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DENSITY OF LOCALIZED STATES IN HYDROGENATED AMORPHOUS SILICON DETERMINED BY QUASISTATIC CAPACITANCE OF METAL/a-Si:H/SiO_2/c-Si STRUCTURES

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A method for estimating the density of states in the band gap of hydrogenated amorphous silicon (a-Si:H) is presented. It is based on a comparison between the experimentally measured and the calculated quasistatic capacitance-voltage dependence of a metal/a-Si:H/SiO_2/c-Si structure.

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1. Introduction

The electrical characteristics of devices based on hydrogenated amorphous silicon (a-Si:H) are mainly controlled by the electronic states in the gap. Thus, a knowledge of such gap states is not only important from a fundamental point of view - for understanding the physics of the material - but also for all a-Si:H based device applications, e.g. thin film transistors and solar cells. It has been shown that the quasistatic capacitance method, applied to metal-insulator-semiconductor structures, is a powerful tool for studying study the defects in a-Si:H [1-3].

In this work, we present results concerning the dependence of the calculated quasistatic capacitance-voltage curve (qs C-V) of a metal/a-Si:H/silicon dioxide/crystalline Si structure (M/a-Si:H/SiO_2/c-Si) on the density of states (DOS) in the gap of the a-Si:H. We used a this structure instead of the usual MIS one because of the difficulty of obtaining a high quality dielectric layer on amorphous silicon. The C-V dependences were obtained after numerical solution of Poisson's equation in the whole M/a-Si:H/SiO_2/c-Si system. For the deep defects related to dangling bonds, we used the defect-pool model [4]. This numerical approach was used to evaluate the DOS in an a-Si:H thin film deposited by the PECVD method.

2. Physical model and numerical procedure

The schematic cross-section of the M/a-Si:H/SiO_2/c-Si structure used in the simulations and experimental measurements is shown in Fig. 1. The theoretical qs C-V characteristics are calculated, after solving Poisson's equation, as the variation of the total charge ΔQ_T caused by a small change ΔV_G in the applied bias voltage V_G $C(V_G) = \Delta Q_T / \Delta V_G$. Poisson's equation:

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$$\frac{\partial}{\partial x}(\varepsilon(x)\frac{\partial}{\partial x}\psi(x)) = -\rho(x) \tag{1}$$

was solved numerically in one dimension, using the finite difference method in the amorphous and the crystalline silicon. Here ψ is the potential, ε is the dielectric permittivity and ρ is the charge density. The following boundary conditions were used: continuity of the electrostatic potential at the semiconductor/oxide interfaces and thermal equilibrium at the metal/semiconductor interfaces.

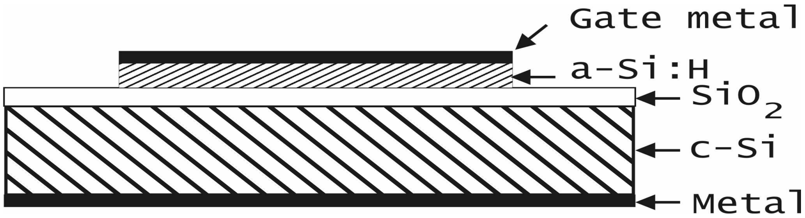

Fig. 1. Schematic cross-section of the M/a-Si:H/SiO$_2$/c-Si structure.

The charge density in the a-Si:H layer has three components, due to free carriers, and those trapped in band tails and deep states. For the valence and conduction band tail distributions, we used exponential dependencies. The dangling bond (DB) contribution to ρ was calculated using the defect-pool expression [4]:

$$D(E) = \gamma\left[\frac{2}{f^0(E)}\right]^{\beta kT/E_{v0}} P\left(E + \frac{\beta\sigma^2}{E_{v0}}\right) \tag{2}$$

where *D(E)* is the density of DB states,

$$\gamma = \left[\frac{N_{v0}2E_{v0}^2}{2E_{v0}-kT}\right]^{\beta} H^{1-\beta}\exp\left[-\frac{\beta}{E_{v0}}\left(E_p - E_v - \frac{\beta\sigma^2}{2E_{v0}}\right)\right], \tag{3}$$

$$f^0(E) = \frac{2\exp\left(\frac{E_F - E}{kT}\right)}{1 + 2\exp\left(\frac{E_F - E}{kT}\right) + \exp\left(\frac{2E_F - 2E - U}{kT}\right)}, \tag{4}$$

$$P(E) = \frac{1}{\sigma\sqrt{2\pi}}\exp\left[\frac{-(E-E_p)^2}{2\sigma^2}\right] \tag{5}$$

