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Mathematical Model-Based Evaluation Methodology for Environmental Burden of Chemical Mechanical Planarization Process

Hyunseop Lee[1], David Alan Dornfeld[2], and Haedo Jeong[1,#]

1 School of Mechanical Engineering, Pusan National University, San 30, Changjeon-dong, Kumjeong-ku, Busan 609-735, South Korea
2 Department of Mechanical Engineering, University of California, Berkeley, California 94720-1740, USA
Corresponding Author / E-mail: hdjeong@pusan.ac.kr, TEL: +82-51-510-3210, FAX: +82-51-518-8442

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Chemical mechanical planarization (CMP) is an essential manufacturing process in semiconductor fabrication. Chipmakers continue to adopt CMP for device planarization or surface finishing of substrate materials. Evaluating the environmental impact of the CMP process may contribute to the greening of the semiconductor process. In this paper, we propose a mathematical model-based evaluation method to determine the environmental burden of the CMP process. We adopted our previously reported material removal rate (MRR) model for CMP and modified it to incorporate the effect of the slurry flow rate and process temperature. The established model was compared with the experimental results. The environmental burden of the CMP process was evaluated by converting the electric energy consumption, slurry consumption, and ultrapure water (UPW) consumption into their carbon dioxide equivalents (CDEs). The results showed that the slurry consumption strongly impacted the CDE of the CMP process. The results of this study may help optimize the process parameters for a sustainable CMP process.

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1. Introduction

For manufacturers, the current challenge is to meet increasing environmental demands for production while using less material and energy.[1] The semiconductor industry also has to consider global environmental regulations on pollution. Most research on sustainable manufacturing of semiconductors has been conducted in high-level studies; however, lower-level guidelines may better aid manufacturers in improving their factories to facilitate environmental sustainability.[2] Prior to making changes in a process, the environmental burden has to be measured and evaluated.

Gutowski et al.[3] summarized the specific energies of various unit manufacturing processes such as machining, grinding, abrasive waterjet, and injection molding. Narita et al.[4] proposed an environmental burden analyzer for machine tools based on numerical control (NC) simulation. Diaz et al.[5] provided a specific energy model for a machine tool. Hu et al.[6] developed an online energy monitoring (OEEM) system for machining systems.

Chemical mechanical planarization (CMP) is the main process in semiconductor manufacturing because of its global and local planarization ability[7,8] and surface smoothing ability.[9] The CMP process is recognized as one of the dirtiest and most expensive processes in semiconductor fabrication. The wastewater of the CMP process is composed of several kinds of organic and inorganic materials. Reducing slurry consumption has been reported to be more significant than saving electric energy in the CMP process.[10]

In this paper, we propose a mathematical model-based evaluation method to determine the environmental burden of the CMP process. A case study on the effect of the slurry flow rate on the environmental burden was performed based on the methodology.

2. Methodology for Evaluating Environmental Burdens

Fig. 1 shows the schematic of the material flow in the CMP process, including post-CMP cleaning, based on a dry-in/dry-out process flow. First, electric energy is used to operate the CMP machine and post-CMP cleaner. CMP slurry and UPW, which are categorized as short-

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lifespan CMP consumables, are supplied from the fabrication facility.[10] Long-lifespan CMP consumables such as the polishing pad, conditioner, retaining ring, and backing film are required for conducting and sustaining the CMP process.[10] In the post-CMP cleaning process, ultrapure water (UPW), cleaning chemicals, and a polyvinyl alcohol (PVA) brush are consumed.[11] From the perspective of post-CMP cleaning, the UPW and cleaning chemicals are short-lifespan consumables, and the PVA brush is the long-lifespan consumable. In this study, our focus was on the material flow and energy consumption relevant to the CMP process, especially the material flow of short-lifespan consumables and electric energy consumption.

The CMP process has so many process parameters that mathematical modeling of the material removal rate (MRR) is very complicated. Thus, a semi-empirical model may be more useful to express or estimate the material removal of the CMP process. Establishing a CMP model has many advantages: not only to optimize the process and predict the results but also to evaluate the environmental burden of using electric energy and consumables.

The proposed mathematical model-based evaluation method for the environmental burden of the CMP process has three steps: (1) establish the mathematical MRR model, (2) assess the consumed energy and consumables for the concerned process time, and (3) evaluate the environmental burden as the carbon dioxide equivalent (CDE). Fig. 2 shows the flowchart of the model-based evaluation for the environmental burden of the CMP process.

