中國機械工程學刊第四十一卷第六期第 713~723 頁(民國一百零九年)
Journal of the Chinese Society of Mechanical Engineers, Vol.41, No.6, pp.713~723 (2020)

Theoretical Simulation and Regression Analysis for Abrasive Removal Depth of Chemical Mechanical Polishing with Pattern-free Polishing Pad at Different Volume Concentrations of Slurry and Experiment

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Keywords: abrasive removal depth, regression model, volume concentration, pattern-free polishing pad, chemical mechanical polishing (CMP)

ABSTRACT

Considering that the contact area between the asperity peak surface of pattern-free polishing pad and wafer is of Gaussian distribution, the paper dippd silicon wafer in slurry at different volume concentrations at room temperature, and then performs atomic force microscopic (AFM) experiment. The paper calculates the specific down force energy (SDFE) values of silicon wafer dipped in slurry at different volume concentrations at room temperature. Then the paper substitutes these values in an innovatively established theoretical model of abrasive removal depth in chemical mechanical polishing (CMP) by pattern-free polishing pad with slurry at different volume concentrations. Then the paper makes a comparison between the simulation calculated abrasive removal depth value per minute obtained from calculation and the result of average abrasive removal depth per minute obtained from CMP experiment by pattern-free polishing pad. Finally, the calculated result obtained from theoretical simulation is proved to be reasonable. Furthermore, the paper proposes a correction concept for the average difference ratio of the simulation result to the experimental result, making the abrasive removal depth value per minute obtained from simulation after compensatory correction become closer to the experimental result. The paper, giving consideration for slurry at different volume concentrations at room temperature, also establishes a new regression model and a new equation of average abrasive removal depth per minute in CMP by pattern-free polishing pad at different down forces and rotational velocities, and with slurry at different volume concentrations so as to make it close to the experimental result. The paper also completes the compensatory regression equation after adding the effects of slurry at different volume concentrations, and makes analysis.

Paper Received September, 2020. Revised November, 2020. Accepted December, 2020. Author for Correspondence:Zone-Ching Lin.

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INTRODUCTION

The chemical reaction of slurry would affect the abrasive depth of silicon wafer, and can make the abrasive removal depth of silicon wafer increased when the abrasive particles polish the silicon wafer. Besides, slurry at different concentrations would affect the softening feature of the chemical reaction layer of silicon wafer, and would further affect the silicon wafer’s abrasive removal depth done by the abrasive particles, leading to effects on the abrasive removal depth per unit time of silicon wafer receiving chemical mechanical polishing (CMP). CMP is a kind of very complicated fabrication behavior. Preston (1927) proposed the first theoretical model of CMP wear, which was expressed as MRR=KPV, where MRR is material removal rate; P is the pressure applied; V is relative velocity of wafer to polishing pad; and K is Preston constant. As seen from the above equation, material removal rate is related to the pressure applied and relative velocity. Yu et al. (1993) firstly proposed that the contact between the asperity of polishing pad and wafer surface should be considered, and explored the relationship between static contact and removal rate. Besides, Yu et al. (1994) also proposed the combined effects of polishing pad with asperity and fluid dynamics of abrasive fluid on CMP process. The contacts explored above were all under a supposition that the asperity distribution on polishing pad surface was of Gaussian distribution; the peak of its asperity was circular; and the polishing pad did not have a pattern groove. Besides, Liu et al. (1996) took statistical method and elasticity theory as the foundation, and derived a mechanical wear model of wafer surface. They indicated that this model was related to pressure, relative velocity, nature of abrasive particles and nature of the material to be polished. They also argued that removal rate was related to the elasticity modulus of slurry particle and wafer surface material. Chekina and Keer (1998), employing the concept of contact mechanics, analyzed the relationship between wafer surface morphology and contact pressure in the CMP wearing process under steady conditions, and determined that the effect of planarization is related to geometric unevenness on a surface and different surface materials. In addition to the published literature relating to CMP wearing studies, Xie and Bhushan (1996) intended to know the wear model of removal rate in mechanical polishing process, proposed how the size of abrasive particles, polishing pad and contact stress were related to removal rate, and proved their theoretical model by experiments. Jiang et al. (1998) suggested giving consideration to two-body wear model under the condition of asperous surface contact, and defined the wear energy of material. They supposed that the asperity peak of asperous surface was conic, and the asperity distribution was Gaussian distribution. Besides, Jongwon et al. (2003) further discussed about a contact deformation effect model for abrasive particles and derived a volumetric removal model for individual abrasive particle. Lin and Chen (2005) developed a binary image pixel numerical analysis method to calculate polishing frequency and polishing times for chemical mechanical polishing of polishing wafer. Lin and Huang (2012) studied the use of CMP sapphire wafer, and used the wafer removal caused by chemical reaction in the contact of slurry with SiO_2 content and substrate to observe the change in the removal amount and surface morphology of wafer when there are different down forces, different rotational velocities, use of polishing pads with different morphologies, such as hole-pattern polishing pad and pattern-free polishing pad, different abrasive particle sizes and different volumetric concentrations of slurry. They also matched with the regression analysis theory. Focusing on the equation MRR=KPV proposed by Preston for polishing of glass, they made improvement. However, they did not establish a theoretical model for calculation of abrasive removal depth. Kim and Jeong (2004) studied and analyzed the relative velocity of polishing velocity, and derived the relative abrasive length of each position on wafer to polishing pad. Atomic force microscopy (AFM), invented by G. Bining et al. (1986), is a kind of scanning probe microscopy generally used for measurement and observation of the surface morphology of conductor and non-conductor, so that the related scholars explored the measurement and application of AFM. It was proved by the related scholars that applying AFM probe as a fabrication tool to perform mechanical cutting was a quite useful technique in fabrication of nanostructures, such as semiconductor, optoelectronic component and metallic surface (Tseng et al.,2008).

