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Chemical mechanical planarization operation via dynamic programming

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Abstract

In this paper, the impact on non-planarization index by the down force and rotational speed during a SiO_2 or Cu CMP process was investigated. Since the magnitudes of down force and rotational speed have limits, we choose the dynamic programming approach because of its ability to achieve constrained optimization by the down force and rotational speed. The duration and the amount of input were computed based on the chemical mechanical polishing model by Luo and Dornfeld [J. Luo, D.A. Dornfeld, IEEE Trans. Semiconduct. Manufact. 14(2) (2001) 112–132.] when the other parameters were fixed. Experiments done for blanket wafers based on dynamic programming operation and conventional constant removal rate operation was compared with each other. The non-planarization index could be improved consistently by dynamic programming operation versus constant removal rate operation. The improvement ranges from 2% to 39% improvement over the base recipe of constant removal rate in all experiments as shown in Tables 3 and 6. The thickness removal error is consistently smaller by constant removal rate operation versus dynamic programming operation in all experiments as shown in Tables 3 and 6. To get the best performance of both planarization and thickness removal, it is recommended that planarization step and overpolish step in SiO_2 and Cu CMP should use different mode of operation, i.e., dynamic programming operation during planarization step for minimizing non-planarization index and constant removal rate operation during overpolish step for minimizing thickness removal error. The incremental time calculation for eliminating thickness removal error during overpolish step can be done using the thickness error and removal rate derived from Luos' removal rate model based on constant wafer pressure and platen speed at the end of planarization step.

Our contribution is a new approach for CMP. Standard CMP uses constant removal rate operation in both planarization step and overpolish step. Our new approach uses dynamic programming operation during planarization step and constant removal rate operation during overpolish step.

Keywords: Chemical mechanical planarization; Dynamic programming; Non-planarization index; Copper dishing; Oxide erosion

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1. Introduction

Chemical mechanical planarization (CMP) is a widely accepted technique to provide a globally planarized surface for microelectronic wafer fabrication nowadays. CMP was developed during the early 1980s when multilevel interconnect technology was pushed to the limits of circuit density and performance. This technique produces excellent planarization across the wafer surface and improves both photolithography and deposition process [1]. In recent years, the device levels and densities increased continuously, at the same time the problem of resistance–capacitance (RC) time delays which can appreciably slow down circuit speeds must be solved quickly. As a result, copper has emerged as the optimal interconnect material because of its low resistivity and high electromigration resistance compared with aluminum [2,3]. Patterned Cu lines are produced by a damascene process when using Cu as an interconnect material. In the damascene process, the dielectric is patterned, followed by the barrier and metal deposition. The barrier is required to prevent the rapid diffusion of the

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Cu into the dielectric. The final step in this process is CMP that removes the excess metal and provides global planarization. Fig. 1 schematically shows a single layer Cu interconnect structure before and after CMP. Two key problems in Cu pattern wafer CMP, namely copper dishing and oxide erosion, generate surface non-planarity which gives rise to problems in integrating multiple layers of metal. Copper and oxide thinning results in increased RC delay which leads to inferior device performance. Therefore, we focus on the experiments for SiO_2 and Cu CMP.

Several research efforts have been reported on modeling the CMP process and the most well known equation is the Preston's equation [4]. Preston's equation reflects the influence of process parameters including wafer pressure and relative velocity. In the last several years, the revised Preston's equations concentrated on different elements of CMP. For example, Zhang and Busnaina [5] proposed an equation taking into account the normal stress and shear stress acting on the contact area between abrasive particles and wafer surfaces. Tseng and Wang [6] showed that the removal rate is proportional to the terms $P^{5/6}$ and $V^{1/2}$. Zhao and Shi [7,8] consider the effects of the pad hardness and the contact between wafer and pad. Luo and Dornfeld [9] assumed an indentation-sliding model for the penetration of the pad and included an empirical accommodation of chemical reaction at the wafer surface. Compared with experiment results, the Luo and Dornfeld model more accurately predicts the removal rate. (Therefore, the Luo and Dornfeld model will be employed to predict thickness removal rate in this paper).

Most of the research work on CMP is focused on removal mechanism and slurry chemistry. Chiu et al. [10] applied the concept of soft landing of a spacecraft to CMP operation. Therefore, the CMP operation can be formulated as a minimum time optimal control problem. They treat the oxide surface as the landing surface, the polishing pad as a fly vehicle, and the removal rate as the vertical velocity. The equations describing the thickness removal process can be expressed as:

$$\begin{bmatrix}\dot{H}\\ \dot{RR}\end{bmatrix}=\begin{bmatrix}0&-1\\0&0\end{bmatrix}\begin{bmatrix}H\\ \mathrm{RR}\end{bmatrix}+\begin{bmatrix}0\\1\end{bmatrix}a$$

$$-a_{\max}\leqslant a\leqslant a_{\max}$$

where H is the thickness of material to be removed, RR the removal rate, and a the rate of change of the removal rate. The constraints in removal rate and rate of change of removal rate are applied because the parameters of CMP machine have physical limit, e.g., platen speed, wafer pressure, and slurry flow rate. They also set the final condition to $\mathrm{H}(t_f) = 2000$ Å and $\mathrm{RR}(t_f) = 2000$ Å/min in order to reduce the dishing and erosion according to the experimental data proposed by K. Wijekoon and S. Tsai etc. [17]. Fig. 2 shows that copper dishing and oxide erosion are proportional to platen speed and wafer pressure. Once the landing point is reached ($\mathrm{H}(t_f) = 2000$ Å), the polisher continues the removal with the smaller removal ($\mathrm{RR}(t_f) = 2000$ Å/min) until the end point is detected. Fig. 3 shows the result of optimal operation. Through their inspiration, we plan to use dynamic programming as our method of optimal operation in this research.

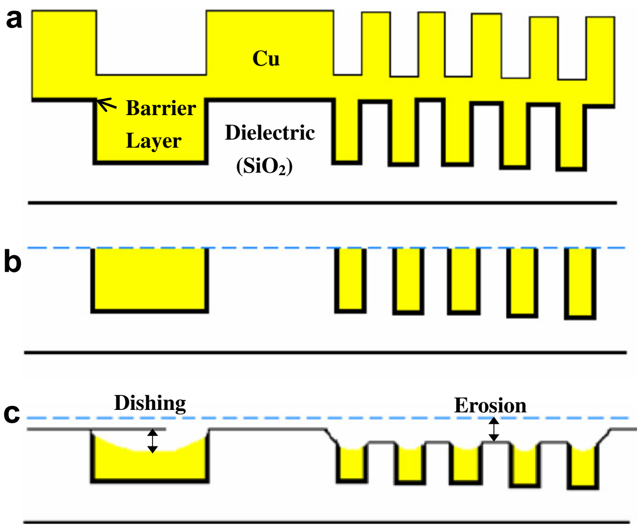

Fig. 1. Schematics of a single layer Cu interconnect: (a) before polishing, (b) ideal case after polishing and (c) real case after polishing.

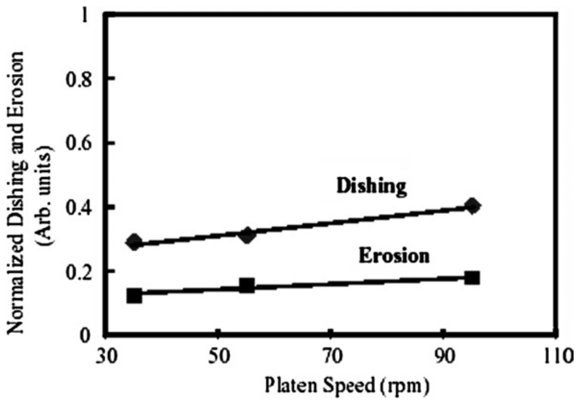

Fig. 2a. Dependence of copper dishing and oxide erosion on platen speed. Wafer pressure was kept constant [17].

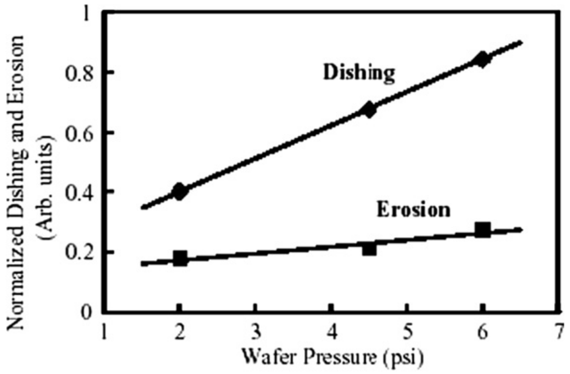

Fig. 2b. Dependence of copper dishing and oxide erosion on wafer pressure. Platen speed was held constant [17].