and $\beta = E_{v0}/(E_{v0} + kT)$. In Eqs. (2)-(5), E_{v0} is the characteristic decay energy of the valence band tail, N_{v0} is the density of states at the valence band edge, H is the hydrogen concentration, P(E) is the energy distribution of the sites which would form defects at energy E (the defect-pool function), E_F is the Fermi level, k is the Boltzmann constant, T is the temperature and U is the correlation energy of the amphoteric dangling bond states. P(E) is assumed to be a Gaussian distribution, centered at E_p and having a characteristic width σ. The above equations represent the density of DB states at equilibrium, which is maintained for temperatures above the equilibration temperature T*. In all calculations, we used T* = 500 K to determine D(E), even at temperatures below T* because the equilibration time is very long and D(E) is assumed to be frozen in. For the one-electron density of states due to dangling bonds, we used the approximation [4]:

$$g(E) \approx D(E + kT\ln(2)) + D(E - U - kT\ln(2)) \tag{6}$$

The total one-electron density of states is a sum of gap states due to dangling bonds and states due to the conduction- and valence-band tails.

3. Results and discussion

3.1. Calculation results

In order to study the influence of some physical parameters on the DOS and on the shape of the qs C-V curve, we calculated the C-V dependencies of a M/a-Si:H/SiO_2/c-Si structure with 100 nm thick SiO_2 and 0.4 μm thick a-Si:H. In the presented results, the following parameters were taken as fixed: the DOS at the valence- and conduction-band edges: $N_{v0} = 2 \times 10^{21}$ $cm^{-3}eV^{-1}$, $N_{c0} = 1 \times 10^{21}$ $cm^{-3}eV^{-1}$, the a-Si:H band gap: $E_G = 1.9$ eV, the Fermi level with respect to the VB edge: $E_F - E_v = 1.05$ eV, the hydrogen concentration: $H = 5\times10^{21}$ cm^{-3} and the correlation energy: U = 0.2 eV. The c-Si was taken to be n^+ doped, with $N_d = 1\times10^{18}$ cm^{-3}.

Fig. 2 shows the one-electron density of states in the a-Si:H layer calculated at two values of E_{v0} at room-temperature, 45 and 55 meV. We assumed that the valence-band-tail slope is temperature dependent $E_{v0}^2 = E_{v0(T=0)}^2 + (kT)^2$ [5] which gives values for E_{v0} at T* of 56 and 65 meV. The defect-pool parameters were: $E_p - E_v = 1.27$ eV and $\sigma = 0.178$. Fig. 3 shows the calculated normalized C-V curves corresponding to the DOS distributions in Fig. 2. C_i is the capacitance of the thermal SiO_2. It can be seen that variation of the density of states spectrum has a strong influence on the shape of the qs C-V curve. The influence of the defect-pool parameters E_p and σ on the qs C-V dependence is shown in Figs. 4 and 5. Here, E_{v0} was kept constant at 45 meV. The curves in Fig. 4 were obtained for a constant defect-pool position $E_p - E_v = 1.27$ eV, for two values of the characteristic width $\sigma = 0.178$ and 0.14 eV. The curves in Fig. 5 were calculated at a fixed $\sigma = 0.178$ eV, for two values of the defect pool center $E_p - E_v = 1.27$ and 1.37 eV. In both cases, a sharp minimum of the capacitance at positive voltage is observed. This corresponds to a minimum of the DOS in the lower part of the a-Si:H gap (since in our case a positive gate voltage is applied to the a-Si:H layer, shifting the valence band closer to the Fermi level).

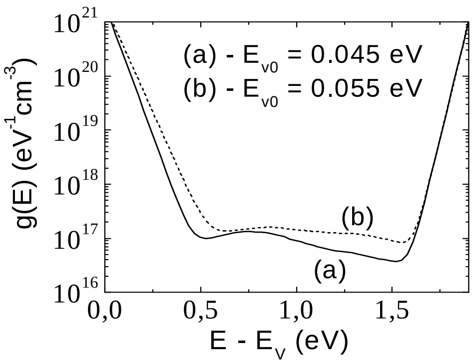

Fig. 2. One-electron density of states in the a-Si:H layer calculated at: (a) E_{v0} = 45 meV, (b) E_{v0} = 55 meV.

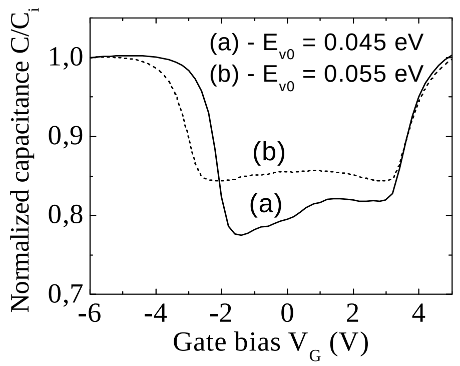

Fig. 3. Calculated normalized qs C-V dependencies Corresponding to the one-electron DOS shown in Fig. 2.

