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Publication date	2019-07-03
Original Citation	Caruso, E.; Lin, J.; Monaghan, S.; Cherkaoui, K.; Gity, F.; Palestri, P.; Esseni, D.; Selmi, L.; Hurley, Paul K. (2019) 'Investigating electrically active defect distributions in MOS structures based on inelastic tunneling interaction with border traps and a nonlocal model for interface traps', INFOS 2019, Cambridge University, UK. 31 June-3 July, Forthcoming.
Type of publication	Conference item
Link to publisher's version	https://infos2019-conf.org/
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Download date	2026-09-08 03:08:24
Item downloaded from	https://hdl.handle.net/10468/7854

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Investigating electrically active defect distributions in MOS structures based on inelastic tunneling interaction with border traps and a nonlocal model for interface traps

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1. Abstract

This work demonstrates that when inelastic band-to-trap tunneling is considered, border traps aligned with the semiconductor bandgap play a significant role in the C-V/G-V dispersion of a MOS structure. In addition, for the case of quantization, a non-local model for interface states is required. The model is used to evaluate the energy/depth distribution of border traps in a n-$In_{0.53}Ga_{0.47}As$ /Al_2O_3 MOS system.

2. Introduction

For MOS structures which exhibit a high density of interface states (ITs) and border traps (BTs) (e.g., narrow band gap III-V MOS), the multi-frequency capacitance-voltage (C-V) characteristics often exhibit a frequency dispersion from depletion to inversion, commonly attributed to an interface trap response, and an accumulation frequency dispersion attributed to border traps aligned at, or above, the majority carrier band edge [2-5]. Based on this approach it is difficult to simulate the full C-V/G-V response, especially the frequency dependent "humps" in the region of weak inversion [3,5]. Building on the work of [4] we highlight: i) the importance of using BTs aligned to the semiconductor bandgap and ii) the need to use a nonlocal model to describe capture and emission from interface defects when quantization effect are taken into account.

3. Device and Model Calibration

The experimental samples are Ni/ 6 nm Al_2O_3/ 2 µm n-$In_{0.53}Ga_{0.47}As$/n-InP MOS structures with a nominal S doping concentration of $4x10^{17}$ cm^{-3} [6]. The C-V/G-V characteristics have been measured varying the gate bias (V_G) from accumulation to inversion. For each V_G, we performed the AC measurements from 1 MHz to 1 kHz. In this way, transient effects due to traps dynamics are minimized yielding experimental measurement conditions closer to the simulation environment. Simulations are performed using Sentaurus™ [7], including Fermi-Dirac statistics and multi-valley with non-parabolic band structure. Quantum corrections of the carrier density are taken into account via the modified local density approximation MLDA [8]. The inelastic nonlocal band-to-trap tunneling models from [9] is used. The traps dynamic parameter used in simulations are reported in **Tab. 1**.

4. Experimental Results and Simulations

Since the determination of the interface ($D_{IT}(E)$) and border ($D_{BT}(z,E)$) traps distribution is based on the deviation of the experimental C-V response from the ideal case, it is instructive to first consider the multi-frequency C-V characteristics of the ideal InGaAs MOS structure with and without the quantization model for electrons (**Fig. 1**). As expected, quantization reduces the accumulation capacitance due to the shift of the charge centroid from the interface (**Fig. 2a**).

Fig. 3 compares the experimental C-V with simulations (without quantization) including $D_{IT}(E)$ within the InGaAs bandgap and $D_{BT}(z,E)$ traps at energies primarily above E_c in the InGaAs, shown in **Fig. 4**. Excellent agreement with the accumulation frequency dispersion can be achieved using the border trap energy/depth distribution shown in **Fig 4b.** However, the peak width of the "humps" in weak inversion cannot be reproduced, as also reported in [5]. An important point in relation to the simulation of the ITs, is that the model typically used to describe ITs response, is based on applying the SRH theory, developed for a bulk semiconductor, to the interface. In this case, the calculation of the emission rate is local and relies on the carrier density at the interface [7]. As show in Fig. 2, when quantization is accounted for, the electron concentration drops dramatically at the interface for all bias regions. For this reason, simulations that include quantization, and interface defects, must use a nonlocal model for interaction of the defects states with electrons/holes in the semiconductor. In this case, all electrically active defects in the MOS system (at the interface and into the oxide) are interacting with the semiconductor free charge through an inelastic tunneling process.