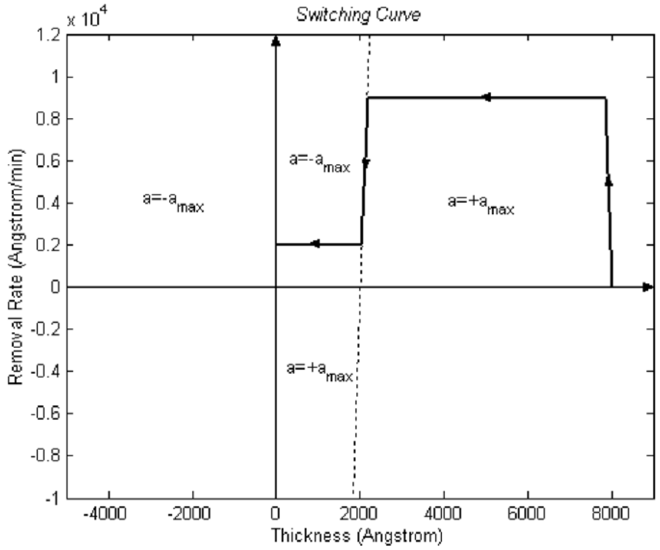

Fig. 3. Trajectory for $RR_{max} = 9000$ Å/min, $H_{small} = 2000$ Å, and $RR_{small} = 2000$ Å/min [10].

Lin and Chi [11] employed the sliding-mode control to set the operation profile of CMP process through “Dynamic Tuning” method to enable the CMP process behave closer to the soft landing. However, the experimental verification may be hard to carry out because of the continuous time control and the lack of available operation mechanism. Hence, the dynamic programming control will be employed to deal with the discrete time control. Dynamic programming was developed by Bellman and his colleagues in the 1950s [12]. The method of dynamic programming will be explained in Appendix A of this paper. It has the advantage of dealing with constrained inputs. That means the problem of available operation mechanism can be solved for constrained inputs and multiple finite stages CMP. Experiments based on dynamic programming were carried out in this research for both $SiO_2$and Cu blanket wafers.

In this paper, the removal rate representation will be presented in Section 2. In Section 3, the simulation results via dynamic programming will provide the basis of dynamic programming of wafer pressure and platen speed as part of recipe for CMP tool. The experimental results for CMP operation via dynamic programming were obtained and discussed in Section 4. Section 5 is for conclusion.

2. Removal rate representation

In this work, the equation proposed by Luo et al. [9] will be employed, that is

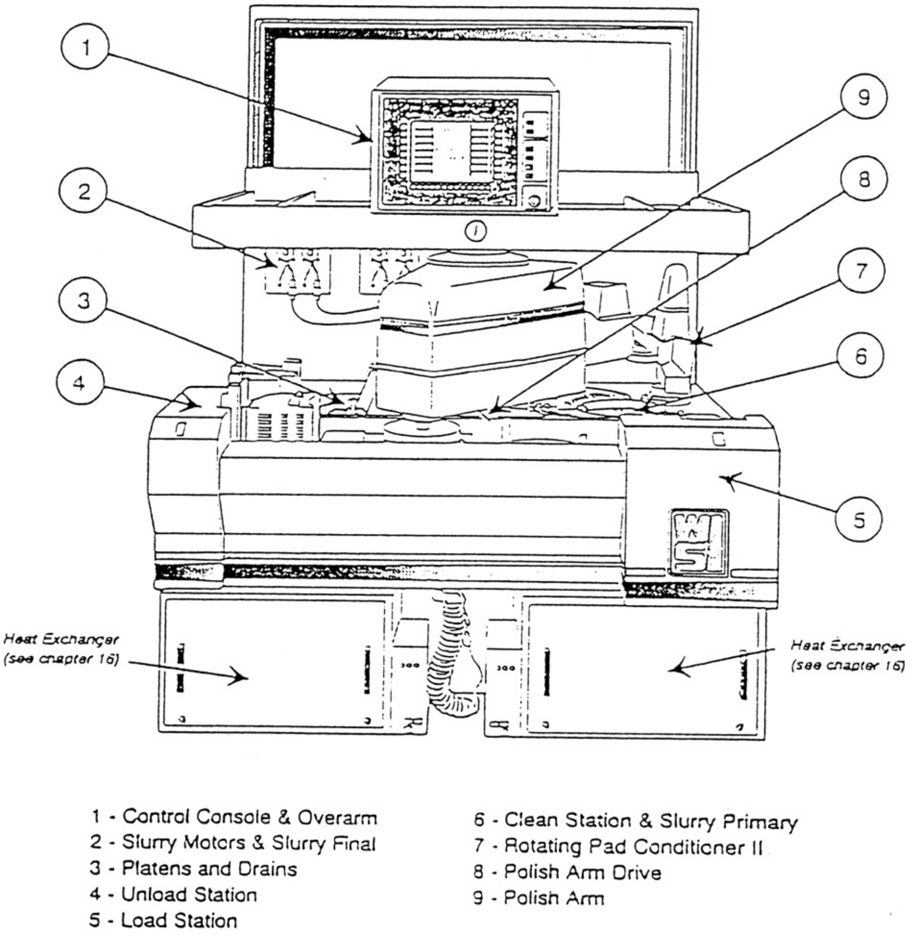

Fig. 4. The perspective front-view of CMP system – Westech 372M tool (source of information: Westech 372M operator manual).

$$\mathrm{RR} = C_2\left(1 - \Phi[3 - C_1 P_0^{1/3}]\right)\sqrt{P_0}V + \mathrm{RR_C},$$

where RR denotes the removal rate; P_0 is applied wafer pressure; V is the angular velocity of wafer carrier and the pad platen; Φ is normal cumulative distribution function; C_1 and C_2 are constants representing the properties of abrasives, pad and wafer; $\mathrm{RR_C}$ is material removal due to chemical reaction.

2.1. SiO_2 wafer CMP process

In SiO_2 wafer CMP process the material removal due to chemical reaction, $\mathrm{RR_C}$, is small compared with the mechanical removal but the material removal due to chemical etch in Cu wafer CMP process may need to be considered for more accurate results. Therefore, we ignored the chemical etch effect in the simulation of SiO_2 wafer CMP process. Furthermore, we modified the power of V from 1 to 6/10 which is based on Tsai's thesis [13] and the value of V is the platen speed of wafer carrier and pad platen. The experiments were carried out on the Westech 372M CMP tool as shown in Fig. 4. Experimental samples were prepared on p-type, (100)-oriented, 6 in. (150 mm) diameter silicon wafers. The thermally grown silicon dioxide film was obtained by wet oxidation (ASM/LB45 furnace system), in which the silicon was exposed to an ambient of H_2 and O_2 at 980 °C. The polishing sample for blanket SiO_2 wafer CMP experiment is a SiO_2 film layer grown to 9000 Å thickness by this furnace system. The structure of the SiO_2 blanket wafer is shown in Fig. 5. Two sets of experimental removal rate results are used to solve for the values of C_1 and C_2 by means of an iteration method of trial and error and the removal rate can be written as

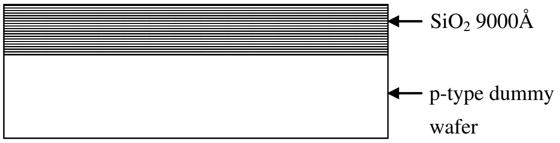

Fig. 5. The Structure of SiO_2 blanket wafer.

$$\mathrm{RR} = 8257\left(1 - \Phi[3 - 0.322 P_0^{1/3}]\right)\sqrt{P_0}V^{(6/10)}.$$

Fig. 6 shows the model prediction and experimental observations of the effects of the wafer pressure and platen speed.

