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Modeling of ion-bombardment damage on Si surfaces for in-line analysis

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ABSTRACT

Structures and mechanism of ion-bombardment damage on silicon wafers exposed to plasma were investigated comprehensively. By using molecular dynamics simulations high-resolution transmission electron microscopy, and composition analysis by high-resolution Rutherford backscattering spectroscopy, features such as gradual transition from the SiO_2 surface to the Si substrate and interface roughness were addressed. On the basis of these findings, the optical model that addresses the characteristics of plasma-damaged Si surfaces is given for ellipsometric analysis. The proposed model includes an interface layer modeled as a mixture of SiO_2 and Si phases. A part of the interface layer could not be removed by wet-etching, signifying the distinct features of the interface layer that are difficult to remove. The proposed model is anticipated to be practical for in-line monitoring of plasma-induced damage.

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1. Introduction

With rapid advancement in plasma etching technology, electronic device feature sizes have shrunk in accordance with the scaling law [1,2]. As the junctions in source/drain extension regions have become dramatically shallower, issues known as *ion-bombardment damage* and *silicon (Si) recess* can no longer be neglected [3–6]. Ion-bombardment damage, classified as one of the plasma-induced damage (PID) mechanisms [3], is illustrated in Fig. 1. The damage includes interstitial atoms, strained network, contaminations due to etchant species [4], and dislocation of silicon atoms in the lattice [5]. During the etching of gate electrodes and offset spacers, the underlying silicon substrate is damaged and oxidized, which is subsequently wet-etched in the post-treatment [7,8]. Moreover, it is believed that the layer with the ion-bombardment damage is easily oxidized and removed, resulting in a recessed structure [5,7]. The thickness of the damaged layer is estimated to be several nanometers, which will be in conflict with the device design margin as the feature size of devices shrinks rapidly [9].

The structure and defects induced by ion bombardments on the scale of 1–1000 keV are relatively well-studied [10–12], partly because of their importance in ion-implantation applications. Plasma etching processes deal with ions in the lower energy range (50–200 eV), where the effects of ion bombardments may differ. For the lower energy range (10–100 eV), many of the existing works focus on applications such as ion-assisted epitaxy [13,14]. Although plasma etching is concerned with ions with energies similar to epitaxy, there have been few reports on the characteristics and practical evaluation methodology of PID. Earlier studies exist where the damaged-layer thickness was optically evaluated as a layer of SiO_2 [5,15]. However, considering the nature of the damaged layer, it is clearly inaccurate to assume its optical properties to be of bulk SiO_2. An analysis methodology that is both consistent with the characteristics of PID and practical for in-line use is required. In this paper, we studied PID by argon plasma so as to eliminate chemical reactions and focus on the physical effects. The structure, composition, and removability were comprehensively studied, and the optimal model was established.

2. Simulation and experimental details

2.1. Molecular dynamics (MD) simulation

In order to investigate the formation mechanism and the physical structure of the damaged layer, we applied a classical MD simulation [16,17]. Stillinger–Weber type interatomic potential model for Si–O–Ar systems were applied [18,19]. To reproduce a practical condition, we constructed a scheme consisting of four simulation phases: (1) a Si (100) structure with 1472 ($=8\times8\times23$) atoms was prepared. (2) Low-energy O atoms were directed towards the structure surface until saturation, to emulate natural oxidation. (3) Ar^+ ions were impinged on the surface at certain incident energy (E_i) for 1000 times. Ar^+ ions that may remain beneath the surface were removed in this simulation. (4) Low-energy O atoms were directed to emulate post-etch natural oxidation. Simulation domain was 2.17 nm in side length with periodic boundaries. E_i was varied, to simulate different bias voltages.

2.2. Plasma exposure

N-type Si (100) wafers (0.02 Ω cm) were placed on an inductively coupled plasma (ICP) reactor stage and were exposed to argon plasma. Chamber pressure was 20 mTorr. Exposure time was 30 s.

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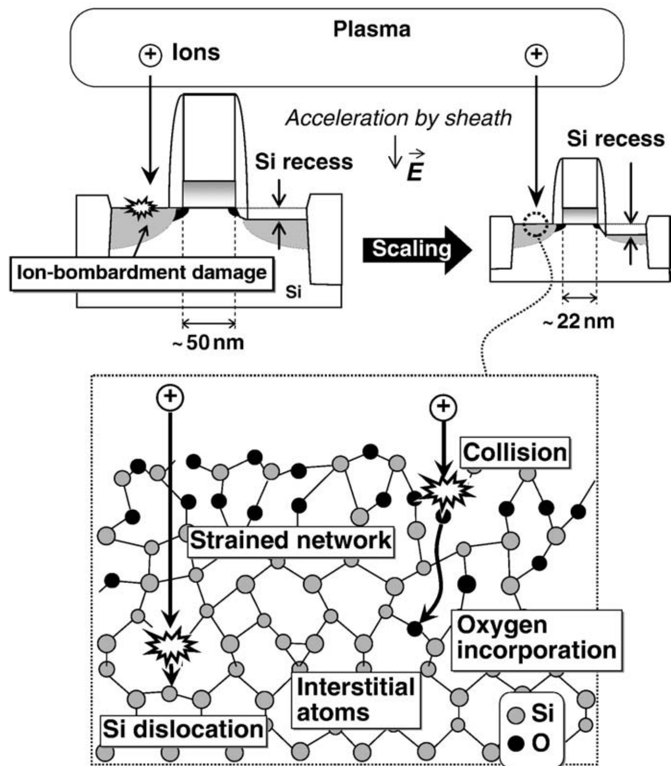

Fig. 1. Schematic illustration of ion-bombardment damage and the Si recess. The recess depth does not scale along with device dimension as it is determined by plasma parameters. This makes the recess much more significant and problematic in scaled devices.