3. Mathematical models for CMP process

3.1 Mechanical Contact Model

In this study, the particle indentation deformation associated with the pad was assumed to be elastic, and the deformation associated with the film on the wafer was assumed to be plastic based on Wang's nonlinear and micro-contact model.[12] ξ is the ratio of the indentation depth of a particle into the polishing pad ($\delta_p(D)$) to the particle diameter D ($\xi = \delta_p(D)/D$). According to Wang et al., ξ can be obtained by solving[12]

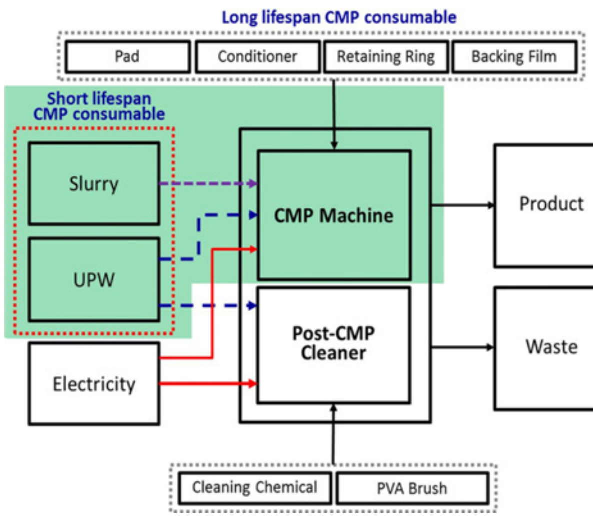

Fig. 1 Schematic of material flow in CMP process including Post-CMP cleaning

$$\left(\frac{H_f}{E_{ap}}\right)^2 = \frac{(4\xi+(2\xi-1)(-3+\sqrt{9+24\xi}))^2}{8\pi^2(2-2\xi)^2(-3+\sqrt{9+24\xi})} \tag{1}$$

where H_f is the hardness of the film and E_{ap} is the composite elastic modulus of the pad and particle.

The equivalent indentation depth of a single particle of diameter D into the film surface can be obtained from the relationship shown below.[12]

$$\delta_w(D) = \left(1-\frac{\xi}{2}\right)D \tag{2}$$

S(D) is the cross-sectional removal area for the chemically reacted film surface and is written as

$$S(D) = \frac{4}{3}K(T)\sqrt{\delta_w(D)D} = \frac{4}{3}K(T)\left(1-\frac{\xi}{2}\right)^{3/2}D^2 \tag{3}$$

where $K(T)$ is a temperature-dependent parameter indicating the chemical reaction along with the process temperature.

3.2 Kinematic Model

The relative velocity between a point on the wafer and the pad can be expressed as[13,14]

$$v_{re}(r_w,t) = \sqrt{r_0^2\omega_p^2 + r_w^2(\omega_w-\omega_p) + 2r_0 r_w \omega_p(\omega_p-\omega_w)\cos(\omega_w t)} \tag{4}$$

where r_w is the distance of a point on the wafer from the wafer center; t is the process time; r_0 is the distance between the center of the polishing pad and the wafer; ω_p is the angular velocity of the polishing pad; and ω_w is the angular velocity of the wafer.

The time-averaged relative velocity of an arbitrary position on the wafer from the wafer center can be obtained by[14]

$$\bar{v}_{re}(r_w) = \frac{1}{T_w}\int_0^{T_w} v_{re}(r_w,t)dt \tag{5}$$

where T_w is the rotational period of the wafer ($T_w = 2\pi/\omega_w$).