2.2. Cu wafer CMP process

The experimental samples were prepared on p-type, (100)-oriented, 6 in. (150 mm) diameter silicon wafers. The thermally grown silicon dioxide film was obtained by wet oxidation (ASM/LB45 furnace system), in which the silicon was exposed to an ambient of H_2 and O_2 at 980 °C. The polishing sample for blanket Cu wafer in CMP experiment is a two-layer film structure of Cu/Ta with thickness of 20,000/500 Å sputter deposited by ULVAC SBH-3308 RDE sputter system on the silicon wafer which is covered with a 1000 Å thick thermally grown SiO_2 film. The under layer of 500 Å Ta is used as an adhesion promoter for the copper deposition since copper itself does not adhere well on the thermal oxide. The structure of the Cu blanket wafer is shown in Fig. 7. Two sets of experimental removal rate results are used to solve for the values of C_1 and C_2 as we did for the SiO_2

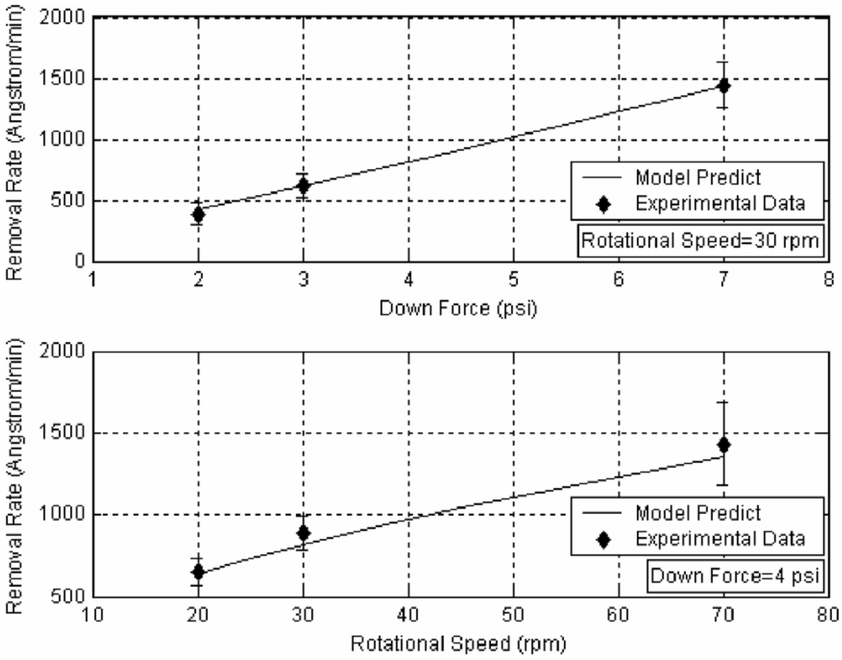

Fig. 6. The model prediction and experimental observations of the effects of the wafer pressure and platen speed for SiO_2 blanket wafer.

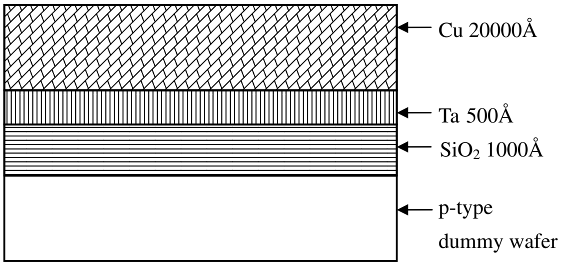

Fig. 7. The structure of Cu blanket wafer.

wafer CMP process. Furthermore, we adopted the original power of V to 1 based on our experimental data. Platen speed and carrier speed were all equal to the platen speed, V. The only difference was that we had to consider the chemical etching rate in the equation. The chemical etching rate was obtained by experiment and the procedure was presented in Section 4.2. The measured etching rate was about 14 Å/min. It is quite small compared to the overall removal rate. The main reason was that we added a higher concentration of citric acid. According to Liu's thesis [14], as the concentration of citric acid in the HNO_3-citric acid slurry increased, the etching rate of copper in the HNO_3-citric acid slurry was suppressed. The citric acid behaves like BTA (Benzotriazole) in preventing copper corrosion in the HNO_3-based solution. The BTA is a common Cu corrosion inhibitor since it can be absorbed on Cu surface to form a passivation layer. It is helpful to a Cu damascene structure because of the low etching rate at the recessed region of the Cu film. Furthermore, the removed thickness was only 6000 Å, hence we hoped that the chemical removal rate was not too high. Therefore, we omitted the chemical removal rate here. Thus, the removal rate representation will be

$$\mathrm{RR} = 30,503\left(1 - \Phi[3 - 0.0113 P_0^{1/3}]\right)\sqrt{P_0}V$$

Fig. 8 shows the model prediction and experimental observations of the effects of the wafer pressure and platen speed.

3. Simulation via dynamic programming

3.1. Design

From Larson and Casti [15], the procedure of dynamic programming can be concluded into three steps. First, calculate the equivalent discrete time domain state equation which describes the CMP process; second, determine the cost function in order to compute the minimum cost and find the optimal control inputs; the final procedure is the iterative computation. We used a very simple concept to obtain the state space model of removal rate for our simulation. The differential equation of the thickness being polished is equal to the removal rate and we made the removal rate to be the input. The equation is written as

$$\dot{h} = \frac{\mathrm{d}h}{\mathrm{d}t} = -\mathrm{RR} = -u$$

where h is the thickness, RR the removal rate, u the input. We assumed that there were only seven values of the input (include 0) because of restrictions on the Westech 372M CMP tool and the sampling period T here was fixed to 1 s. The cost function L was determined as

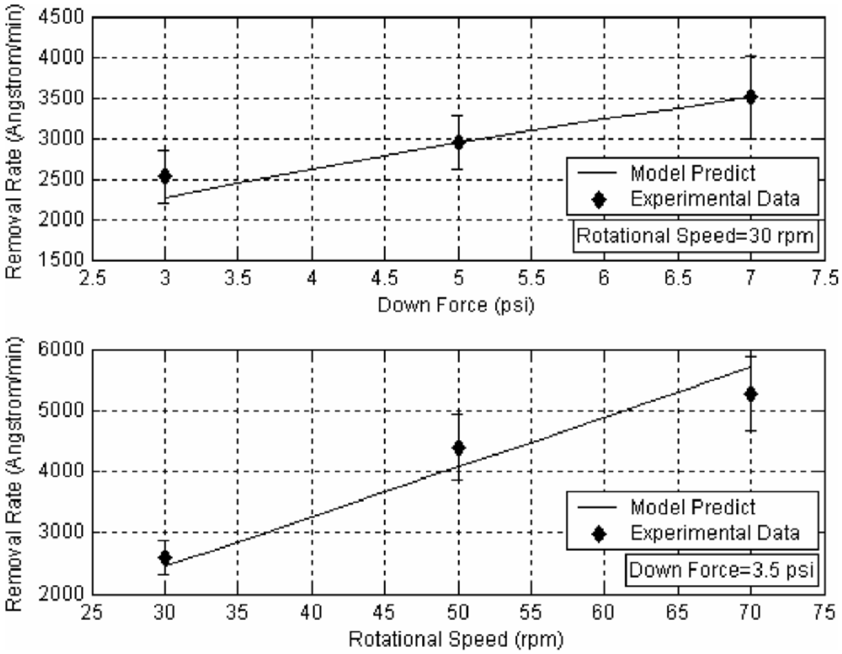

Fig. 8. The model prediction and experimental observations of the effects of the wafer pressure and platen speed for Cu blanket wafer.

$$\mathrm{L} = \frac{1}{2} q h^2(k) + \frac{1}{2} r u^2(k) + \frac{1}{2} s h_N^2$$

where k is the stage, N is the final stage, q is the weighting factor of transient state, r is the weighting factor of input, and s is the weighting factor of final state. The weighting factor of transient state means the penalty factor for the speed of approaching to the final state. The weighting factor of admissible input means the penalty factor for translational wafer pressure and rotational torque provided to CMP tool. The last weighting factor s of final state means the penalty factor for final state which describes the extent of under-polishing. In this study, we want the admissible input to decrease slowly based on the concept of soft landing operation which was proposed by Chiu et al. [10]. The values of these weighting factors were determined by an iteration method of trial and error to get successive decrease pattern of admissible inputs which also minimize the cost function L.