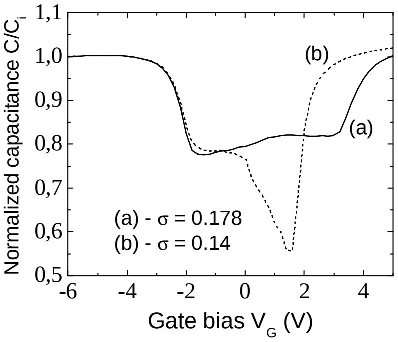

Fig. 4. Normalized qs C-V curves calculated at: E_{v0} = 45 meV, $E_p – E_v$ = 1.27 eV and (a) σ = 0.178 eV (b) σ = 0.14 eV.

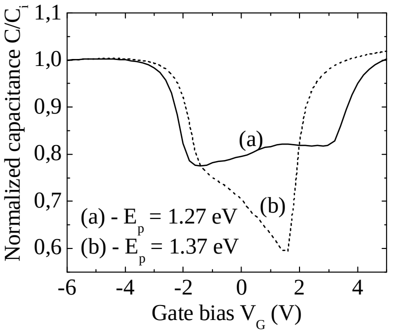

Fig. 5. Normalized qs C-V curves calculated at: E_{v0} = 45 meV, σ = 0.178 eV and (a) $E_p – E_v$ = 1.27 eV (b) $E_p – E_v$ = 1.37 eV

3.2. Experimental results

Experimental structures similar to that shown in Fig. 1 were fabricated by thermal oxidation of n^+ doped crystalline Si with a resistivity in the range 0.006-0.015 Ω cm, followed by PECVD deposition of the a-Si:H film. The thickness of the thermal SiO_2 was 88 nm. The undoped a-Si:H (with a thickness of about 380 nm) was deposited using 10% SiH_4 diluted in H_2 under the following conditions: a frequency of 13.56 MHz, a gas pressure of 65 Pa, an applied power density of 70 $mWcm^{-2}$ and a substrate temperature of 250 ^oC. Al metallization of the a-Si:H was carried out through a mask, and capacitors with a diameter of 1 mm were formed. Al was also used as a back contact to the crystalline silicon.

Fig. 6 shows the experimentally measured qs C-V curve, together with the theoretical curve calculated using E_{v0} = 0.045 eV, E_{c0} = 0.03 eV, E_G = 1.75 eV, σ = 0.185 eV, $E_p – E_v$ = 1.32 eV and U = 0.155 eV. The experimental curve is shifted by about 2.5 V in the negative direction, for better comparison with the calculated one. The reason for this shift is the positive charge which exists in the experimental structure and is not yet included in our simulation procedure. This charge is the sum of the fixed positive charge in the thermal SiO_2 and the charge in the interfacial regions of both insulator/semiconductor interfaces. Fig. 7 shows the one-electron density of states in the a-Si:H, as obtained with the parameters used to fit the experimental curve.

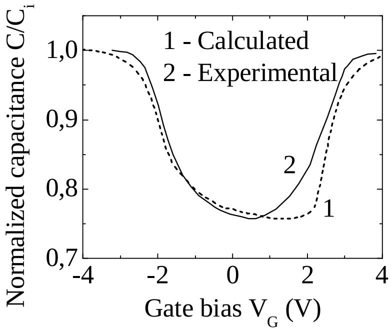

Fig. 6. Theoretical qs C-V dependence (curve 1), obtained as the best fit to the experimentally measured one (curve 2).

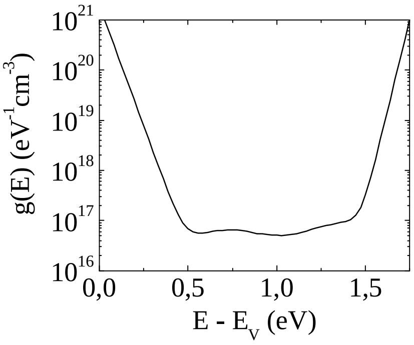

Fig. 7. One-electron density of states in the PECVD a-Si:H layer, obtained with the parameters used to fit the experimental data.

4. Conclusions

The results of our calculations show that the shape of the qs C-V curve of a M/a-Si:H/SiO_2/c-Si structure strongly depends on the density of states profile in the a-Si:H gap. By fitting the experimentally measured qs C-V curve to a theoretical one, the density of the localized states in the gap of the hydrogenated amorphous silicon can be estimated.

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