a whole temperature range studied in the present work. Since the bias voltage in these two diodes is mostly supported by the depletion layer of a-Si:H due to low resistivity of p c-Si substrates, the reverse current is reasonably considered as a generation current judging from the proportionality between J_R and $(V_p-V)^{1/2}$.5)



Fig. 5. Forward current-temperature characteristics of samples 4, 5, 6 and 7.

§3. Summary

The main results we have obtained are summarized as follows:

1) The abrupt heterojunction model is valid for our amorphous-crystalline Si heterojunctions.

2) The electron affinity of undoped a-Si:H is estimated as 3.93 ± 0.07 eV.

3) The forward current, described as $\exp(-\Delta E_{af}/kT)$ x exp(AV), can be explained by tunneling process.

4) The reverse current, which is described as $exp(-\Delta E_{ar}/kT) \times (V_{D}-V)^{1/2}$, is reasonably considered as a generation current.

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Fig. 6. $J_R^{-(V_D^{-V})^{1/2}}$ characteristics of samples 4 and 5.