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Electrical Properties OF Cs Covered Real Si Surfaces

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The conductivity and the electron mobility in inversion layers on etched Si surfaces covered with Cs have been measured at temperatures between 80 and 400 K.

The temperature dependence of the electron concentration can be explained by following energy level scheme at the surface. (1) Acceptor-like trap levels of 1.9×10^{12} cm^{-2} exist at 0.3 eV below the conduction band. (2) Cs-associated donor levels whose concentration decreases from 1.9×10^{12} cm^{-2} to zero with the increase of the adsorbed Cs lies at $0.098 \sim 0.070$ eV. (3) Cs = associated donor levels whose concentration increases from zero to 2×10^{13} cm^{-2} which is almost equal to the maximum number of adsorbed Cs lies at $0.01 \sim 0.005$ eV.

§1. Introduction

Analysis of the temperature dependence data of the charge carrier concentration is a standard technique to determine the electronic energy level scheme in semiconductors. This classical method has been, however, not necessarily succesful at surfaces due mainly to the difficulty in the separation of the surface from the bulk.[1,2]

A surface inversion layer is separated completely from the bulk electrically by a *p-n* junction. Therefore, one can perform standard transport measurements for the inversion layer to analyse the surface levels.

In the present paper, experimental results of the temperature dependence of the resistivity and the electron mobility in *n*-type inversion layers on etched *p*-type Si surfsce at a various cesium coverages and the electronic level scheme at the surfaces analysed from the data will be presented.

§2. Experimental

Specimens used had n$^+$-circular concentric electrodes on (100) surface of *p*-type Si substrate containing acceptors of 1×10^{15} cm^{-3}. The diameters of the inner and the outer electrodes were 580 and 620 μm, respectively. After taking off the oxide layer in HF, the specimens were etched in the mixture of NH$_4$F: H$_2$O$_2 = 1:1$ for 2 minutes and rinsed in distilled water.

CsCO$_3$ was used as a Cs source. CsCO$_3$ in porous Al$_2$O$_3$ coated on W filaments was thermally decomposed by passing a current through the filaments. Number of adsorbed Cs was estimated from the ionic current between the Cs source and the specimen. Experiments were performed in vacua lower than 1×10^{-7} Torr in a oil free system.

The resistance and magnetoresistance were measured at temperatures, T, between 400 and 77 K, and magnetic fields up to 23KOe.

§3. Results and Discussion

The surface conductivity, σ, at 300 K is shown as a function of the number of adsorbed Cs per unit area, N_{Cs}, in Fig. 1. The surface conductivity was initially about 4×10^{-9} mho/□ and almost constant up to the N_{Cs} reached to 1×10^{12} cm^{-2}. After the N_{Cs} exceeded this critical number, the surface conductivity increased drastically with the increase of the Cs coverage. These results are considered to show that electrons in adsorbed-Cs-associated surface states (Cs states) fall into surface states originally existed in etched Si (trap states) until the trap states are completely filled with electrons and thereafter they are excited to the conduction band. The trap state density estimated from the above mentioned model is about 2×10^{12} cm^{-2}.

The electron mobility, μ, at 290 and 90 K is shown as a function of the number of carriers per unit area, N_s, in Fig. 2. The magnitude of μ for $N_s < 5 \times 10^{11}$ cm^{-2} was about 580 cm^2/v.s which was almost independent of T and N_s. The mobility decreased with the increase of N_s for $N_s > 5 \times 10^{11}$ cm^{-2}. The magnitude of the mobility in the whole region is much smaller than the mobility in Si MOS-FET. Therefore, the impurity scattering is the dominant process in the carrier transport in the
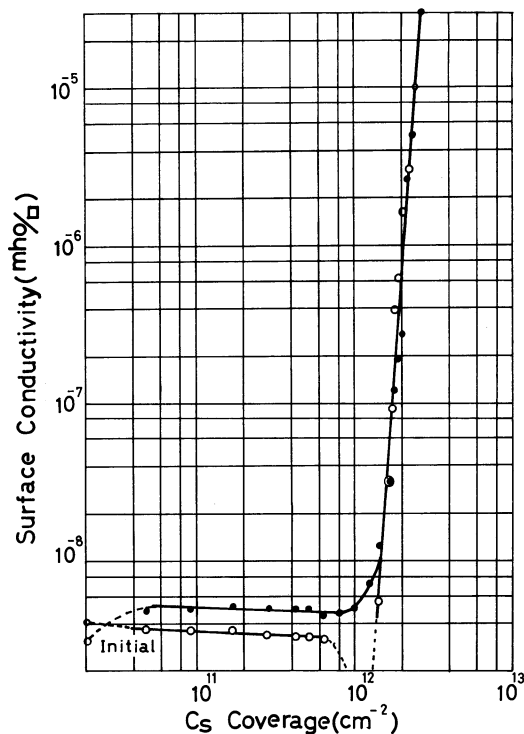
Fig. 1. Surface conductivity of (100) Cs covered real Si surfaces vs Cs coverage at 300 K.