In the above literature, there is no in-depth exploration for establishment of a theoretical model, experiment and regression analysis equation of the abrasive removal depth of silicon wafer being affected by the chemical reaction of slurry at different volume concentrations at room temperature when a pattern-free polishing pad performs CMP of silicon wafer.

THEORETICAL MODEL AND EXPERIMENTAL METHOD FOR SDFE INSIDE THE CHEMICAL REACTION LAYER OF SILICON WAFER DIPPED IN SLURRY AT DIFFERENT VOLUME CONCENTRATIONS AT ROOM TEMPERATURE

The paper considers that in the actual nano-fabrication process, silicon wafer is fabricated in a cutting direction by a downward force energy produced by the cutting tool of probe that presses downward to a certain depth downward force. And the mechanism for silicon wafer to be fabricated is the moving and removal of atomic particles, and this is a model of volume change (2012). Therefore, the paper's $SDFE_{reaction}$ inside the chemical reaction layer of silicon wafer dipped in slurry at different volume concentrations is defined by the product after multiplying the cutting depth by the downward force of the cutting tool of probe applied on the silicon wafer workpiece being dipped in slurry at different volume concentrations. It refers to the quotient after dividing the energy produced in the fabrication process by the volume of the workpiece removed by the downward force of the cutting tool, as shown in equation (1):

$$SDFE_{reaction}(\text{specific downward force energy}) = \frac{F_d \times \Delta d}{\Delta V} \quad (1)$$

where F_d is the downward force of cutting tool applied on the silicon wafer workpiece; Δd is the cutting depth; and ΔV is the workpiece volume removed by the downward force of the cutting tool. Here, the downward force of AFM machine is F_d, which can be obtained from $F_d=k_r d$, where k_r is the spring of AFM machin constant of probe; and d can be obtained by using the setpoint of force-distance curve.

From moving of cutting tool to fabrication of groove, the depth in the middle area gradually inclines to be at a fixed cutting depth. As to the volume removed by moving and downward force of cutting tool, due to fabrication in the abovementioned process, the volume of the distance of the radius R behind the cap of workpiece being pressed in by the probe in advancing direction has been removed. Therefore, the removed volume is half of the cap volume under the cutting depth, and the removed volume is shown as follows (Lin and Hsu,2012):

$$\Delta V = \frac{1}{2}\pi \Delta d^2 \left(R - \frac{\Delta d}{3}\right) \qquad (2)$$

In times of CMP fabrication, when the abrasive particles in slurry are polishing the wafer, the fabrication via polishing and cutting is similar to making of an abrasive depth by each spherical abrasive particle, and is also similar to the foregoing AFM probe's fabrication behavior on silicon wafer. Therefore, if the paper firstly uses scanning electron microscope (SEM) to measure the diameter of the semisphere of AFM probe, and then applies the abovementioned AFM fabrication experiment, with the silicon wafer affected by dipping in slurry at different volume concentrations and at room temperatures, the paper should firstly set the downward force, perform cutting and fabrication, and measure the obtained cutting depth. After that, the paper uses equation (2) to calculate the $SDFE_{reaction}$ value of the chemical reaction layer of silicon wafer dipped in slurry at different volume concentrations at room temperature.