3.2. Simulation results

3.2.1. SiO_2 wafer CMP process

As shown in Fig. 6, the error bars means the non-planarization index (the standard deviation of the removal rates of the nine points on the wafer). The smaller the non-planarization index, the more uniform removal rate

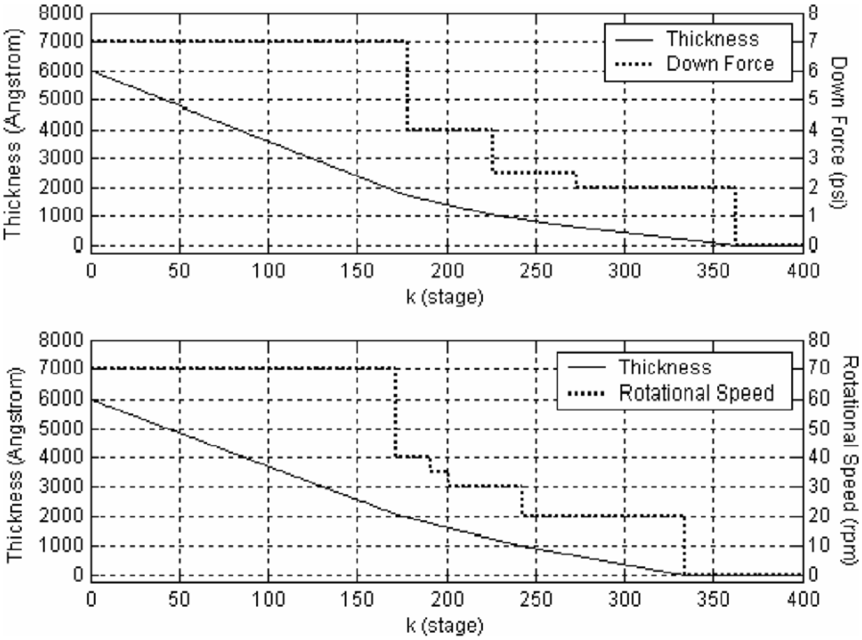

Fig. 9. Simulation result of SiO_2 blanket wafer when the wafer pressure and platen speed as the variable input separately (1 stage = 1 s).

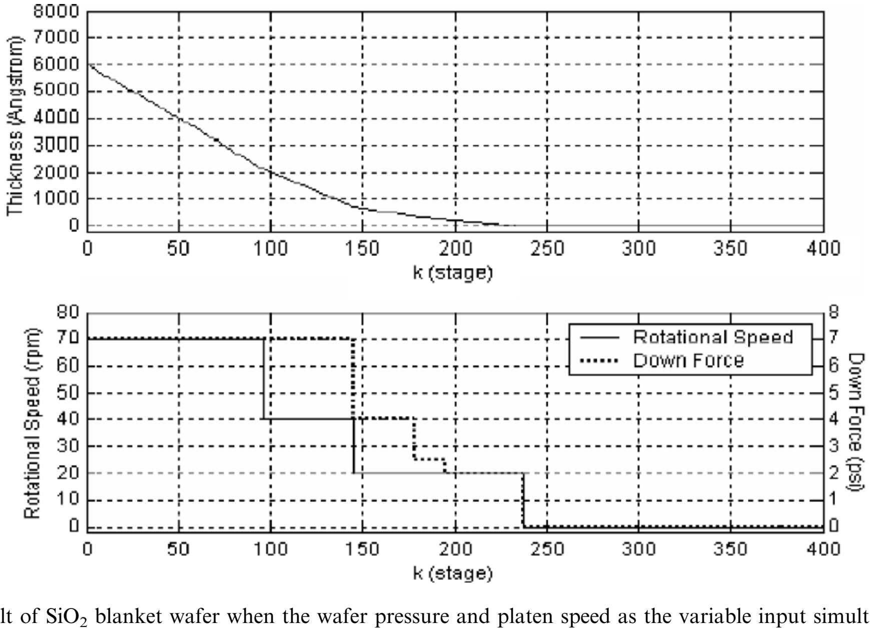

Fig. 10. Simulation result of SiO_2 blanket wafer when the wafer pressure and platen speed as the variable input simultaneously (1 stage = 1 s).

on the entire wafer and it results in more flat surface. Decreasing the wafer pressure or platen speed will decrease the non-planarization index. In order to reduce the wafer pressure or platen speed successively, we choose the weighting factors of final state, transient state and input to be 10000, 1 and 100000, respectively for the case of wafer pressure, and 10000, 1 and 700 for the case of platen speed. For the case of wafer pressure, the platen speed was held at 30 rpm. The initial thickness h(0) was 6000 Å, the result is shown in Fig. 9. According to the result, the process terminated at the 363th stage and the input is 7 psi during 0–177th stage, 4 psi during 178–225th stage, 2.5 psi during 226–272th stage and 2 psi during 273–362th stage. It was the basis of our SiO_2 wafer experiment on wafer pressure. For the case of platen speed, the wafer pressure was held at 4 psi and the result is also shown in Fig. 9.

At the beginning of the CMP process, we hoped that the removal rate was high enough to reduce the time of process and also obtained more flat surface at the end of the process. According to Chen's thesis [16], the platen speed has a great influence on the non-uniformity. For these reasons, we attempted to apply both inputs. We chose the weighting factors of final state, transient state, wafer pressure and platen speed to be 10000, 1,50000 and 1000, respectively. The result of dynamic programming is shown in Fig. 10.

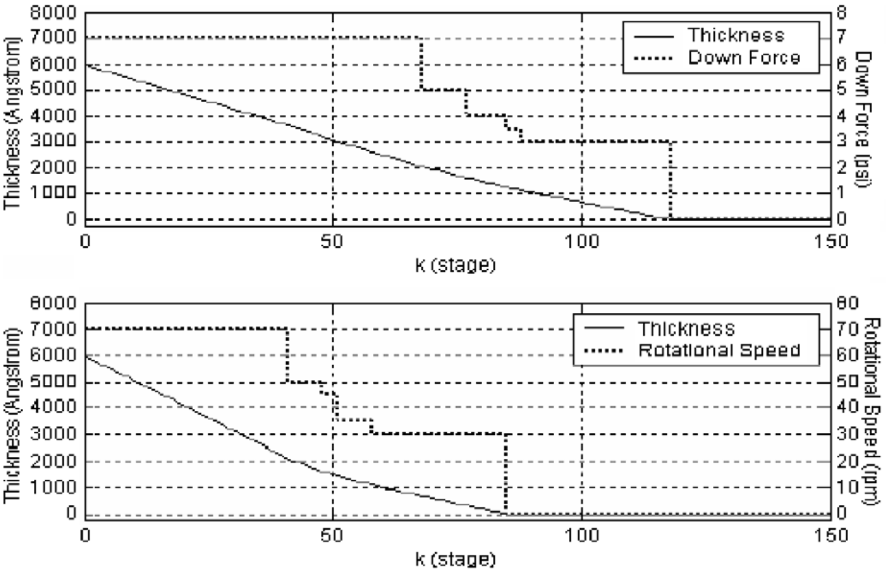

Fig. 11. Simulation result of Cu blanket wafer when the wafer pressure and platen speed as the variable input separately (1 stage = 1 s).

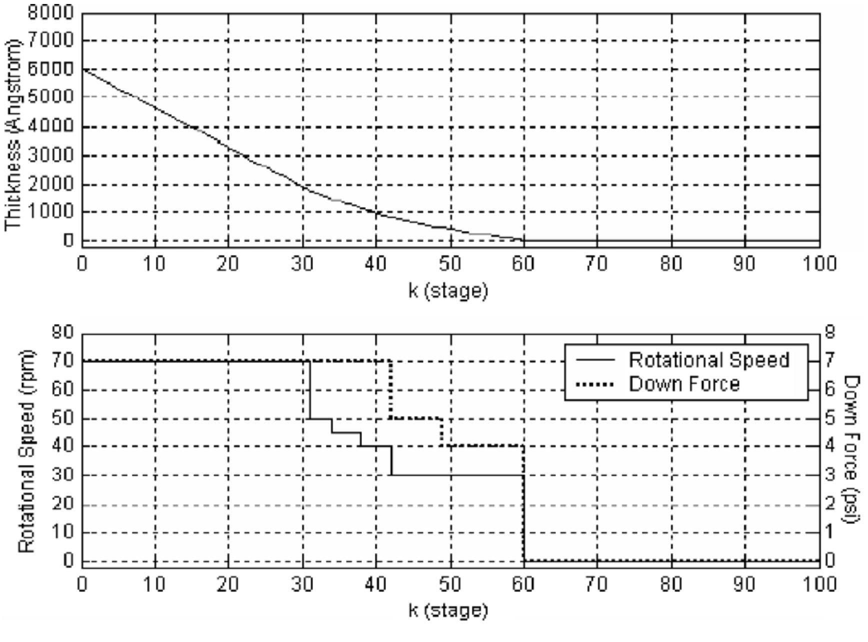

Fig. 12. Simulation result of Cu blanket wafer when the wafer pressure and platen speed as the variable input simultaneously (1 stage = 1 s).

