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EVIDENCE FOR MULTIPHONON EMISSION FROM INTERFACE STATES IN MOS STRUCTURES

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Transient capacitance measurements on MOS structures give strong evidence for a temperature-dependent capture cross-section for electrons at the continuously distributed interface states. A theoretical model that explains this behavior is lattice-relaxation multiphonon emission.

IT IS NOW generally accepted that the distribution of surface states at the silicon/silicon-dioxide interface is continuous in the silicon forbidden energy band with the density increasing towards the band edges [1]. A large amount of experimental information has been obtained in recent years by various techniques which are mainly based on capacitance–voltage measurements [1, 2]; these techniques give no information on the variation of the capture cross-section of interface states. Capture cross-sections have been investigated using the frequency dependence of the conductance in MOS structures [3]. Analyses have been presented which suggest a strong decrease of the capture cross-section with energy near the band edges. This apparent behavior could not be explained until present. The results of conductance measurements are strongly dependent on the evaluation technique which moreover has to take into account surface potential fluctuations due to the random distribution of the fixed oxide charge.

In this paper, we present results obtained using deep-level transient spectroscopy (DLTS) [4] to measure interface states in MOS structures. The DLTS technique has been extensively used to study deep levels in bulk semiconductors [4–7]. Unlike the conductance measurement, the transient capacitance measurement is independent of the surface potential fluctuation in MOS structures. Reliable results are therefore obtained in the vicinity of the band edges. For electron capture and emission from interface states, we find that the capture cross-section is independent, or perhaps weakly dependent on energy, but strongly dependent on temperature. Since in the conductance measurement the temperature has also been varied, an alternative interpretation of the drop of the capture cross-section near the band edges can also be obtained from the temperature effect. The model that can account for the strong temperature variation of the capture cross-section is lattice relaxation multiphonon emission which has been proposed for bulk levels in GaAs and GaP by Lang and Henry [6].

Transient capacitance measurements were made on MOS capacitors that consisted of SiO_2 thin films thermally grown on epitaxial silicon wafers. The wafers consisted of *n*-type epilayers on degenerately-doped, (100)-oriented, *n*-type substrates. Low resistivity substrates were used to minimize series resistance in the MOS structure. The measurement technique is illustrated schematically in the insert in Fig. 1. The measurement involves pulsing an MOS capacitor from depletion into strong accumulation to populate the interface states with electrons. After returning to the depletion bias point, the capacitance decays with time as the occupation of the interface states returns to its equilibrium distribution. The DLTS signal C_s is obtained by forming the difference of two gated sampling signals at delay times t_1 and t_2 $(= 2t_1)$ during the capacitance transient. At low temperatures (< 300 K) the signal is dominated by electron emission from interface states. The emission signal is monitored as the temperature is scanned from 78 to 300 K. Representative results are shown in Fig. 1.

For a continuous distribution of interface traps, the emission signal C_s is given by

$$C_s(t_1, T) = c \int_{-\infty}^{\infty} N_{ss}(E) \exp(-e_n t_1)[1 - \exp(-e_n t_1)]\, dE$$

with

$$e_n = \sigma_n v_{th} N_c \exp(-E/kT),$$

where c is a proportionality constant, N_{ss} is the interface-state density at an energy E below the conduction band, σ_n is the electron capture cross-section, v_{th} is the mean thermal velocity of electrons, N_c is the effective density of states in the conduction band, k is Boltzmann's constant, and T is the absolute temperature. For an

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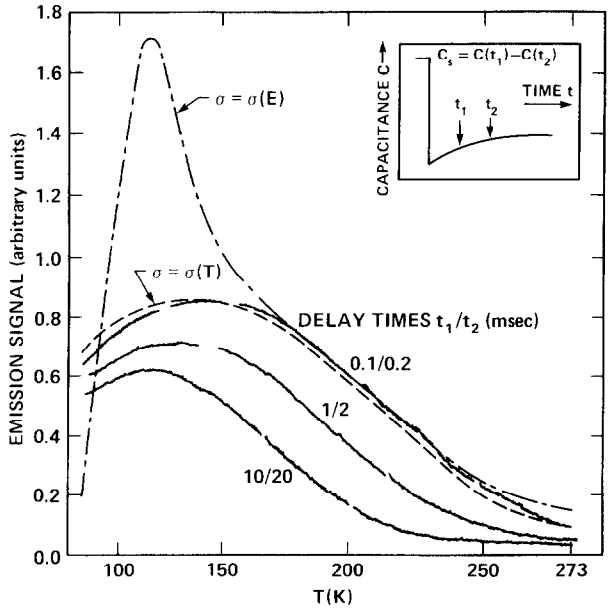

Fig. 1. DLTS emission spectra for an MOS structure. The parameters are the delay times t_1 and t_2 ($= 2t_1$) of the sampling gates. Computed curves are shown for the short gate times (0.1 ms/0.2 ms) for a temperature dependent (dashed curve) and an energy-dependent (dash–dot curve) capture cross-section. The insert schematically illustrates the capacitance transient measurement.

