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First-Principles Approach to the Reliability Issues of MOS Gate Oxides

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INTRODUCTION

Negative-bias temperature instability (NBTI) is one of the important issues in reliability of metal-oxide-semiconductor (MOS) devices. Understanding the mechanism of the NBTI is demanded to design a higher-performance and more reliable device. Though the extensive studies have been done [1], the causes for some dependence of the NBTI on stress conditions have remained unknown. For example, the origin of the electric-field dependence is not established yet.

We have investigated the charged species that causes the electric field dependence of NBTI by a first-principles calculation.

CALCULATIONAL METHOD

We took a hydrogen-originated NBTI and considered the specific role of hydrogen paying attention to the difference of the Si/SiO_2 and Si/SiO_xN_y interfaces. Hole-trapping energy (an energy required to trap a hole into the interface) and hydrogen-migration energy (an energy required to migrate a H atom from one place to another in the interface trapping a hole) were calculated for the two interfaces. We used the molecular models of the interfaces (Figures 1 and 2) and a first-principles density functional theory program, deMon [2].

RESULTS AND DISCUSSION

The obtained hole-trapping and hydrogen-migration energies are listed in Tables I and II. The Si/SiO_xN_y interface needs less energy to trap a hole than the Si/SiO_2 interface does. This corresponds to the fact that the N incorporation into the Si/SiO_2 interface enhances the NBTI. The hole-trapping energy at the O or N site in the interfaces is lower than that at the Si-H site or at the O or N vacancy, showing that hole trapping can occur most easily at the O or N site. On the other hand, the generation of a proton and a Si dangling bond from the hole-trapping Si-H site was calculated to be energetically less favorable to the generation of a H atom and a hole-trapping Si atom by 5.8 eV. We conclude that the hole trapping, an initial step of the NBTI, occurs at the O or N site in the interface, not at the Si-H site. The H atom should play a role in the following step of the NBTI.

The hydrogen migration from Si to O or an O vacancy trapping a hole destabilizes the hole-trapping state of the Si/SiO_2 interface by about 0.4 eV, while the migration from Si to N trapping a hole stabilizes the Si/SiO_xN_y interface by 0.1 eV. This difference in the hydrogen-migration energies is another reason for the enhancement of NBTI by the N incorporation into the interface.

Next, we investigated the possibility of reducing activation energy by electric field in the case of hydrogen migration at a $Si(100)/SiO_2$ interface. The calculated energies of the interface along the assumed path (Fig. 3) of hydrogen migration are listed in Table III. The effect of electric field (either forward or backward) on the neutral state is negligible. The activation energy of the hole-trapping state, even without electric field, is significantly smaller than those of the neutral state. We conclude that the Si-H bond dipole is not the origin of the electric field dependence of the NBTI. A good correspondence between the hole-trapping energies and the NBTI tendencies of the dielectric materials implies that the rate-limiting step of the

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NBTI is a hole trapping in the interface. So, the electric field dependence of NBTI may be explained by the hole-trapping rate under an applied electric field.

CONCLUSION

Hole trapping, the initial step of the NBTI, occurs at the O or N atom in the Si/SiO_2 or Si/SiO_xN_y interface. The electric field dependence can be explained by the hole-trapping rate in the interface under the electric field.

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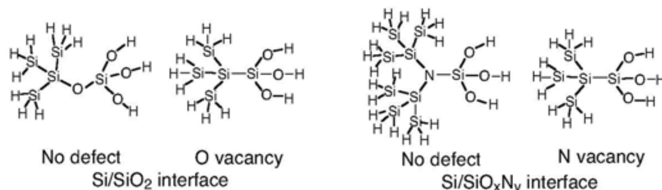

Fig. 1. Molecular models of Si/SiO_2 and Si/SiO_xN_y interfaces. The O-vacancy and N-vacancy structures are the same.

Table I. Hole-trapping reaction energies of Si/SiO_2 interfaces with and without hydrogen migration.

