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Energy Dependence of the Electron-Capture Cross Section of Gap States in Undoped a-Si:H Films

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Isothermal capacitance transient spectroscopy (ICTS) has been employed to measure the energy dependence of the electron-capture cross section of continuously distributed defect levels in undoped a-Si:H film for the first time, via the proposed novel structure. For undoped a-Si:H films, experimental results show that the electron-capture cross section of defect levels initially decreases exponentially, reaches a minimum, and then increases exponentially with energy depth measured from the mobility edge of the conduction band. This v-shaped distribution of the electron-capture cross section of continuously distributed defect levels in undoped a-Si:H film is different from that in phosphorous-doped a-Si:H film. This means that mechanisms other than multiphonon emission can be dominant in the electron-capture process in the gap states in undoped a-Si:H film.

KEYWORDS: undoped a-Si:H, energy dependence of electron-capture cross section

Detailed information on the nature of gap states in a semiconductor, *e.g.*, a-Si:H, is needed to understand the electronic properties of the material and also for relevant devices. The capture cross section of the gap states for electrons and holes is one of the most important parameters in recombination and trapping kinetics. Isothermal capacitance transient spectroscopy (ICTS) has been considered a useful method for determining the density-of-state distribution $g(E)$ and the capture cross section of continuously distributed gap states. Owing to measurement under the isothermal condition, it is easy to separate the temperature dependence from the energy dependence of the capture cross section. This technique had been successfully applied for investigating the gap states of phosphorous-doped a-Si:H films.[1-4] However, it is still limited in the applications to semiconductor films with low resistivity. For high-resistivity semiconductor (HRS) films, *e.g.*, undoped a-Si:H, high series resistance appears in the conventional Schottky configuration, and the RC time constant for charging and discharging the depletion layer capacitance would be too long for the high-frequency capacitance sensing signal.

In earlier work, a novel metal/HRS/n-type low-resistivity c-Si structure which has the space-charge region entirely covering the HRS film and penetrating into the c-Si substrate was proposed for substitution of the conventional Schottky configuration for determining $g(E)$ by the ICTS method.[5] Carriers charged and discharged the depletion layer capacitance through the low-resistivity c-Si substrate and metal without passing through the HRS film. Hence, the depletion layer capacitance, which reflects the space charge in HRS film, can be measured at high frequency without the influence of the high resistance of the HRS film. Thus, the ICTS method can be used to determine the $g(E)$ of HRS film. Nevertheless, the energy dependence of the electron-capture cross section of continuously distributed defect levels in undoped a-Si:H remains to be studied.

In this study, the pulse-filling measurements of the novel Au/undoped a-Si:H film/n-type c-Si substrate structure are performed. The result shows that the energy dependence of the electron-capture cross section of defect levels in undoped a-Si:H is different from that in phosphorous-doped a-Si:H film.

For our structure, the ICTS signal $S(t)$ is modified as

$$S(t)\equiv t\cdot\frac{df^*}{dt} \tag{1}$$

with

$$f^*(t)=1/C^2(t)-1/C^2(\infty), \tag{2}$$

where t is time, and $C(t)$ is transient depletion-layer capacitance, and $C(\infty)$ is the steady-state capacitance. For a system of continuously distributed defect levels, the relationship between $S(t)$ and $g(E)$ for an electron trap is given by

$$g(E(t))=\frac{-1}{kTB}\cdot S(t) \tag{3}$$

and

$$E_c-E(t)=kT\cdot\ln\left[v_n(E(t))\cdot t\right] \tag{4}$$

where $B=x_a^2/\varepsilon_a\varepsilon_c A^2 N_D$, x_a is the thickness of undoped a-Si:H film, A the junction area, N_D the doping concentrations of c-Si substrate, ε_c and ε_a the permittivities for c-Si and undoped a-Si:H film, respectively, E_c the mobility edge of the conduction band, $v_n(E(t))=N_c\cdot\sigma_n(E(t))\cdot v_{th}$ is the attempt-to-escape frequency of electrons, N_c the effective density of states in the conduction band, $\sigma_n(E(t))$ the electron-capture cross section of defect level $E(t)$, and v_{th} the electron thermal velocity. In the derivation of eq. (3), it is assumed that the voltage filling pulse width W_f is wide enough to saturate the initial conditions. However, if W_f decreases, $S(t)$ should decrease in proportion to the decrease in the number of carriers trapped at energy level $E(t)$ during the filling pulse. We can therefore determine the electron-capture rate at energy level $E(t)$ by using

$$S(t,\ W_f)=S(t,\ \infty)\cdot\left[1-\exp\left[-W_f/\tau(E(t))\right]\right], \tag{5}$$

where

$$\tau(E(t))=\frac{1}{n\cdot\sigma_n(E(t))\cdot v_{th}}=\frac{N_c}{n}\frac{1}{v_n(E(t))}, \quad (6)$$

with n the carrier concentration in the undoped a-Si:H film during the filling pulse. $S(t, \infty)$ is the value of $S(t, W_f)$ at $W_f=\infty$. It is noted that eq. (5) is based on the assumption that the electron-emission process is slower than the electron-capture process within the duration of the filling pulse. Namely, eq. (5) is valid only when $W_f \ll 1/e_n$, where e_n is the electron emission rate.

