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Assessment of Ion-Bombardment Damage in Plasma-Exposed Si by Interface Layer Thickness and Charge-Trapping Defects

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1. Introduction

Plasma etching technology has enabled rapid advancement of the microelectronic industry, but meanwhile has given rise to an issue known as *plasma-induced damage* (PID) [1–3]. *Ion-bombardment damage*, one of the PID mechanisms, is caused by energetic ions from the plasma physically damaging the Si substrate (Fig. 1). The damage can degrade MOSFET performance in several ways: One is by the formation of *Si recess* [2]. Its depth is typically several nanometers and will be in conflict with the device design margin. Another form is the charge-trapping *latent defects* that remain after post-etch processes [3]. In order to minimize the negative effects of the damage, accurate analysis techniques are extremely in need.

In this study, the forms of the damage mentioned above are studied. Structural picture and formation mechanisms of the damage are studied in detail by using molecular dynamics (MD) simulations, and optical and electrical techniques. Thickness and energy band structure of the damaged layer are investigated by spectroscopic ellipsometry (SE). The charge-trapping defects are detected by capacitance-voltage (C-V) measurements.

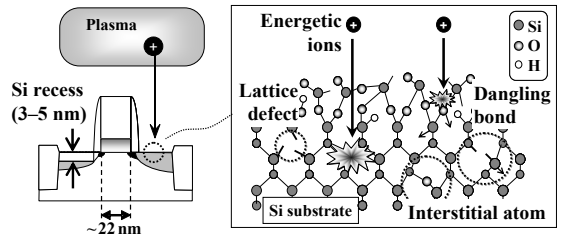

Fig. 1 Ion-bombardment damage and Si recess mechanisms.

2. Simulational/Experimental Procedures

Molecular Dynamics (MD) Simulations

Formation mechanism and physical structure of the damage were simulated using classical MD [4]. Ar plasma was utilized in this work so as to eliminate chemical reactions and focus on the physical effects. Stillinger–Weber type interatomic potentials for Si–O–Ar systems [5] were applied. To reproduce the "practical" structures and processes, we constructed a scheme consisting of four phases: (i) Si (100) structures with 1152 (= 8 × 8 × 18) atoms were prepared. (ii) Low-energy O atoms were impinged on the surfaces until saturation, to emulate natural oxidation. (iii) Ar^+ ions were impinged on the surface at incident energy E_i for 1000 times. (iv) Low-energy O atoms were impinged to emulate post-process natural oxidation. The number of covalent bonds was determined for each Si atom by analyzing the distance of neighboring Si–Si pairs.

Plasma Exposure and Optical/Electrical Measurements

N-type (100) Si wafers (0.02 Ωcm) were mounted on an ICP (inductively coupled plasma) chamber stage. The wafers were exposed to Ar plasma for 30 s. 13.56 MHz rf bias was applied to the stage. Bias power was ranged from 0 to 300 W, to vary the mean energy of ions (E_i) impinging onto wafer surface. Plasma density and electron temperature were determined by using a Langmuir probe, to estimate E_i and the ion flux.

SE measurements were carried out to investigate the surface structure. Measured data was fitted with a four-phase optical model: ambient / SiO_2 surface layer (SL) / interface layer (IL) / crystalline Si (*c*-Si) substrate. We have shown preliminarily that the inclusion of IL is indispensable, and that modeling it as a composite of SiO_2 and *c*-Si is suitable for practical in-line monitoring [6]. This model is supported by *lower unbiased estimator* which indicates "good fit" and its correlation with the thickness determined by HR-TEM. As shown later, the presence of this partially-oxidized structure will be confirmed by MD simulations.

C-V measurement was performed by a mercury probe system with various modulation frequencies to quantify the areal density N_{dam} of the trap sites. If we apply charge-sheet model [7] to the damaged structures, the obtained bias voltage shift ΔV_b of the C-V curve can be expressed as

$$\Delta V_b = \frac{qN_{dam}}{\varepsilon_0 \varepsilon_{SiO_2}} d_{SL}, \quad (1)$$

where q is the elementary charge, and d_{SL} is the thickness of the surface layer determined by SE. Thus, N_{dam} can be estimated by ΔV_b.

3. Results and Discussion

Interface Layer Thickness

Figure 2 illustrates the results of MD simulations, comparing under different E_i. Incident ions were observed to scatter atoms and disarrange the crystalline structure beneath the SiO_2 surface layer (SL). One should note that this partially-oxidized disordered region is assigned as the interface layer (IL) between SL and the substrate, which is also identified by spectroscopic ellipsometry (SE) as below.

The thickness of the surface structures (SL and IL) can be experimentally determined by SE. It has been shown [3,6] that the total layer thickness ($d_{SL} + d_{IL}$) saturates at approximately 5 nm (consistent with widely observed

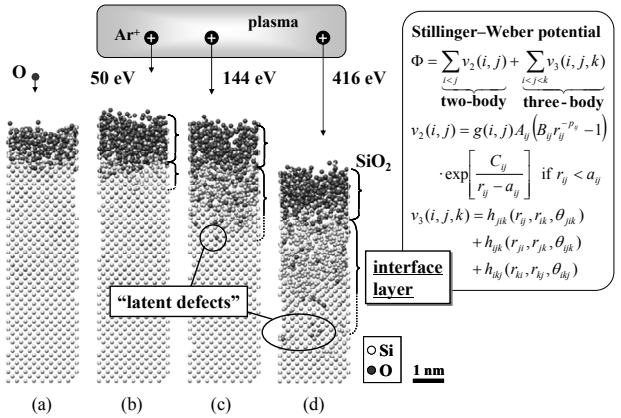

Fig. 2 Results of the MD simulations. (a) After natural oxidation (phase ii). (b)–(d) After incidence of Ar^+ ions (E_i shown) and post-process oxidation (phases iii & iv).