The slurry used in the paper is produced by Allied High Tech Product, Inc., with the diameter of its abrasive particle at 50nm and its volume concentration at 50%. The slurry with volume concentration 50% has the following implied meanings: for example, if the total volume of a slurry is 100 c.c., the slurry at volume concentration 50% represents that the volume of an abrasive particle is 50c.c. Therefore, a slurry at volume concentration 40% implies that the volume of its abrasive particles accounts for 40% of the total volume of the slurry. In other words, the volume of abrasive particles in 100c.c. of slurry made by Allied High Tech Product, Inc. is 50c.c. Therefore, it is required to add 25c.c. of deionized water to the slurry in order make the total volume of the slurry to be 125c.c. Right now, since the volume of abrasive particles is 50c.c., the volume of the abrasive particles accounts for 40% of the total volume of 125c.c.

According to the abovementioned blending method in making a slurry with volume concentration 40%, we can obtain different kinds of slurry at 30%, 20% or 10%. In the aspect of control of dipping time, after dipping a single-crystal silicon substrate in slurry, a meter is used as a tool to measure time, and count the dipping time of 30 minutes.

SIMULATION MODEL OF ABRASIVE REMOVAL DEPTH OF SILICON WAFER OF CMP BY PATTERN-FREE POLISHING PAD

Focusing on the experiments with the same experimental parameters, the paper conducts CMP experiments for 5 times. In each experiment, polishing is carried out for 20 minutes, and then the paper finds the average abrasive removal depth value per minute in the experiment.

The paper's theoretical model of abrasive removal depth is that silicon wafer is firstly cut into multiple elements, and then the paper calculates the relative abrasive removal length per minute of the corresponding polishing pad of each element of silicon wafer as well as the number of moving times per minute for the contact of each element with the polishing pad. The paper also combines with the SDFE theory-based abrasive depth calculation model of a single abrasive particle. First of all, the paper applies the theoretical equation of relative moving between silicon wafer and pattern-free polishing pad, and then calculates the relative moving length per unit time between silicon wafer and polishing pad. Relative moving length represents a length in which there are abrasive particles polishing the wafer. After that, the paper calculates the effective contact area between the asperous surface of polishing pad and each element on the silicon wafer surface.

Subsequently, the paper uses an abrasive contact model of single-element multiple abrasive particles. Using this contact model, the contact force of single abrasive particle with wafer per unit time can be calculated. After that, based on the contact force and according to the $SDFE_{reaction}$ theory, as well as the $SDFE_{reaction}$ value of the chemical reaction layer of silicon wafer dipped in slurry at different volume concentrations obtained in AFM experiment, the paper calculates the abrasive removal depth of a single abrasive particle. Furthermore, the paper calculates the effective removal volume and average abrasive removal depth of a single element. Furthermore, the paper calculates the effective abrasive removal volume of silicon wafer per unit time by dividing the effective abrasive removal volume of silicon wafer by the area of wafer, thus acquiring the abrasive removal depth of silicon wafer per unit time.

Calculation Method of the Contact Area Between Asperity Peak of Polishing Pad and Wafer

Currently, the concept of the commonly used statistical surface contact mechanics theory was firstly developed by Greenwood and Williamson (1966). This theory includes a supposition that the contact between two surfaces is Hertz contact; the contact surface is semispherical; and the height of surface asperity is of Gauss distribution. Compared to the surface roughness of wafer, the surface roughness of polishing pad is much greater. Therefore, the contact surface between polishing pad and wafer can be considered a contact between an roughness surface (polishing pad) and a smooth surface (wafer). The paper of Qina et al. (2004), the asperity peak of pattern-free polishing pad was supposed to be of Gaussian distribution, and the wafer was supposed to be a flat surface. As to the derived contact area between polishing pad and wafer as well as the equation of load, they supposed that abrasive particles were embedded on the polishing pad only on the contact area between the asperity peak of polishing pad and wafer, to perform polishing of wafer. Under this model, in order to use pattern-free polishing pad, the paper cuts the silicon wafer into single elements, with each element in the size of 1mm*1mm, as shown in Figure 1. When the silicon wafer is rotating, each element have continuous relative turning contacts with the pattern-free polishing pad.

