Modeling of Electron Beam Charging of an Insulating Layer on a Silicon Substrate*

Kaoru Ohya† and Hideaki Kuwada
Institute of Technology and Science, The University of Tokushima, Minamijosanjima 2-1, Tokushima 770-8506, Japan
(Received 25 October 2010; Accepted 2 February 2011; Published 26 March 2011)

Charging effects caused by secondary electron (SE) emission near a 100-nm-high SiO$_2$ step on a Si substrate are investigated. The system was irradiated by a 1-keV electron beam. We modeled SE emission by performing dynamic and self-consistent calculations of electron transport inside and outside the system. The model accounts for the electric field generated by positive and negative charges in the SiO$_2$ step. Positive charging of the SiO$_2$ step reduces the total electron yield to unity during irradiation. When the irradiation position is moved close to the step, charging decreases strongly and the electron yield increases sharply due to additional SE emission from the side wall of the step. When the Si substrate is irradiated with the electron beam, many SEs re-enter the side wall of the SiO$_2$ step so that the wall surface becomes negatively charged. This negative charging deters other SEs from re-entering the step. Consequently, the reduction in the total electron yield of the Si substrate near the wall is more localized than that without charging. [DOI: 10.1380/ejssnt.2011.112]

Keywords: Electron–solid interaction; Scanning electron microscopy; Insulating films; Nanoscale imaging; Monte Carlo simulation

I. INTRODUCTION

Silicon dioxide (SiO$_2$) is the most commonly used insulator in integrated circuit devices based on silicon (Si). Due to shrinking device dimensions, electron beams (EBs) have been increasingly used in device fabrication for performing inspection, metrology, and failure analysis. The small size and complexity of devices demands EB systems (e.g., scanning electron microscopes) with nanoscale resolutions and effective material contrast for structural and compositional analysis.

Insulators can become either positively or negatively charged by EB irradiation depending on various parameters. Charging effects are a critical problem when analyzing insulating materials since they produce undesirable distortions in secondary electron (SE) images. We have recently developed a Monte Carlo model for SE emission from SiO$_2$ that accounts for charging induced by EB irradiation [1]. It performs self-consistent calculations to model primary electron (PE) and SE transport, space charge creation, and the resultant electric fields in the material and in vacuum. This model has been applied to a very thin SiO$_2$ layer on a Si substrate. Calculated changes in pseudo-SE images with PE energy reproduced experimental observations of thermally oxidized layers with thicknesses of 24-106 nm on a Si wafer [2]. Thick SiO$_2$ layers on Si become positively charged during irradiation by 300-1600-eV EBs, and attract emitted SEs back to the surface. Consequently, the total electron yield is reduced to unity. Positive charging is reduced for thin layers (< 60 nm) and the total electron yield recovers to the yield (> 1) without charging. The surface voltage is sensitive to variations in the layer thickness of several tens of nanometers.

In this paper, we investigate charging effects on structured surfaces on a subnanometer scale. We model a SiO$_2$ step on a Si substrate. The surface was irradiated with a zero-diameter EB and total electron yields at various points on the SiO$_2$ step and the Si substrate were calculated.

II. SIMULATION MODELS

Figure 1(a) shows the 100-nm SiO$_2$ step on a Si substrate used in this simulation. A thick insulating layer with an infinite lateral dimension will be either positively or negatively charged by EB irradiation depending on the ratio of emitted to incident electrons. The number of emitted electrons includes both SEs and backscattered secondary electrons (BSEs). In this study, the total electron yield is greater than unity because the incident PE energy is chosen to be 1 keV. Therefore, the surface becomes positively charged during EB irradiation. The step is 250 nm long and 500 nm wide. These dimensions are larger than the lateral distributions of PE and SE trajectories in SiO$_2$.