From the measurement of $S(t, W_f)$ for different W_f's, $\tau(E)$ can be experimentally obtained using eq. (5). On the other hand, the characteristic energy E_p relating to the broad peak of $S(t, \infty)$ and the value of $v_n(E_p)$ are estimated from the temperature dependence of the positions of the peak in $S(t, \infty)$, according to eq. (4) under the assumption that v_n is independent of temperature. Hence, the value of N_c/n can be determined from the relation $N_c/n=v_n(E_p)\cdot\tau(E_p)$. Once the value of N_c/n is known, the energy dependence of $v(E)$, and automatically that of $\sigma_n(E)$ can be obtained by $v_n(E)=N_c/n\tau(E)$ and $\sigma_n(E)=v_n(E)/(N_c\cdot v_{th})$, respectively.

The undoped a-Si:H films used in the present experiment were deposited in a plasma-enhanced-chemical-vapor-deposition (PECVD) system. The thickness of the undoped a-Si:H film is 1200 Å, the dark conductivity is $2.8\times10^{-12}\,\Omega^{-1}\cdot\mathrm{cm}^{-1}$ and the optical gap (E_o) determined from Tauc plots is 1.72 eV. After a-Si:H film deposition, a layer of Au film of area $0.1\times0.1\ \mathrm{cm}^2$ was evaporated and patterned. The detailed process procedure was described in an earlier report.[5]

The transient capacitance signals $C(t)$ after applying the injection voltage pulse are measured at 280 K. Figure 1 shows the ICTS signals for different W_f's under the conditions of steady reverse bias $V_R=-1.5$ V and filling pulse voltage $V_f=2.3$ V. The ICTS signals $S(t, W_f)$ increase with an increase of W_f and saturate for W_f longer than 50 ms. It is noted that a bump in $g(E)$ corresponding to the saturated ICTS signal $S(t, \infty)$ is observed. Then, these ICTS signals at a specific measurement time t for different W_f's are used to determine $\tau(E(t))$. Figure 2 shows a semilog plot of $S(t, \infty)-S(t, W_f)$ vs W_f for four different time values, where the value of $S(t, W_f=90\ \mathrm{ms})$ is taken as $S(t, \infty)$. Although a nonexponential behavior which has a long tail with varying capture time due to the slow capture of carriers on the edge of the depletion region[6,7] is observed, eq. (5) is still valid for shorter W_f. The values of $\tau(E(t))$ are therefore calculated from the initial slope of this semilog plot, as indicated by dotted lines in Fig. 2. On the other hand, from the measurement of temperature dependence of $S(t, \infty)$, the energy level E_p and the value of $v_n(E_p)$ are estimated to be $E_c-0.66$ eV and $1.61\times10^{13}\,\mathrm{s}^{-1}$, respectively. The value of N_c/n is accordingly determined to be 1.5×10^8. Thus, the energy dependence of $v(E)$ as well as the corresponding $\sigma_n(E)$, calculated under $N_c=10^{20}\,\mathrm{cm}^{-3}$ and $v_{th}=10^7$ cm/s, which are usually assumed in a-Si:H,[8-10] can be obtained and are shown in Fig. 3. $\sigma_n(E)$ initially decreases exponentially, reaches a minimum, and then increases exponentially with energy depth measured from the mobility edge of the conduction band. Similar V-shaped distribution of $\sigma_n(E)$ was also found by Kida *et al.* for the undoped a-Si:H film, using current transient spectroscopy.[11] As for the n-type-doped a-Si:H film, Okushi *et al.*[4] reported a different behavior in which $\sigma_n(E)$ monotonically decreased exponentially with energy, and the multiphonon emission was suggested to predominate in the electron-capture process in these deep gap states in doped a-Si:H film. In accordance with our results, it seems that mechanisms other than multiphonon emission can be dominant in the electron-capture process in the gap states in undoped a-Si:H film. This implies that doping will modify the atomic structure of the a-Si:H film and change the electron-capture process in gap states.

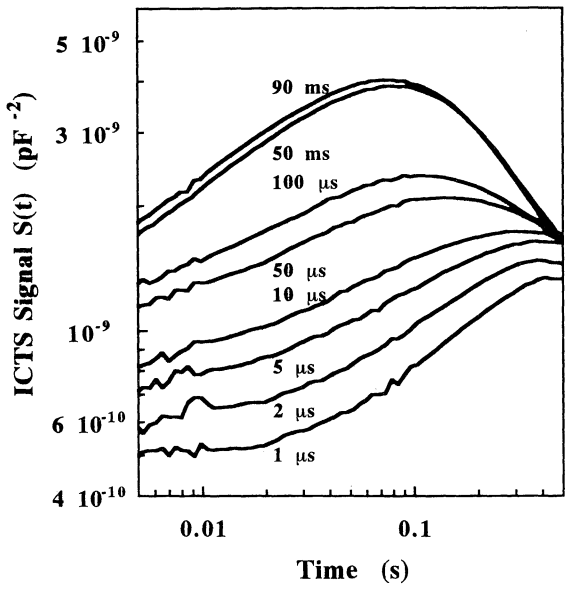

Fig. 1. ICTS Signals for various voltage filling pulse widths W_f.