13.56 MHz bias was applied to the wafer stage. Bias power was ranged from 0 W (no bias) to 400 W, to vary the energy of ions impinging onto the wafer surface. Mean energy of incident ions (E_i) was estimated as $E_i = e(V_p - V_{dc})$; where e is the elementary charge, V_{dc} (<0) is the dc self-bias voltage monitored with an oscilloscope, and V_p is the plasma potential determined by plasma diagnostics using a Langmuir probe [20]. V_p was 11.1–15.2 V for the conditions studied here. Electron density was 3.0–3.1 × 10^{11} cm^{-3}. Electron temperature was 3.1–3.7 eV.

2.3. Composition analyses by HRTEM and HRBS

Three of the samples were examined by using cross-sectional high-resolution transmission electron microscopy (HRTEM). To determine the composition stoichiometry of the damaged layer, one of the samples (E_i = 128 eV) was examined by using high-resolution Rutherford backscattering spectroscopy (HRBS) using a 300 keV He^+ beam at scattering angle of 55°. The depth profiles of the atomic concentrations were obtained by simulation fitting.

2.4. Ellipsometry measurements

Spectroscopic ellipsometry (SE) is an optical, non-destructive method that can investigate wafer surface structures in atomic scale, and is widely used as in-line monitors. Measurements were carried out in the photon energy range of 1.60–5.50 eV at 0.05 eV intervals. SE measures the changes in amplitude (Ψ) and phase (Δ) between the p and s components of polarized light reflected from the sample, as described by the fundamental equation of ellipsometry [21,22]:

$$\rho = \frac{r_p}{r_s} = \tan(\Psi)\exp(i\Delta), \quad (1)$$

where r_p and r_s are the reflection coefficients of the p and s components. ρ is a function of the photon energy ($h\nu$), the angle of incidence, the thickness, and the dielectric function of the layers on the sample. To obtain the layer thickness and composition, the ρ spectrum must be fitted with an appropriate optical model that describes the sample structure correctly (discussed later). The best fit was determined by regression analysis to minimize the unbiased estimator σ, defined as

$$\sigma = \frac{1}{\sqrt{M-P-1}}\left\{\sum_{j=1}^{M}\left[\rho_{ex}(h\nu_j) - \rho_{model}(h\nu_j)\right]^2\right\}^{1/2}, \quad (2)$$

where M is the number of measurement points, P is the number of unknown parameters, and ρ_{ex} and ρ_{model} are the experimental and calculated ρ, respectively.

2.5. Wet-etching

In order to emulate the post-treatment by wet-etching and investigate the fate of the defects, a sample damaged by 100-W-bias argon ICP (similar conditions but not the same as the sample for HRTEM observation in section 2.3) was immersed in ≅0.1% diluted hydrofluoric acid (DHF) for tens of seconds at a time, measured by SE immediately after, and immersed in DHF again until the thickness was determined to be constant.

3. Results and discussion

3.1. MD simulation

Fig. 2 shows the results of the MD simulations. Si and O atoms on the topmost region were etched away in higher E_i conditions due to surface sputtering. Incident Ar^+ ions were observed to scatter Si and O atoms and disarrange the crystalline structure. Also, an event was observed where an Ar^+ ion collided with an O atom and caused the O atom to penetrate a few nanometers into the substrate.

The resulting structure can be classified into four layers from the top: (1) amorphous SiO_2, (2) amorphous SiO_x (x<2), (3) crystalline silicon (c-Si) with dislocated Si and interstitial atoms (both Si and O), and (4) c-Si, free of defects. Layer 1 was confirmed to be stoichiometric SiO_2 [graph in Fig. 2c]. The interfacial layers (2 and 3) were virtually nonexistent prior to plasma exposure, only a few monolayers thick for E_i = 50 eV, and increasingly thicker with higher E_i. The transition from layer 2 to layer 3 was gradual, and had roughness of which its height was several monolayers. This structure is compared with the experiments in the following sections.

3.2. Composition and structure

Fig. 3 shows the HRTEM images for the wafers processed under 100, 300, and 400 W biases. For all three samples, nanometer-sized crystallites protruding 1–6 monolayers from the amorphous/crystalline interface towards the surface were observed, causing roughness at the interface. Fig. 4 shows close-up views of the 300 W sample. What seem to be examples of crystallite inclusions are observed, which may coincide with the interface roughness between the layers 2 and 3 in the simulation. Also, in the crystalline region, features which may suggest the presence of defects were observed. On a larger scale, localized shades were observed in the crystalline region, near the interface. These were present only for 300 W and 400 W, and not for 100 W (Fig. 3). These may indicate the presence of strain fields [4,23] or segregated oxygen atoms [23,24] in the substrate. While it is not immediately clear which mechanism was responsible, it should be reminded that the latter was observed in layer 3 in the simulation (Fig. 2). The thickness of the amorphized layer as observed by HRTEM (d_{TEM}) was 4.5 ± 0.1 nm for 100 W and 4.0 ± 0.1 nm for 300 W (including the rough interface). Smaller thickness for 300 W may be attributed to surface sputtering. Disregarding the large wave-like

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