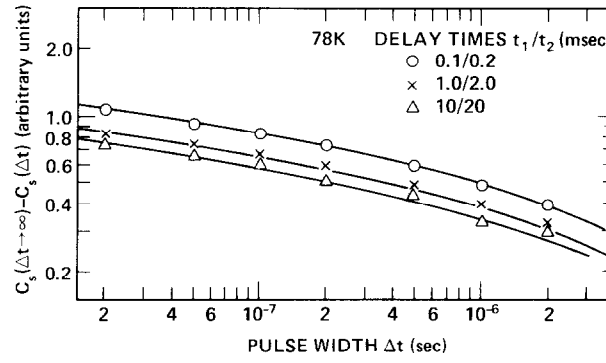

Fig. 2. The difference between the saturated emission signal obtained with long pulse widths ($\Delta t \to \infty$) and the emission signal for shorter pulses is plotted as a function of the filling pulse time Δt. The solid lines are calculated using an energy-independent capture cross-section. The initial free carrier concentration and the interface state distribution were fitted.

energy-independent cross-section, the integral can be solved by assuming that N_{ss} is slowly varying relative to the peaked function of the exponentials. We obtain $C_s(t_1, T) = c\, ln2kTN_{ss}(E_{max})$, where $E_{max} = kT\, ln\,(\sigma_n \nu_{th} N_c t_1/ln2)$. Thus, the emission signal is directly proportional to N_{ss} at the energy E_{max}. Only those interface states within an energy interval ΔE of the order of kT contribute to the emission signal. The broad maximum observed in Fig. 1 is caused by the decrease of the measurement band width ΔE at low temperatures. The temperature scan in Fig. 1 is therefore directly proportional to $kTN_{ss}(E)$.

In this state-of-the-art MOS sample (i.e. $N_{ss} \leqslant 10^{10}$ cm^{-2} eV^{-1} near midgap) no structure is observed in the N_{ss} spectrum. The interface state distribution rises continuously towards the conduction band edge. We have also observed N_{ss} spectra in ion-implanted samples which show peaks superimposed on the continuous spectrum. These results will be discussed elsewhere.

The arguments in favor of a temperature-dependent and energy-independent capture cross-section σ_n are drawn from the following observations:

(1) A computer simulation that assumes a capture cross-section which strongly decreases with energy as shown in [3] and an interface state density which monotonically increases towards the band edge, cannot be fitted to our experimental result. A typical curve shape is shown in the dash–dot curve in Fig. 1. The excess emission signal obtained for an energy-dependent capture cross-section would have to result from the contraction of the time constant spectrum at low energies, which would increase the number of states within the observation band width. If instead a fit of the N_{ss} distribution to the measurement is made, a decrease of the density towards the band edge is needed in disagreement with the result obtained by the conductance technique [3] and other C–V results [1].

For a temperature-dependent cross-section, the experimental results can easily be fitted to an interface-state distribution that increases monotonically towards the conduction band edge (dashed line in Fig. 2). This behavior is consistent with the results of other capacitance techniques [1] and of the conductance technique if one assumes that the variation of the capture cross-section in [3] is primarily due to the temperature effect.

(2) Direct evidence of an energy-independent capture cross-section is shown in Fig. 2. We have measured the emission signal taken at different delay times t_1 as a function of the filling pulse width at a fixed temperature of 78 K where the σ-variation is expected to be strong. In Fig. 2, we have plotted the emission signal difference, $C_s(\Delta t \to \infty) - C_s(\Delta t)$, which is proportional to the number of unfilled interfaces states, as a function of the pulse width Δt for three values of t_1 as indicated by the symbols. For a constant free carrier density, this signal would be a simple exponential decay. In the MOS structure, however, the free carrier density at the surface strongly decreases during the trapping process because of the feedback of the trapped interface charge on the surface potential. The observed time variation for the filling of the interface states therefore differs from the normal exponential

