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Hydrogen in MOSFETs – The Good, the Bad, and the Ugly

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INTRODUCTION

Hydrogen is intentionally introduced in metal-oxide-semiconductor field-effect transistors (MOSFETs) because of a highly beneficial effect at the Si-SiO_2 interface: it passivates the so-called dangling bonds, which results in high carrier mobilities in the channel. Over the years, many undesirable phenomena, observed in MOSFETs under different conditions and causing varying degrees of degradation, have gradually been attributed directly or indirectly to hydrogen. In the last several years, we pursued extensive first-principles calculations of hydrogen configurations and reactions in MOSFETs in the context of pertinent experimental data, both old and new. The calculations were based on density-functional theory, the local-density approximation for exchange-correlation, supercells, and plane-wave basis sets. The key questions were: where, in addition to passivated dangling bonds at the interface, does hydrogen reside? How is it released and in what charge state? How does it migrate? If H is released elsewhere and migrates to the Si-SiO_2 interface, how might it depassivate dangling bonds? Does it get through the interface in one or both directions and what are the consequences? As it migrates, can it induce the formation of other defects? The pertinent experimental data are the so-called bias temperature instability (BTI) and radiation-induced phenomena such as increase of interface trap density and pertinent annealing cycles, deactivation of dopants in Si, and combined radiation/BTI conditions. This talk will summarize a few of the key findings.

DEPASSIVATION OF DANGLING BONDS

It has long been recognized that H is released as H^+ from various sites in the oxide under a variety of conditions (radiation, hot electrons, etc). Under suitable bias, it can travel to the interface, where it depassivates dangling bonds, and potentially crosses the interface, where it can deactivate dopants. It was believed that, in order to depassivate a dangling bond, H^+ must first capture an electron from the Si side and then, as neutral H, migrate until it finds its target, when the reaction Si-H + H → D + H_2 occurs (here D is a neutral dangling bond). Detailed density-functional calculations have demonstrated that H^+ can depassivate directly via the reaction Si-H + H^+ → D^+ + H_2. The result has a significant consequence for modeling depassivation processes because they do not depend on the availability of excess electrons [1].

DEACTIVATION OF DOPANTS IN Si

Dopant deactivation was also believed to require prior neutralization of H^+. In fact, it has been shown that H in Si is a negative-U defect, meaning that neutral H is not the stable species at any value of the Fermi energy. We now have shown [2] that direct deactivation of boron impurities occurs by H^+. We have modeled the process in the presence of bias using Monte-Carlo simulations and showed that the observed strong dependence of deactivation on electric field is due mainly to transport of H+ in the depletion region. The dependence of the deactivated-boron concentration on irradiation bias, as

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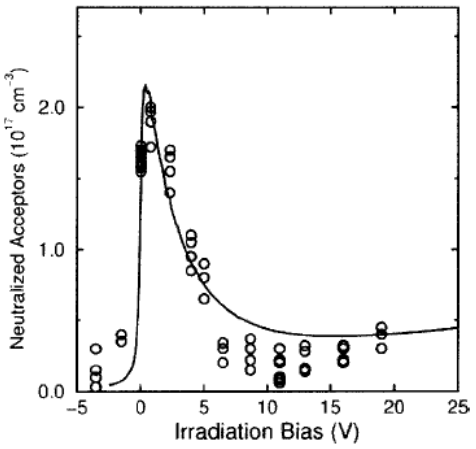

measured by Witczak et al. [3], was accounted by the model (see Figure above, taken from [2]).

NEGATIVE BIAS TEMPERATURE INSTABILITY

The interface trap density has long been known to increase under negative bias (2-6 MV/cm) at moderate temperatures (100-200ºC). Small activation energies (~0.3 eV) are generally attributed to hydrogen-mediated depassivation of dangling bonds (larger activation energies are generally attributed to H_2O-mediated processes). The effect is more pronounced in p-channel MOSFETs under negative bias. It is widely believed that, in the presence of the electric field and excess holes, Si-H at the interface undergoes direct dissociation, i.e., Si-H + $h^+ \rightarrow$ D + H^+. We have shown with parameter-free density-functional calculations [4] that the direct dissociation activation energy in the absence of holes is 2.4 eV (in agreement with the experimental value of 2.6 eV) and that, in the presence of holes, the activation energy only drops to 2.1 eV. We proposed that deactivation must be mediated by H, which in this case, must originate on the Si side. Calculations of H release from dopants suggest that hydrogen attached to the dopant atoms is the likely source. The observed small activation energy, only ~0.3 eV, is the result of quasi-equilibrium that is established by the pertinent reactions. A diffusion-reaction theory developed by Jeppson and Svensson[5] in 1977 was applied. The activation energy is given by $E_a = \frac{1}{2}\Delta E + \frac{1}{4}Q$, where ΔE is the reaction energy of depassivation by H^+, as described earlier, and Q is the diffusion barrier of H^+. Using our calculated values for these energies (ΔE = 0.5 eV, Q = 0.45 eV), we find $E_a = 0.36$ eV. We have confirmed the experimental values with new experiments for both Si-SiO_2 and Si-SON-HfO_2 (an alternate dielectric) and found similar activation energies [6], establishing the generality of the phenomenon. We have also investigated the response of such structures to combined NBTI and radiation and found that the two phenomena can influence each other strongly, and often in surprising ways.

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