Multi-phonon hole-trapping from first-principles

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Introduction One of the most critical degradation effects observed in p-MOSFETs is the negative bias temperature instability (NBTI). It is usually observed when a large negative bias is applied to the gate contact with all other terminals grounded. As the name implies, the degradation depends heavily on the applied voltage and the device temperature.

We have recently suggested a new model for NBTI that fits experimental NBTI stress and relaxation data with very high accuracy,[1] and explains the behavior of small-scale MOSFETs under NBTI stress observed by the time-dependent defect spectroscopy (TDDS).[2] This two-stage model (TSM) understands the occurring degradation as the capture of holes into oxide defects which causes a structural reorganization of the defect's atomic structure, in contrast to the popular reaction-diffusion (RD) model. The exchange of electrons and holes between the defect and the channel, a temperature-activated process in nature, is described within the framework of non-radiative multiphonon (NMP)[3,4] theory. The central actor within the TSM is an oxide defect — usually illustrated as an oxygen vacancy — which undergoes several well defined transitions in the course of degradation and recovery. These transitions require for certain features of the defect's adiabatic potential energy surfaces in the different charge-states. So far, these potentials have been empirically adjusted to fit the experimental data.

This work is a first step towards the analysis of the atomistic roots of the TSM. We focus on the examination of the hole-capture process by evaluating atomistic defect structure models for their multiphonon-properties from first-principles. The defects selected for inspection are the oxygen vacancy and the hydrogen bridge. The former has been previously suggested as the defect causing NBTI and other reliability issues such as radiation damage[5] or 1/f-noise.[6] The hydrogen bridge has been proposed as the defect causing stress-induced leakage current (SILC).[7]

Multiphonon Theory The description of carrier transition processes involving multiple ionic excitations of defects in semiconductors has been studied in detail by several authors.[3,4,8] The theory is based on a quantum-mechanical formulation, derived from perturbation theory and using the Franck-Condon-principle. For hole capture, the capture cross section is expressed as a function of the energy E of the hole in the channel.

$$\sigma(x,E) = \sigma_0(x) \underset{\eta_\mathrm{i}}{\mathrm{ave}} \sum_{\eta_\mathrm{f}} |\langle \eta_\mathrm{f} | \eta_\mathrm{i} \rangle|^2 \, \delta(E_\mathrm{f} - E_\mathrm{i} + E - e_0 x F) \tag{1}$$

$$= \sigma_0(x) \; f(E - e_0 x F) \tag{2}$$

The line-shape function concept, which is usually employed for the description of the optical absorption spectra of bulk defects, is adopted in Eq. 1 for the description of a distribution of hole energies. f is the adapted line-shape function and is determined by the thermal average of the overlaps of the vibrational wave functions $|\eta_\mathrm{f}\rangle$ and $|\eta_\mathrm{i}\rangle$, of the final and initial state (E_f and E_i being the respective energies). The application of an electric field F shifts f by $e_0 x F$, where e_0 is the elementary charge and x is the distance from the silicon substrate. The prefactor σ_0 is determined by the electronic matrix element that depends strongly on the position of the defect inside the oxide and weakly on E and F.

In the present work we apply the usual harmonic approximation to the potential energy surface. Additionally we assume single-mode coupling, treating the reaction coordinate for the hole capture transition as an eigenmode of the system. Consequently, the overlap integral becomes $\langle \eta_\mathrm{f} | \eta_\mathrm{i} \rangle = \langle \omega_\mathrm{i}, m | \omega_\mathrm{f}, n \rangle$, where $|\omega, i\rangle$ is the i-th eigenvector of the harmonic oscillator of frequency ω. This integral is evaluated using the analytic expression from Zapol.[9] The oscillator frequencies ω_i and ω_f as well as the energetic and spatial separation of the harmonic oscillator potentials are determined from first-principles.

Ab initio calculations The electronic structure is described with density functional theory (DFT) using the PBE functional. The calculations have been performed using the Vienna ab initio simulation program (VASP).[10] The host lattice is an orthorhombic alpha-quartz supercell structure containing 72 atoms.[7,11] Alpha-quartz was chosen because it is a well studied reference system for amorphous silica. The wave functions are expanded in a plane-wave basis-set up to 800 eV. The core electrons are represented using PAW pseudopotentials. The determination of defect energies relative to the silicon bands follows the method of Blöchl.[7]

Results The plain solution of Eq. 1 is a series of Dirac impulses as indicated in Fig. 2. Life-time broadening[3] has been introduced in an empirical manner. The prefactor will differ for the two defects although it is assumed to be the same order of magnitude, since they show similar localization of the electron densities. However, it shows that the oxygen vacancy has its maximum capture cross section approximately 1eV above the SiO_2 valence band. At room temperature a non-radiative transition of a hole residing near the Si valence band into this defect requires a deep position within the oxide and a high field to create significant overlap. In contrast, the hydrogen bridge has its maximum trapping efficiency about 0.5eV below the silicon valence band, in good agreement with our expectations for the defect involved with NBTI.

Conclusions Oxide defects were analyzed for their ability to capture holes from the silicon substrate using ab initio DFT. The results for the hydrogen bridge are in good agreement with the assumptions in the TSM. The oxygen vacancy requires a large distance to the channel and high fields for hole capture.

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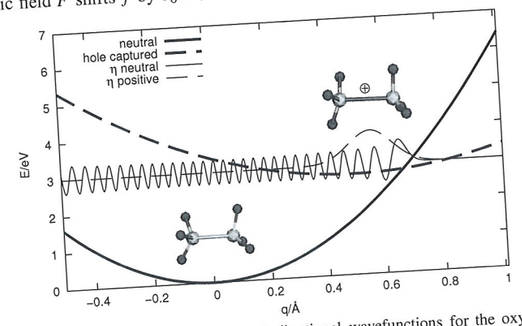

Figure 1: Potentials and examples of vibrational wavefunctions for the oxygen vacancy (hole energy at silicon midgap). q is the reaction coordinate.

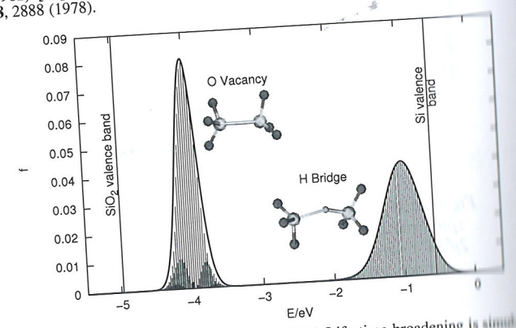

Figure 2: Adapted line-shape function at 300K. Life-time broadening is simulated by smearing with a normal distribution of spread $k_B T$.