The platen speed is decreased first in order to get better non-planarization index when the SiO_2 film thickness is about 2000 Å and followed by the wafer pressure. (The definition of non-planarization index is shown in Section 4.)

3.2.2. Cu wafer CMP process

In order to decrease the wafer pressure or platen speed in the same manner as SiO_2 wafer, we choose the weighting factors of final state, transient state and input to be 10000, 1 and 40000, respectively for the case of wafer pressure, and 10000, 1 and 1200 for the case of platen speed. For the case of wafer pressure, the platen speed was held at 30 rpm. For the case of platen speed, the wafer pressure was held at 3.5 psi. The initial thickness h(0) was 6000 Å and the result is shown in Fig. 11.

As we know that dishing and erosion are proportional to the pressure and platen speed [17], we expected that decreasing the wafer pressure and platen speed would reduce the dishing and erosion of Cu wafer and also obtain better non-planarization index at the end of the process. Nevertheless, only the Cu blanket wafer experiment was done due to lack of Cu pattern wafers. We chose the weighting factors of final state, transient state, wafer pressure and platen speed to be 10000, 1,20000 and 1200, respectively. The result of dynamic programming is shown in Fig. 12.

4. Experiment for SiO_2 and Cu blanket wafer

The experiments were carried out on the IPEC 372M CMP polisher. The slurry formulation of SiO_2 wafer CMP process was prepared by diluting the commercial slurry, Cabot SS-25, with DI water in the ratio of one to one. The copper wafers were polished with a slurry of 2 wt% alumina abrasive, 2 vol% HNO_3 and 0.01 M citric acid slurry.

The CMP removal rates were monitored at nine points along two perpendicular diameters on the entire wafer and the within-wafer non-planarization index is defined as:

$$\text{Non}-\text{planarization index} = \left(\frac{1}{n-1}\sum_{i=1}^{n}(x_i-\bar{x})^2\right)^{\frac{1}{2}}$$

Table 2
Slurry formulation of SiO_2 CMP

	Species	Concentration
Commercial slurry	Cabot SS-25	50 vol%
Dilution	DI water	50 vol%

where x is the removed thickness and $\bar{x}$ is the average removed thickness.

4.1. SiO_2 wafer CMP experiment

The experiments with dynamic programming were compared with the experiments which removed the same thickness at the same duration of polishing with constant removal rate operation. Since the removed thickness and duration of polishing were known, we can compute the value of constant removal rate. The base recipe process parameters for the constant removal rate were found through experiment and are listed in Tables 1 and 2. The experimental results are listed in Table 3.

4.1.1. Change wafer pressure as the admissible input

The duration of polishing was 363 s and the removed thickness was 6000 Å. The required removal rate was 992 Å/min. Because of the fixed platen speed here, the required removal rate was found by changing the wafer pressure to be 4.3 psi. From the experimental results which were listed in Table 3, the constant removal rate operation mode has the better thickness removal but the dynamic programming operation mode possesses 39% better non-planarization index. The model prediction error on the lower wafer pressure caused the inaccuracy of thickness removal. It could be improved by developing more accurate model.

4.1.2. Change platen speed as the admissible input

The duration of polishing was 334 s and the removed thickness was 6000 Å. The required removal rate was 1078 Å/min. Because of the fixed wafer pressure here, the required removal rate was found by changing the platen speed to be 40 rpm. Table 3 revealed the similar phenomenon to the part of wafer pressure. The dynamic program-

Table 1
Process parameters of SiO_2 CMP experiment (constant removal rate base recipe)

Fixed parameter	Base recipe value for wafer pressure as variable input in Fig. 9	Base recipe value for platen speed as variable input in Fig. 9	Base recipe value for both wafer pressure and platen speed as variable inputs in Fig. 10
Wafer pressure	4.3 psi	4.0 psi	4.7 psi
Back Pressure	1 psi	1 psi	1 psi
Carrier speed	30 rpm	40 rpm	52 rpm
Platen speed	30 rpm	40 rpm	52 rpm
Polish time	363 s	334 s	237 s
Slurry flow rate	150 ml/min	150 ml/min	150 ml/min
Pre-wet pad speed	28 rpm	28 rpm	28 rpm
Pre-wet duration	10 s	10 s	10 s
Pre-wet flow rate	300 ml/min	300 ml/min	300 ml/min
Pad	Rodel IC1400	Rodel IC1400	Rodel IC1400

Table 3
SiO_2 wafer experimental result with three kind of admissible inputs via dynamic programming operation

	Average removed thickness (Å)	Thickness removal error from 6000 Å (%)	Non-planarization index (Å)	Non-planarization index improvement (%)
Wafer pressure	5499 Å (5899 Å)	−8.35 (−1.68)	435 Å \(717 Å)	39
Platen speed	6113 Å (5914 Å)	1.88 (−1.43)	518 Å (697 Å)	26
Simultaneously	5875 Å (5957 Å)	−2.08 (−0.72)	487 Å (580 Å)	16

The values in brackets belong to the constant removal rate operation.

Table 4
Process parameters of Cu CMP experiment (constant removal rate base recipe)

Fixed parameter	Base recipe value for wafer pressure as variable input in Fig. 11	Base recipe value for platen speed as variable input in Fig. 11	Base recipe value for both wafer pressure and platen speed as variable inputs in Fig. 12
Back pressure	1 psi	1 psi	1 psi
Wafer pressure	5.1 psi	3.5 psi	4.9 psi
Carrier speed	30 rpm	50 rpm	57 rpm
Platen speed	30 rpm	50 rpm	57 rpm
Polish time	118 s	85 s	60 s
Slurry flow rate	150 ml/min	150 ml/min	150 ml/min
Pre-wet pad speed	28 rpm	28 rpm	28 rpm
Pre-wet duration	10 s	10 s	10 s
Pre-wet flow rate	300 ml/min	300 ml/min	300 ml/min
Pad	Rodel IC1400	Rodel IC1400	Rodel IC1400

Table 5
Slurry formulation of Cu CMP

	Species	Concentration
Abrasive	Al_2O_3 (EXTEC 0.1 μm)	2 wt%
Oxidizer	HNO_3	2 vol%
Complex agent	Citric acid	0.01 M
Dilution	DI water	Remaining balance of slurry

ming operation mode possesses 26% better non-planarization index. The thickness removal was over 6000 Å for dynamic programming because the model prediction was lower than the experimental data on the higher platen speed.

4.1.3. Change wafer pressure and platen speed as the admissible inputs simultaneously

The duration of polishing was 237 s and the removed thickness was 6000 Å. The required removal rate was 1519 Å/min. In order to avoid one-sided emphasis of these two inputs, we simultaneously increased the wafer pressure and platen speed. The final value was found to be 4.7 psi and 52 rpm, respectively. The thickness removal had a little improvement and this might be caused by combining complimentary model prediction error from both platen speed model and wafer pressure model. Nevertheless, the dynamic programming operation still possessed 16% better non-planarization index.

4.2. Cu wafer CMP experiment

We will explain how to calculate the removal rate due to chemical reaction first. The experiment for calculating the removal rate due to chemical reaction was carried out in a circular glass container. Because the slurry was not well stirred, we put a magnet at the bottom of the container to produce the flow of the slurry in order to keep the reaction rate at the surface stable. It also dispersed the abrasive to suspend in the slurry and made the experiment be closer to the real circumstance of polishing. The surface of Cu wafer faced with the magnet and kept a distance with the magnet. We set the time to immerse the wafer in the slurry to 5 min and assumed that the concentration of the slurry was constant during chemical reaction. The base recipe process parameters for the constant removal rate were found through experiment and are listed in Tables 4 and 5. The experimental results are listed in Table 6.

The same comparison between dynamic programming and constant removal rate were done as we did for the

Table 6
Cu wafer experimental result with three kind of admissible inputs via dynamic programming operation

	Average removed thickness (Å)	Thickness removal error from 6000 Å (%)	Non-planarization index (Å)	Non-planarization index improvement (%)
Wafer pressure	7491 Å (6721 Å)	24.85 (12.02)	1204 Å (1225 Å)	2
Platen speed	5406 Å (5948 Å)	−9.9 (−0.87)	615 Å (806 Å)	24
Simultaneously	6814 Å (5772 Å)	13.57 (−3.8)	1034 Å (1153 Å)	10

The values in brackets belong to the constant removal rate operation.