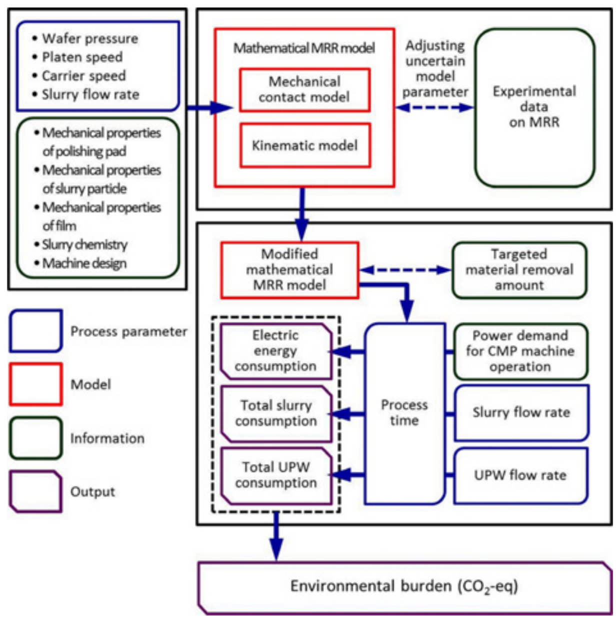

Fig. 2 Model-based evaluation on environmental burdens of CMP process

3.3 Mathematical MRR Model

In this study, we adopted our previously reported MRR model for the CMP process.[15] The model was modified to consider the chemical reaction with regard to the process temperature. Before the mechanical contact between the film material and particle can be considered, the number of particles in the CMP slurry needs to be calculated.

We assumed that the particles are uniformly located in the CMP slurry with distance l between particles. The distance between particles can be calculated from[15]

$$\left(\frac{\sqrt{A_w^T}}{l}+1\right)\left(\frac{X}{A_W^T l}+1\right)=N_p=\frac{6X\rho_s C_a f_p}{\pi D^3\rho_a\int_0^{+\infty}\Phi(D)dD} \tag{6}$$

where $A_w{}^T$ is the apparent wafer-pad sliding area calculated from the total contact area between the rotating wafer and polishing pad during the process time and t_s is the imaginary slurry thickness ($X/A_w{}^T$). X is the total slurry volume during the CMP process; ρ_s is the density of the slurry; C_a is the weight concentration of particles in the slurry; f_p indicates the ratio of particles that flow underneath the wafer, which was not considered in the previous study; D is the particle diameter; and ρ_a is the particle density. $\Phi(D)$ is the probability density function of slurry particles.

By solving Eq. 6, we can obtain the area density of particles (q) as $((A_w^T)^{0.5}/l+1)^2/(A_w^T)$, and the real contact area (A_r) is expressed as[15]

$$A_r=\left(\frac{f_s}{C}\right)\left(\frac{R_p}{\sigma_p}\right)^{1/2}\frac{PA_w}{E_{pw}} \tag{7}$$

where f_s (0.83 for an k-grooved IC1000 pad) is the area density of the up-features divided by the area of the flat pad; R_p is the average radius of curvature of the pad asperity tips; C (= 0.35) is a constant determined from the Greenwood-Williamson model[16] and Qin's research;[17] σ_p is the standard deviation of the pad asperity height distribution; and E_{pw} is the composite elastic modulus of the pad and wafer. P is the applied pressure, and A_w is the nominal area of the wafer surface.

The number of active particles that participate in material removal can be expressed as[15]

$$n_a=qA_r\int_{D_{cr}}^{+\infty}\Phi(D)dD \tag{8}$$

where D_{cr} is the critical diameter of particles that can participate in the material removal process and q is the area density of particles.

Thus, the MRR model for the CMP process can be written as

$$\begin{aligned} MRR &= K(T)\cdot MRR_{mech} \\ &= \frac{4K(T)(\sqrt{A_W^T}+l)^2 f_s R_p^{0.5}}{3A_W^T C\sigma_p{}^{0.5}E_{pw}l^2}\left(1-\frac{\zeta}{2}\right)^{1.5}\int_{D_{cr}}^{+\infty}\Phi(D)D^2dD\cdot PV_{re} \end{aligned} \tag{9}$$

where MRR_{mech} is the pure mathematical removal rate by particles without the aid of chemical reaction and V_{re} is the average relative velocity of the wafer.

$K(T)$ in Eq. 9 is the temperature-dependent parameter expressed in the modified Arrhenius equation, as shown below.[18]

$$K(T)=k\,\exp\left(-\frac{E_{comb}}{k_B T}\right) \tag{10}$$

where k is the thermally independent constant, E_{comb} is the combined activation energy of the process, k_B is the Boltzmann constant, and T is the process temperature.[18] Eq. 10 can be determined by comparing the mathematical model with the experimental results. $K(T)$ implies the change in chemical reaction between slurry chemicals and the target material with the process temperature.

4. Case Study: Effect of Slurry Flow Rate

4.1 Power Demand for CMP Machine Operation

In this paper, a 1.5 μm of SiO_2 film was deposited on 200 mm diameter silicon wafer, and the thickness of the SiO_2 film was measured with a reflectometer. The CMP cycle consists of idling, conditioning, wetting, wafer loading, head dropping, polishing, and wafer unloading, as shown in Fig. 3. The power demand for each operational step was measured with a power meter installed in the power panel at the facility. Table 1 shows the measured required power demand for CMP machine operation.

