$$\rho_I(u_{OB}) = \int_{E_F^a - u_{OB}}^{E_F^a} g(E)dE \qquad (3\text{-}16)$$

and

$$qN_I^* = \rho_I(u_{OB}) \qquad (3\text{-}17)$$

with

$$u_{OB} = E_F^a - E_{OB}^a \quad , \qquad (3\text{-}18)$$

where u_{OB} is the energy variation at $x=W_{OB}$, N_I^* is the density of midgap states between E_F^a and E_{OB}^a in a-Si:H, E_{OB}^a is E_{OB} in the neutral region of a-Si:H. At thermal equilibrium (i.e., V=0 V), when the built-in potential for a-Si:H is larger than the value of $(E_F^a - E_{OB}^a)/q$, $\rho_I(x)$ near the interface exceeds qN_I^* because the Fermi level is below E_{OB} near the interface. This situation near the interface remains the same even when the reverse bias is applied. However, as will be discussed later, the contribution of the excess charges near the interface can be included in the effect of charged states in the near-interface region.

In the depletion region in p c-Si, which is region Ⅲ ($-W_1 \leq x \leq 0$) in Fig. 3.11, the space-charge density is given by $-qN_A$ under the reasonable assumption that the p c-Si has only shallow acceptors whose density is N_A. As a consequence, the space-charge density can be schematically shown in Fig. 3.11(c).

3-3-2. Simulation

Based on the energy-band diagram mentioned above, the C-V characteristics of the amorphous/crystalline semiconductor heterojunction is theoretically considered. Simulations of the C-V characteristics of the amorphous/crystalline semiconductor heterojunctions at 0 Hz were reported,[10-13] but it is experimentally difficult to measure their very low frequency C-V characteristics that would correspond to the simulation data. Moreover, the experimental low frequency C-V characteristics vary with the measuring frequency due to the dielectric relaxation and

trapping/detrapping processes in the amorphous film.

On the other hand, it is easy to measure their high-frequency C-V characteristics, and when the measuring frequency is high enough, the dielectric relaxation process as well as the trapping/detrapping process can be neglected in the amorphous film. So the change in width of the depletion region in the crystalline semiconductor, produced by the dc reverse bias, is only needed to calculate the capacitance. This leads to an accurate simulation of the high-frequency C-V characteristics of highly resistive amorphous/lowly resistive crystalline heterojunctions. The analytical approach here is that the contribution of a-Si:H to the measured capacitance is equal to the geometric capacitance of the a-Si:H film due to its longer dielectric relaxation time, whereas that of c-Si is associated with the depletion width of c-Si. The measured capacitance is essentially the result of two capacitances in series. In the following, discussed is the simulation condition for the high-frequency C-V characteristics of the amorphous/crystalline heterojunction.

The potential u(x)/q for electrons can be derived from the Poisson equation;

$$d^2[u(x)/q]/d^2x = \rho_I[u(x)]/\varepsilon_{s2} \quad , \tag{3-19}$$

where ε_{s2} is the semiconductor permittivity for a-Si:H. The space-charge Q_{rI} per unit area in region I ($W_{OB} \leqq x \leqq W_2$) is given by

$$Q_{rI} = [2\varepsilon_{s2} \int_0^{u_{OB}} \rho_I(u)du]^{1/2} \tag{3-20}$$

and the electric field (E_{rI}) at $x=W_{OB}$ is given by

$$E_{rI} = Q_{rI}/\varepsilon_{s2} \quad . \tag{3-21}$$

In region Ⅱ, Eq. (3-19) can be solved easily with the boundary conditions of $u(0)=u_0$, $-d[u(x)/q]/dx=E_{rI}$ at $x=W_{OB}$, and $u(W_{OB})=u_{OB}$, because $\rho_I=qN_I^*$, where N_I^* is constant in the region.

The value of W_{OB} is calculated as a function of u_0. Then, the width (W_1) of the depletion region in p c-Si is estimated from the charge neutrality;

$$qN_AW_1 = qN_I^*W_{OB} + Q_{rI} \qquad (3\text{-}22)$$

and the reverse voltage is calculated from the relation

$$V_B^* - V = u_0/q + qN_AW_1^2/2\varepsilon_{s1} \quad , \qquad (3\text{-}23)$$

where V_B^* is the built-in potential and ε_{s1} is the semiconductor permittivity for c-Si.