SiO_2 wafer CMP experiment. The parameters for the constant removal rate were also found through experiment.

4.2.1. Change wafer pressure as the admissible input

The duration of polishing was 118 s and the removed thickness was 6000 Å. The required removal rate was 3051 Å/min. Because of the fixed platen speed here, the required removal rate was found by changing the wafer pressure to be 5.1 psi. From the experimental results which were listed in Table 6, the constant removal rate operation has better thickness removal but the dynamic programming operation possesses a little better non-planarization index. However, the difference of non-planarization index between dynamic programming operation and constant removal rate operation is very small and it can be considered within statistical error of experimental data. It also shows that the wafer pressure is not a major factor to influence the non-planarization index in Cu wafer CMP. As shown in Fig. 8, we see that the non-planarization index data under 3 psi and 5 psi is within statistical error with each other. This explains why there is no degradation in non-planarization index when the wafer pressure is decreased from 5.1 psi to 3 psi, i.e., there is no degradation in non-planarization index when Cu wafer CMP process is changed from constant removal rate operation mode to dynamic programming operation mode. The inaccuracy of removed thickness may be caused by the lower predicted value of removal rate on the smaller wafer pressure. It means that the model for Cu wafer CMP process needs to be modified.

4.2.2. Change platen speed as the admissible input

The duration of polishing was 85 s and the removed thickness was 6000 Å. The required removal rate was 4235 Å/min. Because of the fixed wafer pressure here, the required removal rate was found by changing the platen speed to be 50 rpm. Table 6 shows that the dynamic programming operation is 24% better than the constant removal rate operation in terms of non-planarization index. The error of the removed thickness may be caused by higher predicted value of removal rate at faster platen speed and lower predicted value of removal rate at slower speed, there was not enough time to remedy lower removal rate at slower platen speed by higher removal rate at faster platen speed. Therefore removal thickness of dynamic programming operation mode is less than that of constant removal rate operation mode. However, it made a significant improvement of non-planarization index through dynamic programming operation of platen speed. This shows platen speed is a major parameter affecting the non-planarization index of Cu wafer CMP process.

4.2.3. Change wafer pressure and platen speed as the admissible inputs simultaneously

The duration of polishing was 60 s and the removed thickness was 6000 Å. The required constant removal rate was 6000 Å/min. We simultaneously increased the wafer pressure and platen speed to be 4.9 psi and 57 rpm, respectively. The dynamic programming operation still provides 10% improvement of non-planarization index than constant removal rate operation.

4.3. Discussion

Three cases of CMP process to use wafer pressure, platen speed and both wafer pressure and platen speed as admissible inputs were examined in this study. In the SiO_2 wafer CMP experiment, the non-planarization indexes of three cases were all improved and the errors of the removed thickness were within 8%. The model could predict the removal rate well. It illustrated that the multi-step dynamic programming of SiO_2 wafer CMP was feasible to implement. It could further be verified by experiment on IPEC 372M CMP tool.

Slurry chemicals play an important role in the Cu wafer CMP process. The formation of a non-native passivation layer by the passivating chemical (e.g., citric acid) in the slurry, the dissolution of Cu or the abraded materials by abrasives from surface layer are all determined by the chemical environment in the slurry [18]. In the Cu wafer CMP experiment, the result shows that the platen speed is the main factor to influence non-planarization index. When we made the platen speed change, non-planarization index improved 10% at least. It means that the higher the platen speed, the faster the refresh rate of the slurry underneath the wafer and the larger the removal rate. It may also cause worse non-uniformity of the slurry to transport on the entire wafer and influence the non-uniformity of the removal rate. For this reason, the interactions between mechanical and chemical parameters need to be investigated more thoroughly. This also indicated that the current model was not sufficient to describe the entire Cu wafer CMP process. The errors in thickness removal fall between 14% and 25%. There are two ideas to reduce the error in thickness removal. The first way was to modify the model and make it more comprehensive and complete by including interaction between mechanical polishing and chemical reaction. The second way was to get more removal rate data corresponding to every value of the admissible input by experiment to obtain higher degree polynomials regression model.

In the case of both SiO_2 and Cu CMP, we observed that both Tables 3 and 6 reveal that dynamic programming operation performs better than constant removal rate operation in terms of minimizing non-planarization index.

From the removal rate model for SiO_2 wafer in Fig. 6, the standard deviation (or NPI) of removal rate are smaller for lower wafer pressure and platen speed. It means lower wafer pressure and platen speeds generates smaller NPI or better planarization results as is reported in Table 3 for SiO_2 wafer. The relative improvement in standard deviation of removal rate (or relative improvement in NPI) from higher wafer pressure and platen speeds to lower wafer pressure and platen speeds is obvious in Fig. 6 for SiO_2 wafer.

From the removal rate model for Cu wafer in Fig. 8, the standard deviation (or NPI) of removal rate are smaller for lower wafer pressure and platen speed. It means lower wafer pressure and platen speeds generates smaller NPI or better planarization results as is reported in Table 6 for Cu wafer. The relative improvement in standard deviation of removal rate (or relative improvement in NPI) from higher wafer pressure and platen speeds to lower wafer pressure and platen speeds is obvious in Fig. 8 for Cu wafer.

The relative trend of improvement of standard deviation (or NPI) for SiO_2 wafer in Fig. 6 stands out more than the relative trend of improvement of standard deviation (or NPI) for Cu wafer in Fig. 8. This also predicts the benefits of dynamic programming operation on NPI improvements for SiO_2 wafer will also stand out more than Cu wafer.

The standard deviation of removal rate data for SiO_2 wafer in Fig. 6 is smaller than the standard deviation of removal rate data for Cu wafer in Fig. 8. This explains the fact that the percentage value of thickness removal error for SiO_2 wafer is smaller in Table 3 than that of thickness removal error for Cu wafer in Table 6 due to smaller numerator in percentage computation. This also explains the fact that the percentage value of NPI improvement for SiO_2 wafer is larger in Table 3 than that of NPI improvement for Cu wafer in Table 6 due to smaller denominator in percentage calculation.

To get better performance for both global planarization and thickness removal, we recommend that planarization step and overpolish step in SiO_2 and Cu CMP should use different mode of operation, i.e., dynamic programming operation during planarization step for minimizing non-planarization index and constant removal rate operation during overpolish step for minimizing thickness removal error. The incremental time calculation in overpolish step can be done using the thickness error and removal rate derived from Luo's removal rate model based on constant wafer pressure and platen speed at the end of planarization step.

5. Conclusions and future work

5.1. Conclusions

In this study, we focused on the mechanical parameters of CMP process. The wafer pressure and platen speed were taken as the control parameters. We applied the control method of dynamic programming to carry out experiment for CMP process with blanket SiO_2 and Cu wafers. The influence of dynamic programming operation and constant removal rate operation on the non-planarization index for CMP process were compared carefully. We arrived at the following conclusions:

(1) The non-planarization index could be improved consistently by dynamic programming operation versus constant removal rate operation. The dynamic programming operation has 2% to 39% improvement over the base recipe of constant removal rate in all experiments as shown in Tables 3 and 6.

(2) The thickness removal error is consistently smaller by constant removal rate operation versus dynamic programming operation in all experiments as shown in Tables 3 and 6.

(3) To get the best performance of both planarization and thickness removal, it is recommended that planarization step and overpolish step in SiO_2 and Cu CMP should use different mode of operation, i.e., dynamic programming operation during planarization step for minimizing non-planarization index and constant removal rate operation during overpolish step for minimizing thickness removal error. The incremental time calculation for eliminating thickness removal error during overpolish step can be done using the thickness error and removal rate derived from Luo's removal rate model based on constant wafer pressure and platen speed at the end of planarization step.

(4) The platen speed is a more consistent factor to influence the non-planarization index (about 25% improvement over base recipe of constant removal rate) during planarization step using dynamic programming operation as shown in Tables 3 and 6. The removal thickness error (about 1%) is also minimum in overpolish step using constant removal rate operation by constant platen speed and wafer pressure as shown in the third row of Tables 3 and 6.