Hole-trapping site			Hole-trapping reaction	Reaction energy (eV)	Hydrogen-migration energy (eV)
Si-H bond			Si-Si-H →(h+) Si-Si(+)-H	8.87	—
Si/SiO2 interface	No defect	Without H migration	Si-O-Si-O →(h+) Si(+)-O-Si-O	8.14	0.39
		With H migration	Si-O-Si-O⁻, Si-Si-H →(h+) Si(+)-O(H)-Si-O, Si-Si(·)	8.53	
	O vacancy	Without H migration	Si-Si—Si-O →(h+) Si-Si (+) Si-O	8.39	0.38
		With H migration	Si-Si—Si-O, Si-Si-H →(h+) Si-Si-H-Si-O (+), Si-Si(·)	8.77	

Table II. Hole-trapping reaction energies of Si/SiO_xN_y interfaces with and without hydrogen migration.[a]

Hole-trapping site			Hole-trapping reaction	Reaction energy (eV)	Hydrogen-migration energy (eV)
Si/SiOxNy interface	No defect	Without H migration	Si-Si-N-Si-O →(h+) Si-Si-(+)N-Si-O	7.52	-0.10
		With H migration	Si-Si-N-Si-O, Si-Si-H →(h+) Si-Si-N(+)(H)-Si-O, Si-Si(·)	7.42	

[a]The energies for N vacancy are not shown, because the values are the same as those for O vacancy in Table I.

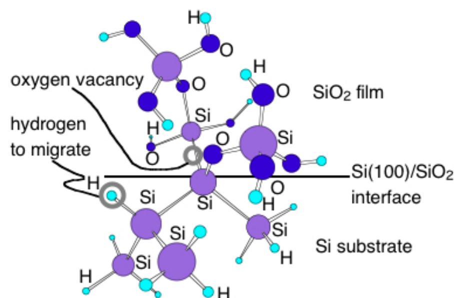

Fig. 2. Molecular model of the $Si(100)/SiO_2$ interface for the calculation of activation energy of hydrogen migration in an electric field.

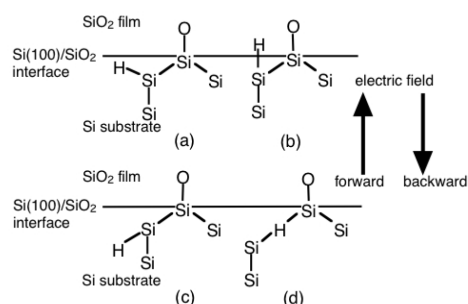

Fig. 3. Definitions of four hydrogen positions and directions of the electric field: (a) the equilibrium structure, (b) the Si-H bond perpendicular to the Si(100) surface, (c) the Si-H bond and the Si-Si bond on the same linear line, and (d) the H atom on the Si-Si bond.

Table III. The energies[a] of the three kinds[b] of H positions in neutral and hole-trapping states of the equilibrium structures and the large lattice distorted structures (LLDSs) under an electric field[c].

charge state	base structure	electric field	energy (eV)[a] H-position (b)[b]	H-position (c)[b]	H-position (d)[b]
neutral	equilibrium	none	0.93	2.23	–
		forward	0.88	2.15	–
		backward	0.87	2.19	–
	LLDS	none	0.91	2.36	1.21
		forward	0.93	2.32	1.20
		backward	0.89	2.39	1.22
hole trapping	equilibrium	none	0.42	1.17	–
	LLDS	none	0.09	1.30	0.03

[a]For the equilibrium base structure, the energy of the fully optimized structure in each charge state with or without an electric field was taken as zero of the energy. For the LLDS base structure in each charge state, the energy of the LLDS whose Si-Si bond length was 3.0 Å keeping the other part the same as the equilibrium structure was taken as zero.

[b]See Fig. 3 for the structures of H-positions (b), (c), and (d).

[c]The electric field strength was 10 MV/cm.