Fig. 3. Surface resistance vs reciprocal temperature at various Cs coverages.
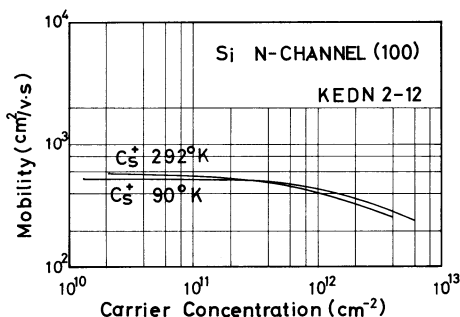

Fig. 2. Mobility of electrons in inversion layer vs surface carrier concentration at 292 and 300 K.

present surfaces.

In Fig. 3, the temperature dependence of the surface resistance for various number of adsorbed Cs are shown. The surface resistance, R, changed as $R = R_0 \exp(\Delta E/kT)$. ΔE decreased from 0.3 eV at $N_{Cs} = 1 \times 10^{12}$ cm^{-2} to almost zero with the increase of N_{Cs}. The data in Fig. 3 can be converted to the temperature dependence of N_s by use of the mobility data.

In what follows, a procedure to obtain energy levels of the trap states and the Cs states will be described. In the first place, the Fermi level at the surface will be determined
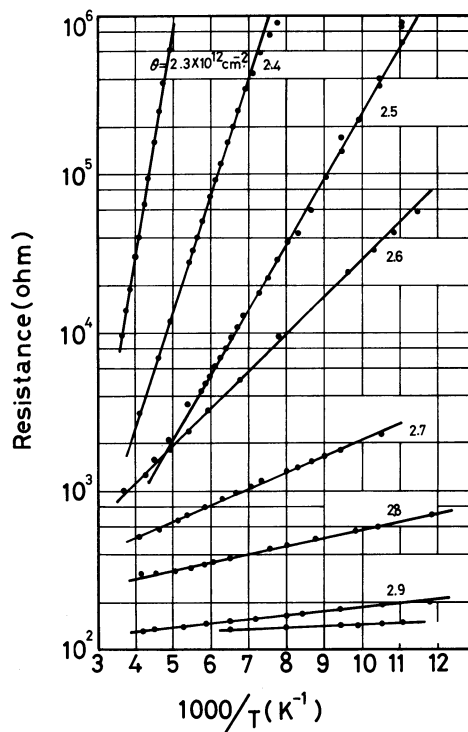
as a function of N_s and T. Secondly, a model surface level scheme will be assumed most simply as far as the experimental temperature dependence can be explained. Finally, on a basis of the electrical neutrality condition, the energy of each surface level will be calculated at various temperatures to fit the experimental Fermi level as a function of the concentration of the level. A set of a concentration and a energy of the surface level which do not vary with temperature will be chosen as the physical quantities to be determined.

The energy levels of electrons in a thin inversion layer are grouped in two dimensional sub-bands whose bottoms are connected with quantized levels in the motion normal to the surface.[4] A self-consistent calculation should be performed to determine the energy levels of the sub-bands. Here, we used in the following calculation, however, eigen values in a inverted triangular potential well in which the constant electric field, E_s, is given by the field at the center of the electron distribution in the inversion layer: $E_s = e(N_s/2 + N_{dep})/\varepsilon_{sc}$, where ε_{sc} the dielectric constant of the semiconductor and N_{dep} the total number of negative charge

per unit area in the depletion layer. The surface carrier concentration is given by

$$N_s = \sum_n \frac{kT}{\pi\hbar^2} v_n m_{dn} \cdot \ln\{1 + \exp\left[(E_F - E_n)/kT\right]\}$$

where v_n the valley degeneracy, m_{dn} the density-of-state mass, E_n the energy level of n-th sub-band bottom. If $(E_F - E_n)/kT \ll -1$, which is fairly well satisfied in the present experiment, the Fermi level is given by

$$E_F = kT\left[\ln N_s - \ln\left\{\frac{kTv_n m_{dn}}{\pi\hbar^2}\sum_n \exp(-E_n/kT)\right\}\right]$$

E_F has been calculated as a function of N_s determined by experiments at various temperatures for various Cs coverages. For N_s less than 5×10^{11} cm^{-2}, the value of E_F is in good agreement with those obtained by classical surface space charge layer calculations.[1,2] The results are represented well by

$$(E_F - E_c)_s = (E_F - E_c)_{s0} - \alpha T.$$

$(E_F - E_c)_{s0}$ and α are shown in Table I, for various N_{Cs}.

In order to explain the surface potential and its temperature variation for various Cs coverages, we have assumed a level scheme at the surface as shown in Fig. 4. Here we have assumed as follows.

1) Three discrete sets of localized surface levels, trap states, lower Cs states and higher Cs states exist at the surface.

2) The trap states are acceptor-like and the two kinds of Cs states are donor-like.

3) The number of the lower Cs states, N_1, is equal to the number of adsorbed Cs, N_{Cs}, when $N_{Css} < N_t$ (the number of the trap states).