The experimental results showed that the power demand did not significantly change with respect to the varying slurry flow rate condition. The average power demand during the polishing step was 1.417 kW under various slurry flow rates. The UPW flow rates in the idling and conditioning steps were 100 and 200 mL/min, respectively. The slurry flow rates in the polishing step varied from 50 mL/min to 350 mL/min, and the slurry flow rate in the wetting step was fixed at 200 mL/min. The polishing pressures were 27.58 kPa for the wafer and 34.47 kPa for the retaining ring. The rotational velocity of the polishing head and platen was 80 rpm. The conditioning force was 22.24 N, and the rotational velocities of the platen and conditioner were 93 and 87 rpm, respectively. The UPW flow rate in the rinsing step was 200 mL/

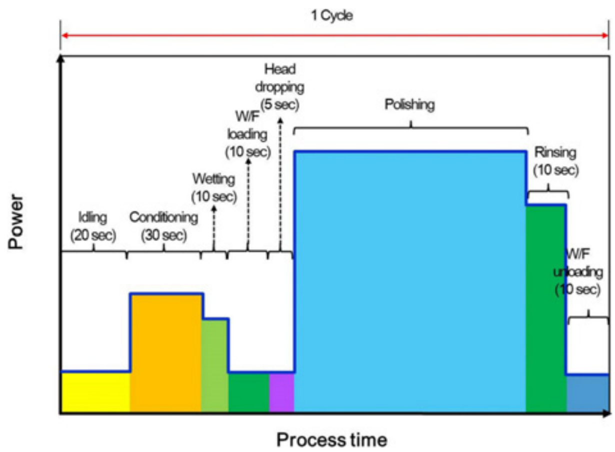

Fig. 3 Schematic of power input at CMP machine over process time and operational steps

Table 1 Power demand for CMP machine operation

Operations	Average power demand (kW)
Idling	0.143
Conditioning	0.921
Wetting	0.753
W/F loading and unloading	0.143
Head dropping	0.143
Polishing	1.417
Rinsing	0.877

min, and the pressures were 9.81 kPa for the wafer and 19.61 kPa for the retaining ring.

During CMP process, the polishing temperature was measured with an infrared sensor at the trailing-edge of the polishing head. The measured signals were displayed on the monitor. The average polishing temperature was used for establishing the temperature-dependent parameter.

4.2 Modeling of MRR

The particle size distribution of silica slurry was measured with a particle size analyzer, as shown in Fig. 4. The left axis is the particle intensity, and the right axis is the cumulative intensity. The particle concentration of the slurry was 12.5 wt%. The material properties of the wafer, pad, slurry followed the previously reported values in.[15] The ratio of particles that flowed underneath the wafer (f_p) was assumed to be 0.05. The critical particle diameter (D_{cr}) was 22 nm.[15]

Fig. 5 shows the relationship between $1/T$ and the temperature-dependent parameter based on the Arrhenius relationship in Eq. 10. In Eq. 10, k is 110717.8, and E_{comb}/k_B is 3339.83 K. These results show that the chemical reaction is affected by the process temperature.[19]

Table 2 shows the modeling and experimental results of MRRs as a function of the slurry flow rates. The modeling results agreed with the experimentally obtained MRRs for changes in the slurry flow rate. The model reflects the cooling effect on MRR by the CMP slurry. Assuming that the total material removal amount (MRA) is 300 nm, we can predict the required polishing time, as shown in the rightmost column of Table 2.

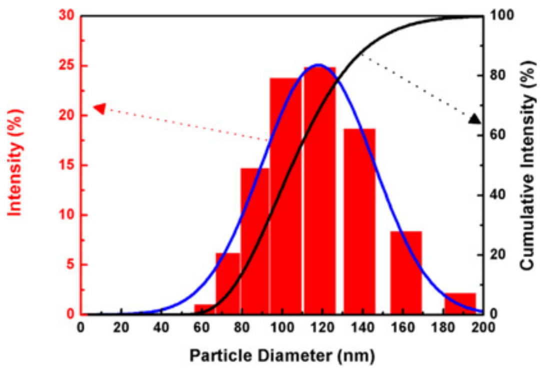

Fig. 4 Particle size distribution of CMP slurry: (left) intensity (%) and (right) cumulative intensity (%)