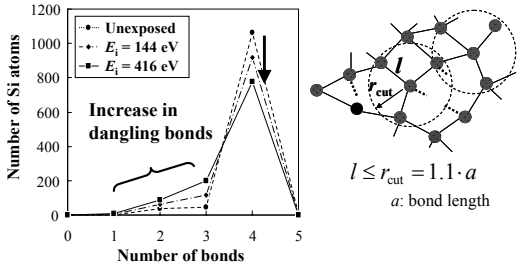

Fig. 3 The number of covalent bonds for each Si atom in the simulation. Number of atoms with less than four bonds indicates the number of dangling bonds, which act as carrier trap sites.

recess depth [2]), and that d_{IL} increases monotonically with E_i. At larger E_i, IL becomes the predominant layer in the surface structure. The increase in d_{IL} observed in both MD and SE indicates that d_{IL} acts as an indicator for the damage and can be useful in predicting the depth of Si recess.

Dangling Bonds and Charge-Trapping Sites

In the MD results (Fig. 2), we can observe disordered Si and interstitial O atoms, in the region where the crystalline structure is largely intact. By analyzing the number of bonds for each Si atom, we found an increase in dangling bonds as shown in Fig. 3. Since dangling bonds are known to trap carriers as gap-states [8], this implies generation of charge-trapping sites by PID.

Pseudo-extinction coefficient ‹κ› calculated from ellipsometric parameters [Fig. 4(a)] assigns these charge-trapping sites. The shoulder near 3.4 eV corresponds to the optical transition energy of Si at Γ- or *L*-point in ***k***-space; larger ‹κ› in the lower-energy region ($h\nu < 3.4$ eV) represents enhancement in absorption of the corresponding photons. This indicates an increase in gap-state density, implying larger charge-trapping defect density. The presence of negatively-charged trap sites was also electrically revealed as ΔV_b to the positive direction. Figure 4(b) shows larger ΔV_b with higher E_i. From eq. (1), the defect density N_{dam} was estimated to be 10^{12}–10^{13} cm^{-2}. A consistent value was also derived from photoreflectance spectroscopy (PRS) [3] as below.

Removal of Damage

A plasma-damaged sample with SE-determined d_{IL} of

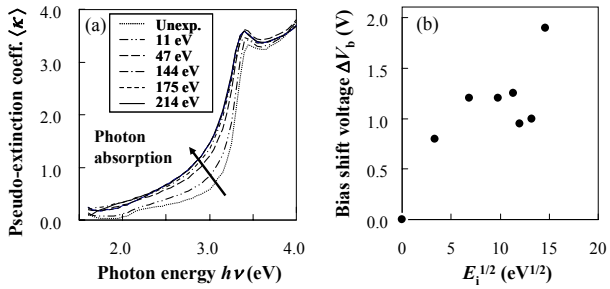

Fig. 4 (a) Pseudo-extinction coefficients of selected samples (E_i is shown). (b) ΔV_b determined by capacitance-voltage test (1 MHz), plotted against square root of incident ion energy.

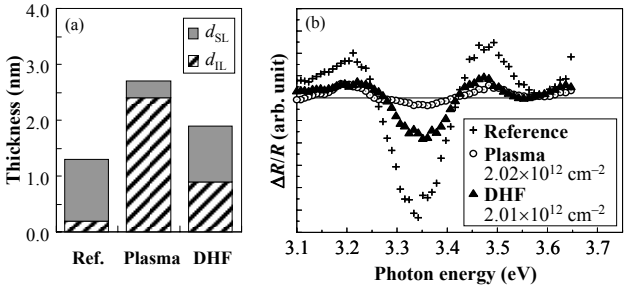

Fig. 5 Measurements before and after DHF treatment. (a) Thickness measured using SE. (b) PRS spectra. Defect density is shown, calculated by Γ-point fitting.

2.4 nm was treated with diluted HF (DHF). We applied PRS to quantify the defect density. The results are shown in Fig. 5. Although d_{IL} decreased after the treatment, the damage did not recover completely. We further found, using SE and PRS, that the damage was not recovered by thermal annealing, and would remain as *latent defects*.

4. Conclusion

Mechanisms of ion-bombardment damage in Si and the recovery process were comprehensively studied. MD simulations clearly projected the presence of interface layer with disordered Si. The SE analysis addressed the absorption of photons, indicating the presence of charge-trapping sites. The density of trap site was estimated to be 10^{12}–10^{13} cm^{-2} from the shift of C-V curves and PRS. Conventional wet-etch stripping or thermal annealing could not completely remove the trap sites. These findings imply that these trap sites in the order of ~ 10^{12} cm^{-2} continue to exist in Si and impact on MOSFET performances.

Acknowledgments

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