4) When $N_{Cs} > N_t$, the higher Cs states whoes number, N_2, is equal to $(N_{Cs} - N_1)$ are
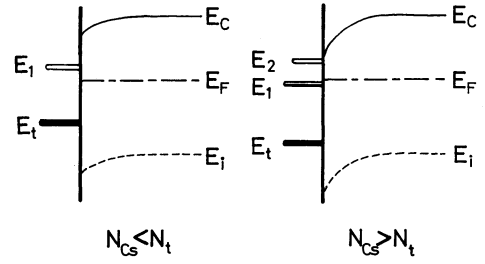

Fig. 4. Schematic band diagram at the Cs covered real Si surface. E_t is the acceptor-like trap states originally existed in the etched Si surface. E_1 and E_2 are donor-like adsorbed-Cs-associated surface states.

created.

Note that two kinds of Cs levels are necessary to explain the experimental temperature dependence of the Fermi level at the surfaces.

Case 1. For $N_{Cs} < N_t$, the electrical neutrality condition is given by

$$N_1^+ - N_t^- = N_s + N_{dep}.$$

Case 1-a. When $(E_1 - E_F) \gg kT$, lower Cs states are fully ionized and α is positive. $(E_t - E_c)_s$ is given by

$$(E_t - E_c)_s = (E_F - E_c)_{s0} - \alpha T + kT \cdot \ln\left(\frac{N_t}{N_1 - (N_s + N_{dep})} - 1\right)$$

$(E_t - E_c)_s$ has been solved numerically as a function of N_t and T and a temperature independent $(E_t - E_c)_s$ for a N_t has been determined for each N_{Cs}.

Case 1-b. As E_F approaches to E_1, lower Cs states are partially ionized. $(E_1 - E_c)_s$ is given by

$$(E_1 - E_c) = (E_F - E_c)_{s0} - \alpha T - kT$$
$$\times \ln\left(\frac{N_1}{N_s + N_{dep} + N_t/\{1 + \exp[(E_t - E_F)/kT]\}} - 1\right)$$

Table I.

No.	$(E_c = E_F)_{s0}$ in eV	α in eV/K	N_t in cm^{-2}	N_1 in cm^{-2}	N_2 in cm^{-2}	$(E_c - E_t)$ in eV	$(E_c - E_1)$ in eV	$(E_c - E_2)$ in eV
1	0.340	3.06×10^{-4}	1.9×10^{12}	1.7×10^{12}	0.0×10^{12}	0.301		—
2	0.304	3.75	1.9	1.9	0.1	0.3060		
3	0.247	2.56	″					
4	0.098	−1.30	″	1.9	0.5	0.3	0.098	0.01
5	0.028	−2.00	″	1.2	1.4	″	0.097	0.01
6	0.030	−1.80	″	1.1	1.6	″	0.085	0.01
7	0.015	−1.60	″	0.7	2.2	″	0.070	0.008
8	−0.002	−2.20	″	0.5	2.6	″	0.070	0.009
9	−0.011	−2.20	″	0.0	3.5	″	—	0.005
10	0.005	−1.70	″	0.0	2.0×10^{13}	″	—	0.005

E_1 and N_1 were determined by the same way to the case 1-a.

Case 2. For $N_{Cs} > N_t$, the electrical neutrality condition is given by

$$N_1^+ + N_2^+ - N_t^- = N_s + N_{dep}.$$

In this case $E_F \gg E_t$, so $N_t^- = N_t$. $(E_1 - E_c)_s$ is given by

$$(E_1 - E_c)_s = (E_F - E_c)_{s0} - \alpha T - kT$$
$$\times \ln \left(\frac{N_1}{N_s + N_{dep} + N_t - N_2 / \{1 + \exp[(E_F - E_2)/kT]\}} \right.$$
$$\left. - 1 \right)$$

$(E_2 - E_c)_s$ is given by the exchange of N_1 and E_1 for N_2 and E_2 in eq. 7, respectively. Cs states were also determined similarly to the case 1-a and b. The results of the calculations are listed up in Table I.

A level scheme proposed by Mönch[3] on the cleaved (111) Si surface with adsorbed Cs has acceptor-like Cs levels at 0.1 eV above E_i. This is lower than the lower Cs levels in the present scheme. He assumed the bulk mobility for electrons in the space charge layer. However, the mobility should be much smaller than the bulk mobility in the space charge layer on the cleaved surface. Therefore, his estimation gives the lower limit of the level.

In conclusion, the surface donor levels associated with adsorbed Cs on etched p-type Si surfaces in $0.098 \sim 0.07$ eV below the bottom of the conduction band for small Cs coverages and changes to $0.01 \sim 0.005$ eV for high Cs coverages which produce a strong inversion in the space charge layer. The former agrees well with a simple hydrogen-like donor model at the surface for 3-DEG (0.106 eV) and the latter can be explained by similar model for 2-DEG (0.016 eV). Co-existence of the two types of levels in the transition region shows probably the inhomogeneity in the Cs coverage.

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