Irrespective of whether a material is conducting or insulating, SE emission can be modeled by a three-stage process [3], which is depicted in Fig. 1(b) for insulating SiO$_2$. The first stage involves generation of internal SEs by PEs penetrating the material. The second stage is transport of these SEs to the surface. In the third stage, the SEs escape over the surface barrier. The Monte Carlo SE emission model simulates PE and SE trajectories in the material based on their mean free paths (MFPs) for collision processes. The PEs enter the material and are elastically scattered by atomic nuclei. They also undergo inelastic energy loss processes (e.g., electron–hole pair creation). The MFP for elastic scattering can be calculated using the screened Rutherford formula. This formula uses the energy-dependent screening parameter, $E_s$, which was obtained by Fitting and Reinhardt [4] ($E_s = 250$ eV for both Si and SiO$_2$). The SEs originate from electron–hole
pairs in the conduction band of Si and from the filled valence band of SiO$_2$. We treat this using an optical data model developed by Ashley [5] that relates the MFP for electron–hole pair creation to the complex dielectric function using optical data for Si and SiO$_2$ [6]. The SEs generate new SEs during electron cascade. The MFP of migrating SEs in SiO$_2$ is also increased by the large band gap energy ($E_g = 9$ eV) of SiO$_2$. Therefore, SEs with energies below $E_g$ cannot create electron–hole pairs and they lose energy only through interactions with phonons in SiO$_2$ [7]. The PEs and SEs that reach the surface and overcome the surface barrier are ejected with reduced energy into the vacuum. This process can be described using the planar surface barrier model. The barrier energy for SiO$_2$ is determined by the electron affinity, $E_A$ (0.9 eV). The barrier energy for Si is given by $\Phi + E_F$, where $\Phi$ is the work function (4.79 eV) and $E_F$ is the Fermi energy (7.83 eV) [8]; this barrier energy is much larger than $E_A$ for SiO$_2$.

Because SEs in SiO$_2$ have a lower surface barrier energy (0.9 eV) and a lower energy loss than SEs in Si, the calculated SE yield is two to five times higher than previously obtained experimental data [9]. Consequently, polarization effects [10] need to be taken into account. This affects low-energy SEs through interactions with ionic cores. This effect is introduced in the form of the probability that SEs are trapped by impurities, defects, or more general polarizability inhomogeneities, $P_p = S_p \exp(-\gamma_p E)$ ($P_p = 1$ if $P_p > 1$). In this case, $E$ is the SE energy. Setting the parameters $S_p$ to 100 and $\gamma_p$ to 0.25 eV$^{-1}$, the calculated SE yield is 1.12 for an incident energy of 1 keV, which is in reasonable agreement with experimentally measured yields (1.02 [11] and 1.18 [12]). The calculated BSE yield ($\sim 0.30$) is also in good agreement with previous experimental results [12].

Any holes created in Si immediately recombine with conduction band electrons or SEs that are not emitted from the surface. However, any charges (i.e., PEs, SEs, and holes) remaining in SiO$_2$ can be fixed so that the material becomes charged. In this study, we subdivided a vacuum–SiO$_2$–Si system into $100 \times 100 \times 100$ cubic cells that have a length of 5 nm, giving a total simulation volume of $500 \times 500 \times 500$ nm$^3$ (Fig. 1(a)). The cells in the SiO$_2$ step correspond to PE, SE, or hole trapping sites, which are assumed to be uniformly distributed with a density of $1/(5 \text{ nm})^3 = 8 \times 10^{18}$ trap sites per cm$^3$. Trapped charges generate an electric field in the SiO$_2$ step and in the vacuum. The electric field in the vacuum bends the trajectories of emitted SEs. The electric field is calculated by solving the three-dimensional Poisson equation. The boundaries of the simulation volume and inside the Si are assumed to be at zero potential. However, at the boundary between the SiO$_2$ step and the vacuum, continuity of the normal component of the electric induction leads to a discontinuous change in the voltage. Classical equations of motion are used to calculate the trajectories of the emitted SEs and BSEs in the vacuum.

Dynamic simulation of the charging process starts with the production of SEs from 100 PEs incident on the SiO$_2$ step and the Si substrate and their subsequent transport in the material and the vacuum. The spatial distributions of trapped charges in the SiO$_2$ and the electric field inside and outside the material are then calculated. Another 100 PEs are incident and the trajectories of the new PEs and SEs are calculated in the electric field. In this case, newly trapped charges drift along the electric field in accordance with the classical equation of motions. A step length of 0.1 nm is employed in the trajectory calculation. If the charge reaches a trap site at the end of a drift step, three possible situations can occur. If the trap site is empty, the charge will be trapped at the site. If it is occupied by a charge with the same sign as the drifting charge, the charge continues on its drift trajectory following the electric field lines. If the trap is occupied by a charge of opposite sign, the charges recombine at this site. In this case, the site becomes vacant and the two charges are removed from the transport process. Finally, the accumulated charge and the resultant electric field are calculated. This sequence is repeated for every 100 PEs. The calculation accounts for the re-entrance of BSEs and SEs that had been emitted from the surface. Re-entering BSEs can penetrate the material again and generate additional SEs. However, re-entering SEs are assumed to be trapped by surface cells because of their low energies.