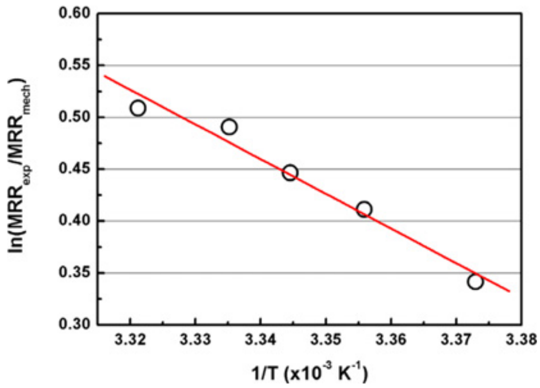

Fig. 5 Relationship between ln(MRR_{exp}/MRR_{mech}) as a function of 1/T(K^{-1})

4.3 Environmental Burdens

The emission rates of carbon dioxide (CO_2), methane (CH_4), and dinitrogen monoxide (N_2O) that are associated with the use of electric energy and reported by the Korean Power Exchange in 2011 were 458.5 gCO_2/kWh, 0.0052 gCH_4/kWh, and 0.0040 gN_2O/kWh, respectively.[20] In terms of the global warming potential (GWP), the CDE of electric energy use was 459.8 CO_2-eq/kWh. The CDEs of UPW and oxide CMP slurry were 0.0104 gCO_2-eq/mL[21] and 0.2704 gCO_2-eq/mL,[22] respectively.

The CDE from the CMP process can be calculated as

$$CDE_{CMP}(t) = CDE_{elec}(t) + CDE_{slurry}(t) + CDE_{UPW}(t) \qquad (11)$$

where $CDE_{elect}(t)$, $CDE_{slurry}(t)$, and $CDE_{UPW}(t)$ are the carbon dioxide equivalents of electric energy consumption, slurry consumption, and UPW consumption, respectively, over process time (t).

The CDE was constant for the operation steps excluding polishing; in the experiment, it was fixed at 17.18 gCO_2-eq. When we polished 300 nm of SiO_2 film, as shown in Table 2, the CDE increases with the flow rate, and the CDE resulting from slurry consumption accounted for the largest portion of the total CDE (Table 3). When the slurry flow rate was changed from 50 mL/min to 350 ml/min, the CDE from electric energy consumption decreased from 32.71 gCO_2-eq to 23.83 gCO_2-eq; however, the CDE from slurry consumption increased from 43.73 gCO_2-eq to 160.59 gCO_2-eq. According to Table 3, the percentage contribution of slurry use increased with the slurry flow rate; however, that of electric energy consumption decreased with respect to the slurry flow rate. Thus, reducing slurry consumption in the CMP process is essential for environmental sustainability. Developing high-efficiency slurry or increasing slurry participation in material removal may help reduce the CDE from slurry consumption.

5. Conclusions

We proposed a mathematical model-based evaluation method to determine the environmental burden of electric energy consumption

Table 2 Modeling results, experimental MRR, and required process time to remove 300 nm of SiO_2 film

Flow rate (ml/min)	MRR_{exp} (nm/min)	MRR_{mod} (nm/min)	Error (%)	Time (min) for MRA 300 nm
50	122.3	123.9702	1.37	2.42
100	164.2	161.7576	1.49	1.85
150	177.4	177.0456	2.00	1.69
250	190.1	189.2167	0.47	1.59
350	185.8	187.3053	0.81	1.60

Table 3 Modeling results, experimental MRR, and required process time to remove 300 nm of SiO_2 film

Flow rate (ml/min)	Carbon dioxide equivalent			
	Total (gCO_2-eq)	Electricity (%)	Slurry (%)	UPW (%)
50	76.175	42.9	54.8	2.3
100	87.468	30.4	67.6	2.0
150	104.308	23.8	74.5	1.7
250	141.575	16.7	82.1	1.2
350	186.153	12.8	86.3	0.9

and the use of short-lifespan consumables by the CMP process. A semi-empirical MRR model based on contact mechanics was adopted to predict the process time to remove the target thickness of the film material. The consumed energy and consumables for a given process time can be estimated from the process conditions. The environmental burden was evaluated according to the consumption of electric energy, slurry, and UPW in terms of CDE. A case study was performed using the proposed method to determine the effect of the slurry flow rate on the environmental burden and show the importance of reducing slurry consumption for environmental sustainability.

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