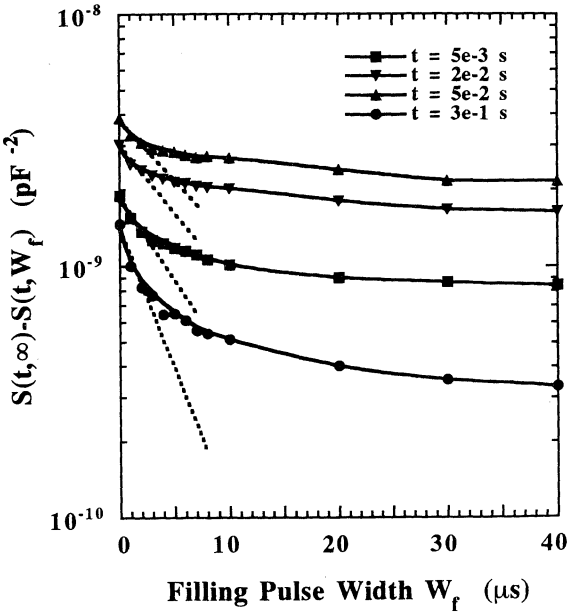

Fig. 2. $S(t, \infty)-S(t, W_f)$ vs W_f for four different values of t obtained from data of Fig. 1.

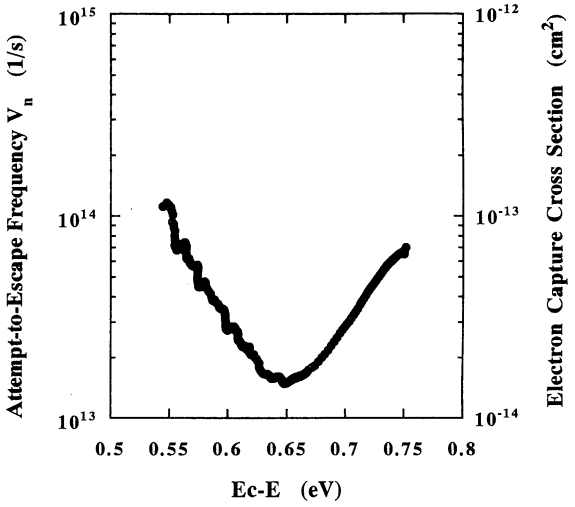

Fig. 3. Energy dependence of the attempt-to-escape frequency $v_n(E)$ and the electron-capture cross section $\sigma_n(E)$ in undoped a-Si:H film with optical gap E_o=1.72 eV.

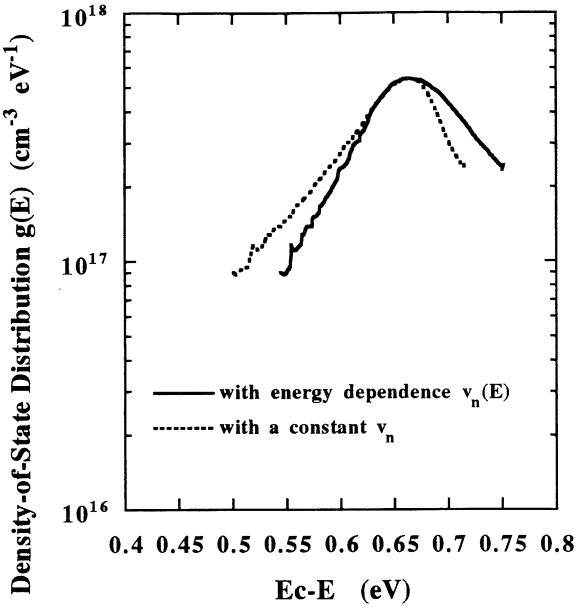

Fig. 4. The density-of-state distribution $g(E)$ for undoped PECVD a-Si:H film calculated with energy dependence of the attempt-to-escape frequency $v_n(E)$ and with constant v_n.

Finally, precise $g(E)$ is obtained by taking into account the energy dependence of $\sigma_n(E)$, as shown in Fig. 4. Obviously, some error will arise if we do not consider the energy dependence of $\sigma_n(E)$.

In summary, the ICTS method is successfully employed for the measurement of the energy dependence of $\sigma_n(E)$ of continuously distributed defect levels in undoped a-Si:H film, via the previously proposed novel structure. It is found that the mechanisms dominating the electron-capture process in gap states in undoped a-Si:H film are somewhat different from those in P-doped a-Si:H film. This means that doping will modify the atomic structure of the a-Si:H film and change the electron-capture process in gap states. In addition, we also find that it is necessary to take into account the energy dependence of $\sigma_n(E)$ in calculating $g(E)$. If the energy dependence of $\sigma_n(E)$ is not considered, incorrect $g(E)$ will be obtained.

Acknowledgments

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