III. RESULTS AND DISCUSSION

Figure 2 shows the total electron yield as a function of the incident position after irradiation with $10^4$ PEs at 1 keV. The step edge is located at a displacement of zero

---

**FIG. 1: Schematic diagrams showing (a) a step of SiO$_2$ formed on a Si substrate and (b) SE emission and charging in SiO$_2$ due to electron irradiation. The dotted square in (a) indicates a cross-section of a 500-nm-wide cubic simulation volume.**
FIG. 2: Electron emission (SE and BSE) yield with and without charging as a function of the incident position of 1-keV electrons. The step edge is located on the origin (see Fig. 1(a)). Negative distances correspond to positions on the SiO$_2$ step surface and positive distances correspond to positions on the Si substrate.

FIG. 3: Trajectories (side view) of SEs emitted due to irradiation of ((a)-(c)) SiO$_2$ step and ((d)-(f)) Si substrate by 100 electrons with energies of 1 keV. Charging on the SiO$_2$ step is not considered. The arrows indicate the irradiation positions.

(see Fig. 1(a)). Negative displacements indicate points on the SiO$_2$ step while positive displacements correspond to points on the Si substrate. When charging is not taken into account, the dependence of the electron yield on the incident position is determined by simple geometric effects [13].

One kind of geometric effect occurs when PEs are incident on the SiO$_2$ step. When approaching the edge of the step, SEs that cannot escape from the surface can be emitted from the side wall of the step. Figure 3(b) shows the trajectories of emitted SEs when charging is not taken into account. Furthermore, high-energy PEs can escape from the side wall and re-enter the Si substrate. These PEs can cause additional emission of SEs from the Si surface (see Fig. 3(c)). This mechanism produces a sharp increase in the total electron yield near the edge of the step on the SiO$_2$ side (Fig. 2).

Another geometric effect is BSEs and SEs re-entering the side wall of the step when PEs are incident on the Si substrate. This is shown in Figs. 3(d), (e), and (f). The re-entrance of BSEs increases the total electron yield due to additional production of SEs inside the wall. However, the re-entrance of SEs reduces the electron yield because some of them are absorbed by the wall. In this case, the BSE yield (0.30) of SiO$_2$ calculated without charg-
FIG. 6: Top views of the charge distribution accumulated in the SiO$_2$ step and the trajectories of SEs emitted from ((a)-(c)) the SiO$_2$ step and ((d)-(f)) the Si substrate. The distributions were calculated for irradiation by 100 electrons at various incident positions for steady-state charging of the SiO$_2$ step. The white and black circles correspond to trapped positive (holes) and negative (SEs and PEs) charges, respectively.

FIG. 7: Charging voltage distributions on the (a) surface and (b) side wall of the SiO$_2$ step for irradiation of the SiO$_2$ step and the Si substrate by 1-keV electrons. The calculation was performed for steady-state charging of the SiO$_2$ step. The arrows indicate the electron irradiation positions.

The electron yield approaches unity at negative positions relative to the step wall ($\leq -50$ nm) after irradiation with 10$^4$ PEs. Because the penetration depth of 1 keV PEs is smaller than the height (100 nm) of the SiO$_2$ step, PEs cannot reach the Si substrate. Therefore, charging cannot be reduced by the Si substrate. Figure 4 reveals that the surface voltage increases with increasing number of PEs until it saturates above $\sim$5,000 PEs at a steady-state value of $\sim$16 V. The steady-state voltage depends on both the incident energy and the SiO$_2$ step height (if it is of the order of tens of nanometers) [2].