By considering D_{BT} aligned with the semiconductor bandgap, as also reported in [4], a nonlocal interface state response produce the C-V shown in **Fig. 5a**. Moreover, the same border trap distribution also predicts the corresponding G-V response (**Fig5b).** The $D_{BT}(z,E)$ used are shown in **Fig. 5c** and **5d**. The general trend of the experimental curves can be reproduced by the simulations, although second-order adjustments on $D_{BT}(z,E)$ are needed to further improve the agreement.

5. Conclusion

This work demonstrates that non-local inelastic tunneling and BTs aligned to the semiconductor bandgap are necessary ingredients to reproduce accurately the C-V and G-V response typically displayed by MOS system with a high density of electrically active defects. The model is applicable to all MOS systems.

Acknowledgements: The research leading to these results has received funding from the European Commission H2020 INSIGHT project No 688784.

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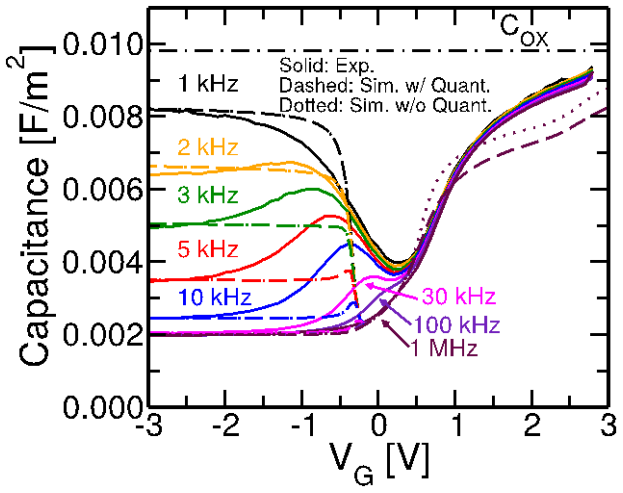

Fig.1: Experimental multi-frequency C-V (solid lines) at 300 K compared with ideal simulations (without traps). Results considering with/without quantization for electrons are reported with dashed and dotted lines respectively. Simulations use a doping value of N_D=4.6·10^{17} cm^{-3} and an *InGaAs minority carrier lifetime τ_g=80 ps. The C_{OX} value used in simulations is shown with the dash-dotted line.*

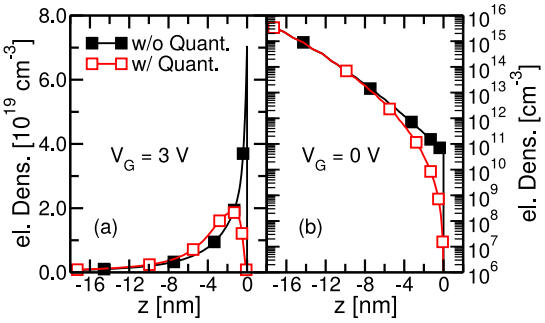

Fig.2: Comparison between the electron densities extracted from simulations of Fig. 1 along the MOSCAP in strong accumulation (a) and in depletion (b). The InGaAs/Al_2O_3 interface is located at z=0 nm.