(5) In SiO_2 CMP, dynamic programming of platen speed during planarization step is followed by constant removal rate operation during overpolish step using platen speed of 20 rpm and wafer pressure of 4.0 psi.

(6) In Cu CMP, dynamic programming of platen speed during planarization step is followed by constant removal rate operation during overpolish step using platen speed of 30 rpm and wafer pressure of 3.5 psi.

(7) Best known method (BKM) for CMP planarization is recommended to use dynamic programming operation of platen speed for coarse control of non-planarization index during planarization step and use constant removal rate operation via constant platen speed and wafer pressure at the end of planarization step for fine control of thickness removal error during overpolish step.

5.2. Future work

Experimental verification of dynamic programming operation needs to be carried out on pattern wafers in the future for different kinds of pattern wafers. The influence on copper dishing and oxide erosion can be compared between dynamic programming and constant removal rate operation. It is conjectured that using dynamic planning operation in planarization step and constant removal rate operation in overpolish step with minimum platen speed

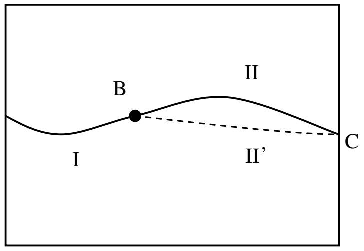

Fig. A.1. Illustration of the principle of optimality.

and/or wafer pressure will minimize the copper dishing and oxide erosion according to experimental results in Fig. 2aa and Fig. 2bb reported by K. Wijekoon and S. Tsai etc. [17].

Appendix A. Optimal control design: dynamic programming

Sociological, economic, and physical pressures in all areas of modern life have generated an accelerated demand for high-level decision-making based upon limited information about the processes being controlled. In 1950s, a systematic and concerted mathematical study of such decision-making situations was initiated by Richard Bellman. This pioneering work was based upon the fundamental system-theoretic notion of feedback, i.e., that decision rules should be based upon the current (and perhaps past) states of the process under study. Bellman and his colleagues continued to develop the feedback decision-making concept under the name of "dynamic programming". The majority of problems of true practical concern were computationally intractable due to the limited state of the computing art at that time. As time goes on, a combination of rapid progress in computer technology, coupled with the development of refined computational procedures, has made it practical for solving a wide variety of problems in economics, engineering, operations research, and mathematics, itself.

A.1. Bellman's principle of optimality

The fundamental concept of dynamic programming originated by Bellman is called the principle of optimality. This principle may conceptually be thought as follows: given an optimal trajectory from point A to point C, the portion of the trajectory from any intermediate point B to point C must be the optimal trajectory from B to C. In Fig. A.1, if the path I–II is the optimal path from A to C, then according to the principle of optimality path II is the optimal path from B to C. The proof by contradiction for this case is immediate: Assume that some other path, such as II′, is the optimum path from B to C, then path I–II′ has less cost than path I–II. However, this contradicts the fact that I–II is the optimal path

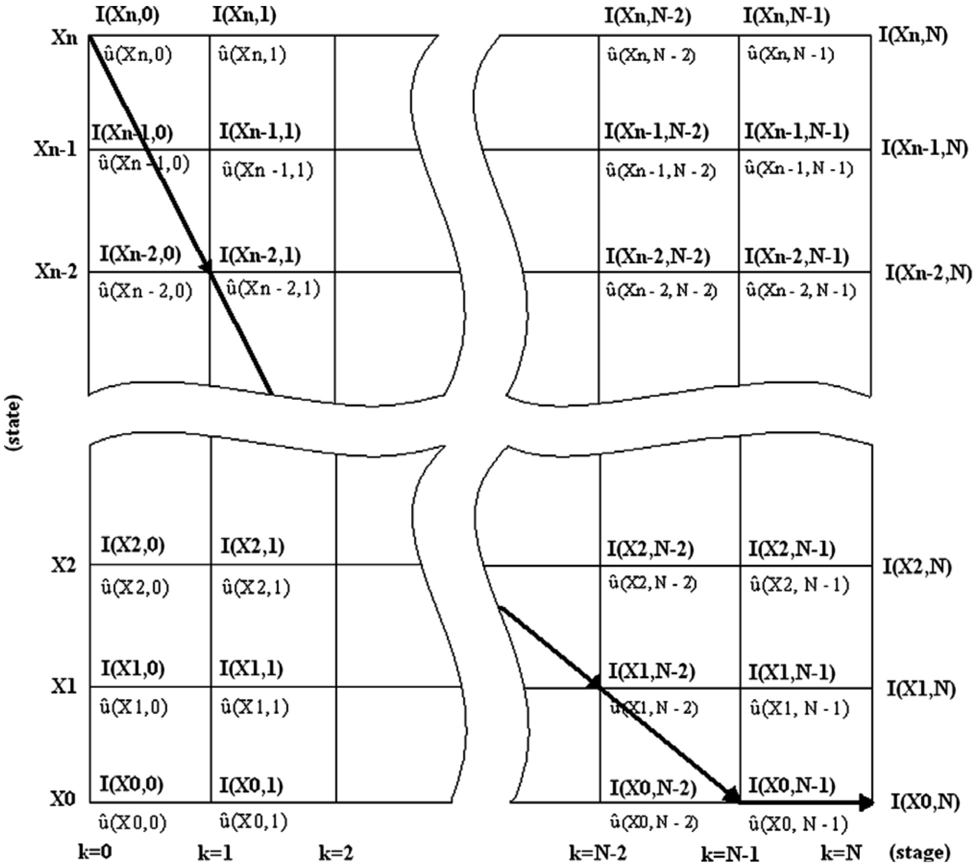

Fig. A.2. Complete result of dynamic programming and recovery of the optimal trajectory from initial state x(0).

from A to C, and hence II must be the optimal path from B to C.

A.2. Dynamic programming

Consider a quantized state $x \in X$, at stage $(N-1)$. At this state, each of the admissible decisions $u^{(m)} \in U$ is applied.

$$X = [x^1 x^2 \ldots x^{n-1} x^n], \quad U = [u^1 u^2 \ldots u^{M-1} u^M]$$

For each of these decisions the cost at the current stage can be determined as

$$\mathrm{L}^{(m)} = \mathrm{L}[x, u^{(m)}, N-1] \quad (m = 1, 2, \ldots, M)$$

Next, for each of these decisions, the next state at stage N is determined from the system equation,

$$x^{(m)}(N) = \mathrm{g}[x, u^{(m)}, N-1] \quad (m = 1, 2, \ldots, M)$$

The next step is to compute the minimum cost at stage N for each of the states $x^{(m)}$. However, in general, a particular state $x^{(m)}$ will not lie on one of the quantized states $x \in X$ at which the optimal cost $\mathrm{I}(x,N)$ is defined. In fact, it may lie outside of the range of admissible states. In the latter case the decision is rejected as a candidate for the optimal decision for this state and stage. If a next state x(m) does fall within the range of allowable states, but not on a quantized value, then it is necessary to use some type of interpolation procedure to compute the minimum cost function at these points.

Assume that the values of the minimum cost at the states x(m) can be expressed as a function of the values of the optimal cost at quantized states $x \in X$.

$$\mathrm{I}[x^{(m)}, N] = \mathrm{P}[x^{(m)}, N, \mathrm{I}(x, N)], \quad \text{all}\, x \in X$$

where $\mathrm{I}(x,N) = \mathrm{L}(x,N)$.

If, as is often the case, no decision is made at $k = N$, the final stage, and hence the cost function at N depends only on the final state, $x(N)$.

The total cost of applying decision $u^{(m)}$ at state x, stage $(N-1)$, can then be written as

$$\mathrm{F}_1^{(m)} = \mathrm{L}[x, u^{(m)}, N-1] + \mathrm{I}[x^{(m)}, N]$$

The minimization can be achieved by simply comparing the M quantities. According to the functional equation, the minimum value will be the minimum cost at state x, stage $(N-1)$.

$$\mathrm{I}[x, N-1] = \min_{u^{(m)} \in U} \left\{ \mathrm{L}[x, u^{(m)}, N-1] + \mathrm{I}[x^{(m)}, N] \right\} \tag{A.1}$$

the optimal decision at this state and stage, $\hat{u}[x, N-1]$, is the control $u^{(m)}$ for which the minimum in Eq. (A.1) is actually taken on.

