Dipoles in SiO_2: Border Traps or Not?

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Border traps are near-interfacial oxide traps that exchange charge with the Si on the time scale of the measurements being performed (1). This charge exchange is typically slower than that for interface traps (2)-(4), so sometimes these defects are called “slow states.” Moreover, border traps typically have a different microstructure than interface traps, although their structures may be similar to bulk oxide traps. Among other impacts to device response, these defects influence MOS 1/*f* noise and stress induced leakage current. As MOS (metal oxide semiconductor) gate insulators have scaled down in thickness, truly bulk-like oxide traps have nearly become extinct, except in parasitic insulators like field oxides, and the buried oxides of SOI (silicon on insulator) devices. So border traps have become increasingly important to MOS performance, reliability, and radiation response.

In this talk, we will re-examine several studies of border traps, their microstructure, and their electrical properties, in view of recent experimental and theoretical studies that may refocus the understanding of past results. An emphasis will be on dipolar defects in SiO_2, which have been observed after devices have been irradiated or subjected to high-field stress. A typical way in which dipolar defects are characterized is through changes in the midgap voltage of MOS capacitors or transistors during switched positive and negative bias annealing. A popular model of these defects, originally proposed by Lelis and co-workers (5), is a hole trapped at an O vacancy defect, which is compensated by an electron that has tunneled into the oxide from the Si. Hence, these defects are properly characterized as border traps. However, in TSC (thermally stimulated current) measurements, a second type of response has been observed. When a device is irradiated at positive bias, there is a significant density of defects for which one observes significant TSC when the device is heated at negative bias, but not when the device is heated at positive bias (6). Moreover, a significant fraction of these defects can be stable during positive or negative post-irradiation anneals up to at least 400 K, but they are removed by annealing at temperatures of ~ 600 K (7). Because this defect is evidently not capable of exchanging charge with the Si, it is apparently not a border trap. It is possible that this defect has been mistaken in much prior work for a recombined electron-hole pair (8). This raises the obvious question of whether the majority of dipoles observed in TSC studies are microstructurally the same as those observed in post-irradiation or post-stress switched-bias annealing studies.

In this presentation, we will review evidence from EPR (electron paramagnetic resonance) studies that suggests that E′ centers (threefold coordinated Si defects) in SiO_2 (9)-(10) can be border traps. However, recent theoretical studies have shown there is a richer than expected variety of E′ centers in SiO_2. For example, three variations are shown in Fig. 1 based on DFT (density functional theory) calculations (11). The moiety in Fig. 1(a) is a dimer defect, the E_δ'. This defect typically does not form a dipole, except when the Si-Si spacing at the center of the complex is stretched well beyond its equilibrium distance (11). The second center in Fig. 1(b) is the well-known E_γ' defect (9)-(11), in which one of the Si atoms has puckered through the plane established by the three nearest neighbor O atoms to back-bond to a fourth oxygen. This defect can form a stable dipole (11). The third type of defect is a variant of the E_γ' which has a similar EPR characteristic, but DFT calculations show this defect now includes a 5-fold coordinated Si atom, and cannot form a stable dipole after irradiation or high-field stress (11).

The impact of these and other (especially hydrogen related) defects will be discussed for MOS radiation response and long-term reliability, and refined models will be described for border traps and dipolar defects in SiO_2. We will also discuss similar defects in alternative dielectrics to SiO_2, with or without a transitional oxide or oxynitride layer at the Si/SiO_2 interface.

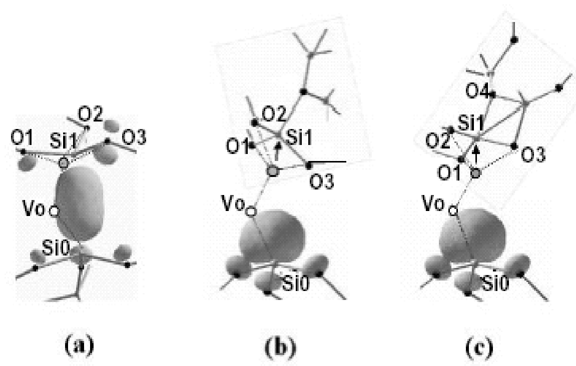

Fig. 1. Schematic illustrations of unpaired electron densities (gray regions) and atomic configurations of (a) a dimer O vacancy center associated with the E_δ' defect, (b) O vacancy center associated with the E_γ' defect (the $E_{\gamma 4}'$), and (c) a second type of O vacancy center also associated with the E_γ' (the $E_{\gamma 5}'$). [After Ref. (11).]

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