Finally, the high-frequency capacitance (C) is estimated as

$$C = S(\varepsilon_{s1}/W_1 + \varepsilon_{s2}/L) \quad , \qquad (3\text{-}24)$$

because of the long dielectric relaxation time of undoped a-Si:H, where L is the thickness of a-Si:H and S is the electrode area.

To calculate N_I^* in Eq. (3-17) it is necessary to know the g(E) in a-Si:H. Because the main midgap states in the a-Si:H are reported to be the dangling bonds, which will be described in Chapter Ⅴ, the g(E) is assumed to have a Gaussian distribution given by

$$g(E) = g_{max}\exp\{-[(E - E_p)^2/2E_W^2]\} \quad , \qquad (3\text{-}25)$$

where g_{max} is the maximum value of the Gaussian distribution, E_p is the energy level of the maximum value, and E_W is the half-width of the distribution.

Next it is necessary to consider the interface states and the states located in the near-interface region that is qualitatively different from the bulk region. Here, one kind of positively charged layer with thickness d_s and density N_s^* are considered. This layer is located between c-Si and a-Si:H, and represents the interface and near-interface regions of the heterojunction. This layer is called an interface layer in this section, and the charge Q_{ss} per unit area is given by $N_s^*d_s$. If

the effect of the interface layer cannot be neglected, Eq. (3-22) becomes

$$qN_AW_1 = qN_I^*W_{OB} + Q_{rI} + Q_{ss} \quad (3\text{-}26)$$

$$= qN_I^*W_{OB} + Q_{rI} + N_s^*d_s \quad . \quad (3\text{-}27)$$

The parameters used in the present simulation are given in Table 3-2 and almost all the parameters are fixed, since the purpose in this section is to understand the physical background of the space-charge density (N_I) as well as the built-in potential (V_B) obtained from the steady-state HMC method which is described in the former section. The value of ε_{s1} is also assumed to be equal to the value of ε_{s2}.

3-3-3. Reliability of steady-state HMC method

Figure 3.12(a) shows the simulated high-frequency C-V characteristics of a highly resistive amorphous/lowly resistive crystalline heterojunction (with parameters of $g_{max}=10^{16}$ $cm^{-3}eV^{-1}$ and $N_A=10^{15}$ cm^{-3}), and Fig. 3.12(b) shows the W_1^2-V relation obtained from the C-V curve given in Fig. 3.12(a) by using Eq. (3-10). According to the steady-state HMC method [Eq. (3-11)], the values of N_I and V_B can be graphically obtained from the slope and the intercept on the abscissa, respectively. The value of N_I obtained in the reverse-bias region ($-6\ V \leqq V \leqq -1\ V$) is 2.5×10^{15} cm^{-3}. This value is close to N_I^* of 2.0×10^{15} cm^{-3} calculated from Eqs. (3-16) and (3-17) using the parameters given in Table 3-2 ($g_{max}=10^{16}$ $cm^{-3}eV^{-1}$). The value of V_B, which is obtained from the intercept of the straight line drawn in the reverse-bias region ($-6\ V \leqq V \leqq -1\ V$) on the abscissa, is 0.21 V. This value is a little lower than the given value of $V_B^*=0.30$ V, because the additional potential u_{OB}/q is necessary to make the space-charge density constant. Figure 3.13 depicts N_I and V_B as a function of N_I^*. Figure 3.14 shows the dependence of N_I and V_B on N_A. From both figures, N_I represents the midgap-state density well, although N_I is a little larger than the given value of N_I^*.

The simulated high-frequency C-V characteristics, in which

TABLE 3-2. Parameters used for simulating high-frequency C-V characteristics.[a,b]

Amorphous film			
Neutral region	Midgap states	Interface layer	Others
$E_C-E_F^a$=0.73 eV $E_C-E_{OB}^a$=0.97 eV	E_C-E_p=0.85 eV E_W=0.10 eV $g_{max}=10^{16}-10^{17}$ $cm^{-3}eV^{-1}$	$N_S^*=0-10^{18}$ cm^{-3} d_S=0 or 50 Å	V_B^*=0.3 V L=1.2 μm S=0.785 mm^2 $N_A=10^{15}-10^{17}$ cm^{-3}

[a] N_I^* is calculated from Eq. (3-16) using the given g_{max}.
[b] N_I and V_B obtained from the steady-state HMC method correspond to the parameters N_I^* and V_B^* for the simulation, respectively.