Figures 5 and 6 show the trajectories of SEs emitted into the vacuum for 1 keV PEs incident on different positions on the SiO$_2$ step and the Si substrate together with the corresponding charge distributions that accumulate in the SiO$_2$. When PEs are incident on the SiO$_2$ step, many holes accumulate near the incident position. Furthermore, due to the electric field above the surface induced by charging, SEs may return to the surface and be reabsorbed by it. The charge distribution in the SiO$_2$ shows good correspondence with the trajectories of the emitted SEs above the SiO$_2$ surface.

When the incident position approaches the edge of the SiO$_2$ step, the charge distribution is strongly influenced by the edge. The total electron yield increases steeply, whereas the surface voltage decreases to zero (see Figs. 2 and 4). Therefore, the effect of charging on the trajectories of the emitted SEs is strongly suppressed (see Figs. 5(c) and 6(c)). The edge effect (i.e., the sharp increase in the electron yield) is also observed when charging is taken into account (Fig. 2). Suppression of the charging effect starts at 50 nm from the edge due to the
reduction in the number of positive charges (i.e., holes) localized near the side wall of the SiO$_2$ step and mixing and redistribution of positive and negative charges. This reduces the electric field in both the SiO$_2$ step and the vacuum. When the incident position is close to the edge, the charges are compensated by SEs emitted from the Si substrate re-entering the step (Fig. 5(c)). This maintains the charge balance between incoming and outgoing electrons. However, the relaxation mechanism is currently not well understood.

However, when PEs are incident on the Si substrate, the edge effect (i.e., SEs re-entering the side wall of the SiO$_2$ step) depends strongly on whether charging is considered or not (see Figs. 5(d) or 3(d), respectively). Although re-entrance of SEs reduces the total electron yield, it also causes the side wall to be negatively charged (see Figs. 5(d)-(f) and 6(d)-(f)). Negative charging of the side wall influences the trajectories of SEs emitted from the Si substrate, causing them to be repelled or reflected from the side wall. These SEs contribute to the total electron yield and negative charging approaches the steady-state value. Therefore, as shown in Fig. 2, the reduction in the total electron yield of the Si substrate is localized near the side wall of the SiO$_2$ step. At locations distant from the wall (Fig. 5(d)), some SEs can return to the Si substrate through negative charging of the wall. Despite the side wall being negatively charged, high-energy BSEs can re-enter the wall and create electron–hole pairs in the SiO$_2$ step.

Figures 7(a) and (b) show the voltage distributions of the surface and the side wall of the SiO$_2$ step, respectively. It shows that the voltage changes from negative to positive when the incident position of the PEs moves from the Si substrate to the SiO$_2$ step. This change occurs due to SEs re-entering the side wall or holes being created in the wall. The negative voltage region shifts from the top to the bottom of the wall as the incident EB beam approaches the wall. However, at most incident positions on the SiO$_2$ step, the positive voltage dominates both the surface and the side wall. At the closest position (~5 nm), the wall is negatively charged near its base, whereas it is positively charged near its top.

IV. CONCLUSIONS

Charging effects caused by SE emission near a 100-nm-high SiO$_2$ step on a Si substrate are investigated. The accumulated positive and negative charge distributions in the SiO$_2$ step, the trajectories of emitted SEs in vacuum, the total electron emission yield, and the surface voltage were calculated for various 1-keV EB irradiation positions. Positive charging of the SiO$_2$ step reduces the total electron yield to unity due to the electric field generated above the step, which leads to emitted SEs being reabsorbed by the step. When the PE incidence point approaches the edge of the step, charging decreases greatly. Consequently, the electron yield increases sharply and additional SEs are emitted from the side wall of the SiO$_2$ step. This is similar to the case without charging. When PEs are incident on the Si substrate, many SEs re-enter the side wall of the SiO$_2$ step causing the wall surface to become negatively charged. This negative charging prevents the SEs from re-entering the wall. As a result, the reduction in the total electron yield near the step edge is more localized to the wall than for the case without charging. These variations in the electron yield, which depend on the incident position on the structured surface, are important when performing structural and compositional measurements of nanoscale materials using EBs. However, comparisons with experiments and parameter studies using different incident energies and different step heights are required to gain a detailed understanding of EB charging of nanoscale insulating layers on various substrates.

Acknowledgments

This work was supported by KAKENHI (19055005).