	ITs	BTs	
	InGaAs/Al_2O_3	InGaAs	Al_2O_3
σ/V_T	10^{-15} cm^2	-	10^{-23} cm^3
m_t	-	0.043 m_0	0.23 m_0
S	-	-	10
$\hbar\omega$	-	-	48 meV

Tab.1: Simulation parameters for ITs and BTs: capture cross section (σ), trap volume (V_T), tunneling mass (m_t), Huang–Rhys factor (S) and phonon energy ($\hbar\omega$).

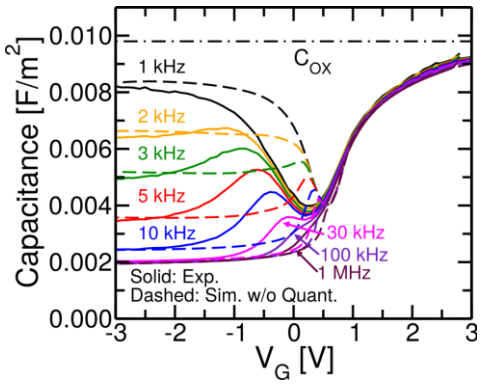

Fig.3: Experimental multi-frequency C-V (solid lines) and simulated one (dashed lines) including D_{IT}(E) and D_{BT}(z,E) shown in Fig. 4. Simulations use N_D=3.0·10^{17} cm^{-3} and τ_g=80 ps.

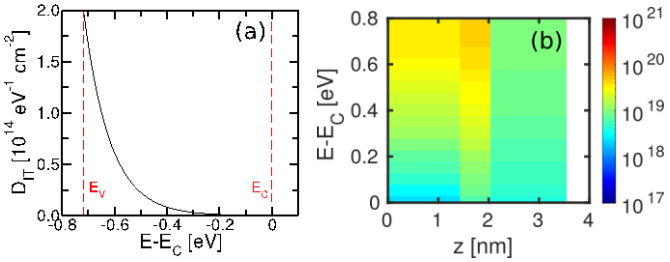

Fig.4: (a) Donor D_{IT}(E) at the InGaAs/Al_2O_3 interface and (b) acceptor D_{BT}(z,E) inside the Al_2O_3. The energy distributions are referred to the InGaAs conduction band (E_C).

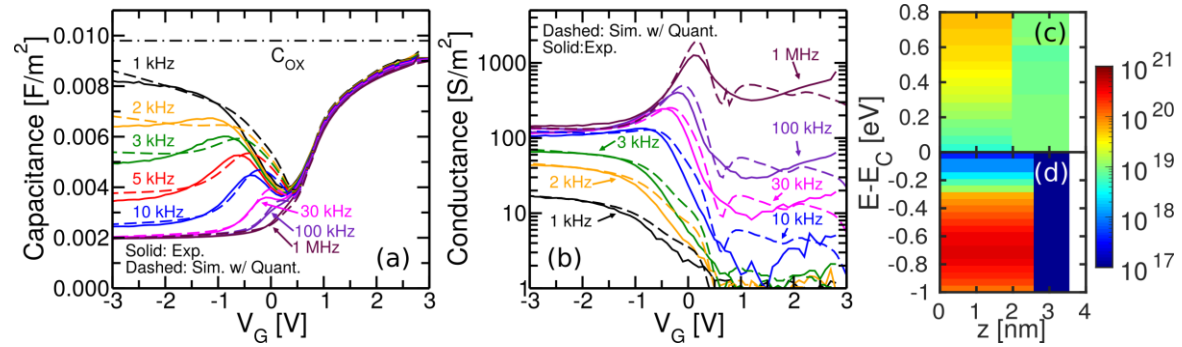

Fig.5: Experimental (solid lines) multi-frequency C-V (a) and G-V (b) compared with simulated data (dashed lines) including quantization correction and nonlocal model for traps. Simulations use (c) acceptor and (d) donor D_{BT}(z,E) inside the Al_2O_3, N_D=3.0·10^{17} cm^{-3} and τ_g=80 ps. The energy distributions are referred to the InGaAs conduction band (E_C).