This procedure is repeated at each quantized state $x \in X$ at stage $(N-1)$. When this has been done, $\mathrm{I}(x,N-1)$ and $\hat{u}[x, N-1]$ are known for all $x \in X$. It is now possible to compute $\mathrm{I}(x,\ N-2)$ and $\hat{u}[x, N-2]$ for all $x \in X$ based on knowledge of $\mathrm{I}(x,\ N-1)$.

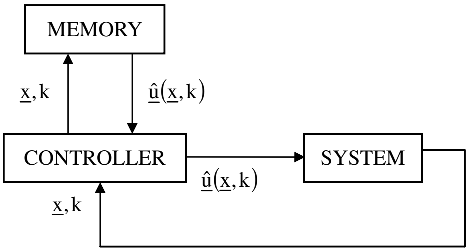

Fig. A.3. A controller based on retrieving the results of the dynamic programming computation from memory.

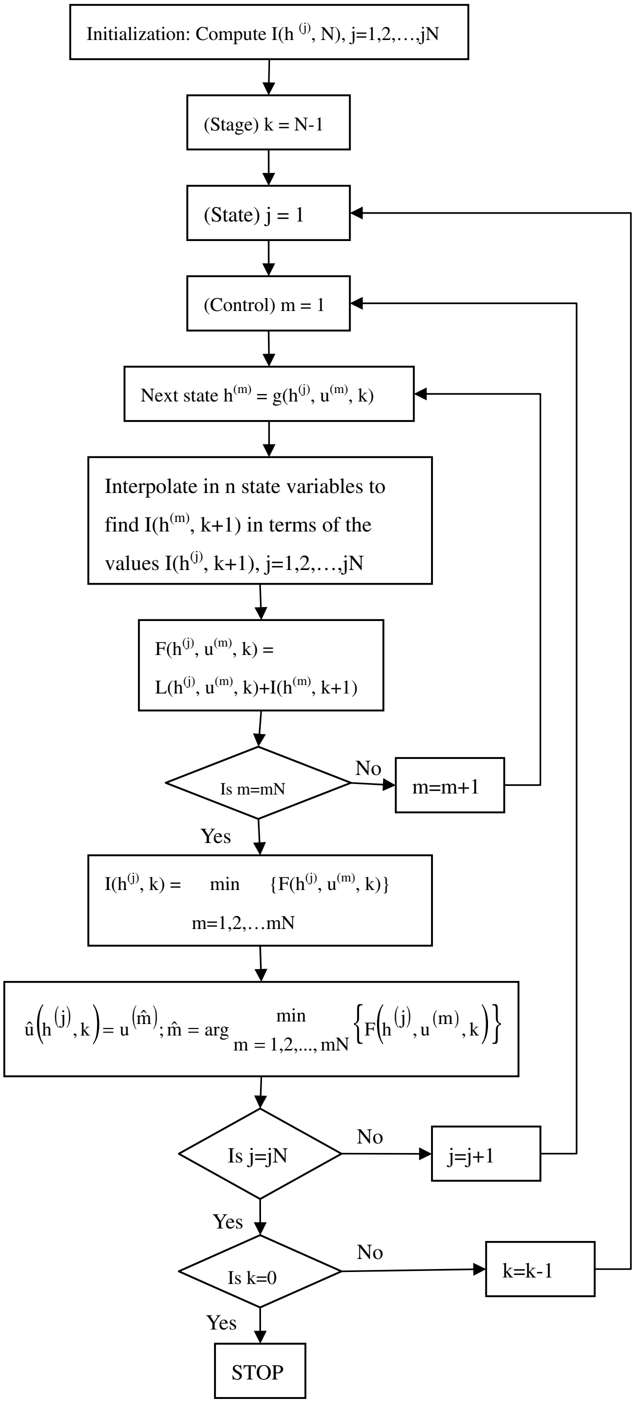

Fig. A.4. Program flowchart of dynamic programming.

The general iterative procedure continues this process. Suppose that I(x,k+1) is known for all $x \in X$. Then I(x,k) and $\hat{u}[x,k]$are computed for all $x \in X$ from

$$\mathrm{I}[x,k] = \min_{u^{(m)} \in U} \left\{ \mathrm{L}[x, u^{(m)}, k] + \mathrm{I}[x^{(m)}, k+1] \right\} \tag{A.2}$$

where $x(m)$ is determined from

$$x^{(m)} = \mathrm{g}[x, u^{(m)}, k]$$

and where I($x^{(m)}$,k+1) is computed by interpolation on the known values I(x,k+1) for all $x \in X$:

$$\mathrm{I}[x^{(m)}, k+1] = \mathrm{P}[x^{(m)}, k+1, \mathrm{I}(x, k+1)], \quad \text{all } x \in X$$

The optimal decision $\hat{u}[x,k]$ is the decision for which Eq. (A.2) takes on the minimum. The iterative procedure begins by computing $\hat{u}[x, N-1]$ and I(x,$N-1$) from the given boundary conditions I(x,N), and it continues until it arrives at $\hat{u}[x, 0]$ and I(x, 0). The complete results of dynamic programming are shown in Fig. A.2. At each state of stage, the optimal decision is written blow, and the minimum cost is written above. Finally, we can find the optimal sequence of decisions starting from the given x(0) and system equation. This is called the recovery procedure and these decisions are the input for our experiments. However, this is based on the system equation when we lack the measurement of state. Our simulated results were done in this manner.

If we could monitor the state and stage of the system, the dynamic programming solution, $\hat{u}[x,k]$, leads to a feedback control or decision policy configuration. One method of implementing this solution is to simply store all the values of $\hat{u}[x,k]$ in memory, monitor the state and stage of the system, and look up the appropriate value of $\hat{u}[x,k]$ as required. This type of implementation is attractive because the dynamic programming calculations can be done offline, and the only operation that needs to be done during the decision interval is retrieval of the appropriate optimal decision. The system configuration is as shown in Fig. A.3.

A.3. Simulation Results

We used the very simple concept to get the equation for our simulation. The differential equation of the thickness being polished is equal to the removal rate and we made the removal rate to be the input. The equation is written as

$$\dot{h} = \frac{\mathrm{d}h}{\mathrm{d}t} = -\mathrm{RR} = -u$$

where h is the thickness, RR the removal rate, u the input. The difference equation version has been computed using a sampling period of T (1 s) is

$$h(k+1) = h(k) - T \times u(k) \tag{A.3}$$

where k is the stage. We assumed that there were only seven values of the input (include 0) because of restrictions on the Westech 372M CMP machine and the sampling period T here was fixed to 1 second. For each of these inputs the cost at the current stage can be determined as

$$\mathrm{L}^{(m)} = \frac{1}{2} q h^2(k) + \frac{1}{2} r u^2(k) \quad (m = 1, 2, \ldots, 7) \tag{A.4}$$

and the cost at the final stage N also was determined as

$$\mathrm{I}(x, N) = \mathrm{L}(x, N) = \frac{1}{2} s h_N^2 \tag{A.5}$$

where s is the weighting factor of final state, q the weighting factor of transient state, and r the weighting factor of input. Then we suppose a quantized state $h \in H$ and a admissible inputs $u^{(m)} \in U$ are applied.

$$H = [6000\ 5999\ 5998 \ldots 2\ 1\ 0] \quad (jN = 6001)$$
$$U = [u^{(1)} u^{(2)} u^{(3)} u^{(4)} u^{(5)} u^{(6)} u^{(7)}] \quad (mN = 7)$$

We could get I(h,$N-1$) and $\hat{u}[h, N-1]$ for all $h \in H$ by substituting Eq. (A.3), Eq. (A.4) and Eq. (A.5) into Eq. (A.2) which is presented in Section A.2.

$$\mathrm{I}[6000, N-1], \mathrm{I}[5999, N-1], \ldots, \mathrm{I}[1, N-1], \mathrm{I}[0, N-1]$$
$$\hat{u}(6000, N-1), \hat{u}(5999, N-1), \ldots, \hat{u}(1, N-1), \hat{u}(0, N-1)$$

It is now possible to compute I(h,$N-2$) and $\hat{u}[h, N-2]$ for all $h \in H$ based on knowledge of I(h,$N-1$). The iterative procedure continues until $\hat{u}[h, 0]$ and I(h, 0) have been computed. The program flowchart is shown in Fig. A.4 and the complete results of dynamic programming can be plotted like Fig. A.2. Finally, we can find the optimal sequence of inputs starting from the given h(0) and Eq. (A.3) by means of the recovery procedure.

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