the effect of the interface layer cannot be neglected, Eq. (3-22) becomes
\[ qN_A W_1 = qN_I^* W_{OB} + Q_{RI} + Q_{SS} \]  \hspace{1cm} (3-26)
\[ = qN_I^* W_{OB} + Q_{RI} + N_s^* d_s \]  \hspace{1cm} (3-27)

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 \(\varepsilon_{s1}\) is also assumed to be equal to the value of \(\varepsilon_{s2}\).

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 \(\varepsilon_{max}=10^{16} \text{ cm}^{-3} \text{ eV}^{-1}\) and \(N_A=10^{15} \text{ cm}^{-3}\)), 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 \((-6 V \leq V \leq -1 V)\) is \(2.5 \times 10^{15} \text{ cm}^{-3}\). This value is close to \(N_I^*\) of \(2.0 \times 10^{15} \text{ cm}^{-3}\) calculated from Eqs. (3-16) and (3-17) using the parameters given in Table 3-2 \((\varepsilon_{max}=10^{16} \text{ cm}^{-3} \text{ eV}^{-1})\). The value of \(V_B\) which is obtained from the intercept of the straight line drawn in the reverse-bias region \((-6 V \leq V \leq -1 V)\) on the abscissa, is 0.21 V. This value is a little lower than the given value of \(V_B^* = 0.30 \text{ V}\), 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 |
| \(E_C-E_F=0.73\) eV | \(E_C-E_F=0.85\) eV | \(N^*_S=0-10^{18}\) cm\(^{-3}\) | \(V_B^*=0.3\) V |
| \(E_C-E_{DB}=0.97\) eV | \(E_W=0.10\) eV | \(d_S=0\) or \(50\) Å | \(L=1.2\) \(\mu\)m |
| \(\varepsilon_{max}=10^{16}-10^{17}\) cm\(^{-3}\) eV\(^{-1}\) | | | \(S=0.785\) mm\(^2\) |
| | | \(N_A=10^{15}-10^{17}\) cm\(^{-3}\) |

\(^a\) \(N_I^*\) is calculated from Eq. (3-16) using the given \(\varepsilon_{max}\).

\(^b\) \(N_I^*\) and \(V_B^*\) obtained from the steady-state HMC method correspond to the parameters \(N_I^*\) and \(V_B^*\) for the simulation, respectively.
Fig. 3.12. Calculated results without interface layer: (a) calculated C-V characteristics and (b) voltage dependence of square of depletion width in crystalline semiconductor. The values of $N_I$ and $V_B$ are obtained from the steady-state HMC method. The solid line is calculated data, and the dashed line is a line extrapolated from high reverse biases.
Fig. 3.13. Dependencies of $N_I$ and $V_B$ obtained from steady-state HMC method on $N_I^*$ without interface layer. The values of $N_I^*$ and $V_B^*$ are parameters for simulating the high-frequency C-V characteristics.
Fig. 3.14. Dependencies of $N_I$ and $V_B$ obtained from steady-state HMC method on acceptor density in crystalline semiconductor without interface layer.

Fig. 3.15. Dependencies of $N_I$ and $V_B$ on density of interface layer.
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the interface layer was taken into account, were similar to those in Fig. 3.12, although the lowest reverse bias, where the discrepancy from the straight line starts to occur, is higher than the reverse bias (about 0.7 V) calculated without the effect of the interface layer. Figure 3.15 shows the dependence of $N_I$ and $V_B$ on the charge ($Q_{SS} = N_S^* d_s$) of the interface layer for $g_{max} = 3 \times 10^{16} \text{ cm}^{-3} \text{eV}^{-1}$ and $N_A = 10^{16} \text{ cm}^{-3}$. In the region of $N_S^* \leq 2 \times 10^{17} \text{ cm}^{-3}$ (i.e., the interface-state density $Q_{SS}$ is less than $10^{11} \text{ cm}^{-2}$), the values of $N_I$ and $V_B$ are quite close to the values of $N_I^*$ and $V_B^*$, respectively, then they increase rapidly with $N_S^*$ in the case of $N_I^* = 5.9 \times 10^{15} \text{ cm}^{-3}$. These increases result from $Q_{SS}$. This critical value of $Q_{SS}$ (or $N_S^*$) increases with an increase of $N_I^*$.

It is clear from the above results that if $Q_{SS}$ is low, the values of $N_I$ and $V_B$ obtained by the steady-state HMC method represent the real midgap-state density and the real built-in potential, respectively.

3.4 Summary

The high-frequency (e.g., 100-kHz) C-V characteristics of undoped (i.e., slightly n-type) a-Si:H/p c-Si heterojunctions have been studied experimentally as well as theoretically. These heterojunctions have been found to form depletion regions in both sides of a-Si:H and c-Si by dc bias voltages, and energy-band diagrams for those heterojunctions with four different resistivities of p c-Si have been presented. Since the measuring frequency is much higher than the reciprocal of the dielectric relaxation time of the high-resistivity undoped a-Si:H, the capacitance in the a-Si:H side is determined by the thickness of the a-Si:H film. That is why the measuring capacitance at the high frequency becomes a series of this capacitance in a-Si:H and the other capacitance which is determined by the width of the depletion region in c-Si. Moreover, the trapping/detrapping processes cannot respond to the high-frequency ac voltage, which easily enables us to analyze the C-V characteristics. The main