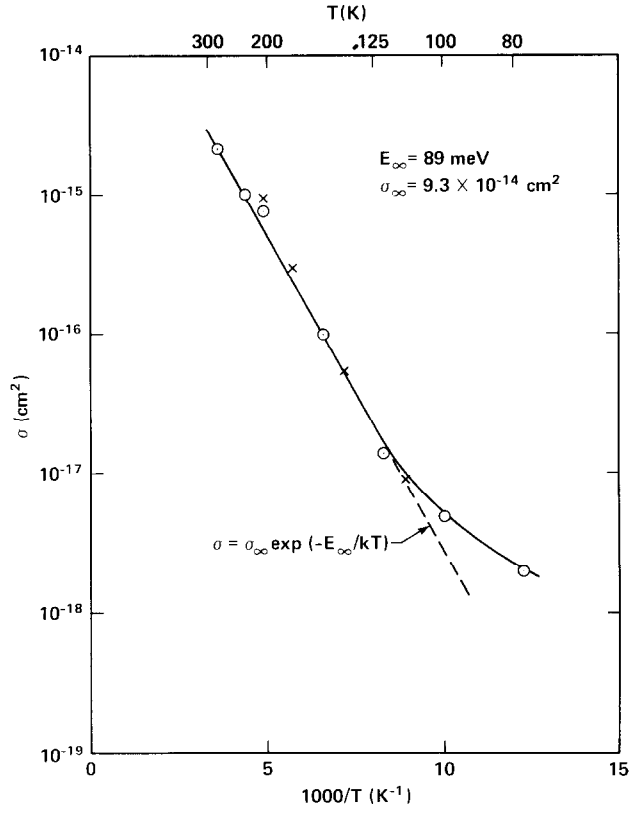

Fig. 3. Temperature variation of the electron capture cross-section of MOS interface states. Circles and crosses correspond to measurements on different capacitor elements on the same wafer.

decay. However, the parallel curves on the log–log plot in Fig. 2 demonstrate that the interface states at the three energies corresponding to the three delay times used in the DLTS technique are filled at the same trapping rate. These states therefore have the same capture cross-section. For a varying capture cross-section, the curves would diverge or cross. The parallel shift itself is due to the change of the interface state density with energy. The delay time constants used in Fig. 2 correspond to an energy range of $\delta E \approx 30$ meV at $E_{\max} \approx 70$ meV below the conduction band. Within this energy range, the capture cross-section is constant within the measurement error of approximately 5%. The interpretation of the conductance measurements in [3] shows a variation of at least a factor of 3 over this range.

(3) The calculated curves in Fig. 2 take into account the time variation of the free carrier concentration at the surface due to the dependence of the surface potential on the trapped interface charge. An energy-independent capture cross-section is assumed for all traps involved, which includes all the states from approximately 70 meV to the band edge. The calculated curves agree with the experimental results.

The capture cross-section variation has been determined from the shift of the three equivalent curves in Fig. 1 by

$$\sigma_n = ln\, 2/[t_1 v_{th} N_c (t_1'/t_1)^{-T'/(T-T')}]$$

where t_1 and t_1', and T and T' are the delay times and temperatures, respectively, where the same arbitrarily chosen interface state density $N_{ss} \propto C_s/T$ is measured. An average σ_n is obtained for the temperature interval $T - T'$, which has to be made narrow when the variation of σ_n is very steep at low temperatures. The result of the temperature variation of σ_n is shown in Fig. 3. The variation can be described by $\sigma_n = \sigma_\infty \exp(-E_\infty/kT)$ at high temperatures where $\sigma_\infty = 9 \times 10^{-14}$ cm^2 as $T \to \infty$ and $E_\infty = 89$ meV.

A theoretical model that can account for the strong temperature variation of the capture cross-section is lattice relaxation multiphonon emission which has been proposed to explain the temperature variation of the capture cross-section of bulk levels in GaAs and GaP [6, 7]. This model assumes a neutral center (acceptor near the conduction band) in which vibrations of a single lattice coordinate linearly modulate the depth of the potential well binding the carrier. For sufficiently large vibrations which are more probable at high temperatures the level can cross into the conduction band and capture an electron. Immediately after capture, the lattice equilibrium position changes leaving the captured carrier in a highly excited vibrational state which rapidly decays by multiphonon emission into the equilibrium state. It is noted that our values of $\sigma_\infty = 9 \times 10^{-14}$ cm^2 and $E_\infty = 89$ meV for the continuous interface states are of the same order of magnitude as for the discrete bulk levels.

At the Si–SiO_2 interface, most deep levels which are caused by the breakage of silicon bonds are removed from the forbidden band by the strong interaction of silicon and oxygen [8]. Band tailing has been proposed to account for the continuous distribution of surface states which is observed experimentally; band tailing states are of acceptor type near the conduction band [9]. Since these states are already caused by a perturbation of the lattice, a lattice relaxation in the multiphonon emission process seems also very plausible. It should be pointed out here that the strong temperature variation observed excludes the "charge model" for interface states which assumes donor-like states with electrons bound to the positive oxide charge [10]. Donor states are only weakly dependent on temperature, and the trapping rate decreases with increasing temperature [6, 7].

In summary, we have employed the DLTS technique to determine the energy and capture cross-section of the continuously distributed interface states

near the conduction band of silicon in MOS structures. We find that the capture cross-section is independent of, or perhaps weakly dependent on, energy and strongly dependent on temperature. The capture process can be described by lattice-relaxation multiphonon emission. This process favors band tailing as a possible origin for the continuous interface state distribution.

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