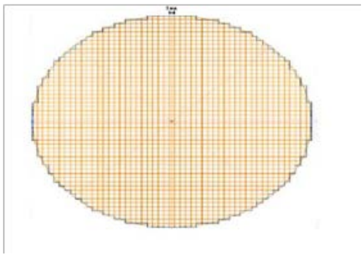

Figure 1 Schematic diagram of the cut elements of silicon wafer

According to the equations of contact area and contact load in the paper of Qina et al. (2004), the paper further corrects the equations, and innovatively proposes the effective contact area *(A_{rs})* equation and contact load (*F*) equation for the contact between the asperity peak of polishing pad and each element of silicon wafer, as shown below. It is supposed that abrasive particles on the polishing pad are embedded only on the effective contact area (A_{rs}) between the asperity peak of polishing pad and wafer, and these abrasive particles are used to polish the wafer.

$$A_{rs} = \eta A_0 \pi \beta \int_h^{\infty} (z-h)\emptyset(z)dz \qquad (3)$$

$$\frac{A_{rs}}{F} = \frac{3\pi\beta^{\frac{1}{2}}}{4E^*} \frac{\int_h^{\infty}(z-h)\phi(z)dz}{\int_h^{\infty}(z-h)^{\frac{3}{2}}\phi(z)dz} \qquad (4)$$

Johnson (1985) used numerical integration to perform integration of equation (4). But for h/σ within a range, the ratio of two integrals is approximately a constant, so that equation (5) can be obtained:

$$A_{rs} = C^{-1}\left(\frac{\beta}{\sigma}\right)^{\frac{1}{2}} \frac{F}{E^*} \qquad (5)$$

$$E^* = \frac{1-{\nu_p}^2}{E_p} + \frac{1-{\nu_w}^2}{E_w}$$

where E^* is equivalent Young's modulus; ν_p is Poisson's ratio of polishing pad; ν_w is Poisson's ratio of silicon wafer; E_p is Young's modulus of polishing pad; and E_w is Young's modulus of silicon wafer.

In equation (5), C is a constant. In the paper of Yu et al. (1993), the constant was derived and calculated. It is known that the ratio h/σ of polishing pad is generally between 0.5 and 3.0 (Johnson,1985). When h/σ is between 0.5 and 3.0, C value is approximately 0.35. The polishing pad used in this paper and the polishing pad used in Johnson (1985) are made by the same company, and of similar model number. Therefore, for the variables of equation (6), the paper refers to the β and σ values of Johnson (1985).

Theoretical Method for Calculation of Abrasive Removal Depth of Single Element of Silicon Wafer

In the paper of Kim and Jeong (2004), pattern-free polishing pad was used to polish wafer. It mentioned that at any point P position on silicon wafer, the relative velocity $v_{w/p}$ of polishing pad is expressed as the following equation:

$$V_{w/p} = \omega_p D_{wp}\sqrt{(\rho\zeta)^2 + 2\rho\zeta cos\phi + 1} \qquad (6)$$

In this paper, we set the central position of each element of silicon wafer at the abovementioned position P on the wafer surface. Therefore, the actual relative abrasive length per minute at the central position of each element on silicon wafer is $\omega_p D_{wp}$. Dividing $\omega_p D_{wp}$ by each element's length L_e of can achieve the relative number of polishing times FF per unit time for the contact between each element and polishing pad. Therefore, $\mathrm{FF} = \frac{\omega_p D_{wp}}{L_e}$.

The paper lets the size of each element of silicon wafer be 1mm×1mm; therefore, L_e=1mm. Right now, the wafer's surface volume Vol that can be removed by abrasive particle is shown in Figure 2 and expressed as the following equation:

$$\mathrm{Vol} = A_p * \ell \qquad (7)$$

where

Vol: volume of wafer removed by a single abrasive particle per unit number of polishing times

A_p : cross-sectional area of abrasive depth δ_{aw} of a single abrasive particle

ℓ : moving length of abrasive particles per unit time

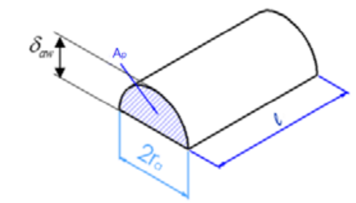

Figure 2 Schematic diagram of abrasive removal volume of single abrasive particle on the corresponding polished wafer

The paper supposes that the abrasive particles on the effective contact area in each of the cut element of silicon wafer are distributed evenly. Therefore, the moving length ℓ per unit time of a single abrasive particle within each of the cut element of silicon wafer is expressed as the following equation:

$$\ell = \omega_p D_{wp} \tag{8}$$

where:

$$A_p \approx \frac{1}{2}\cdot\delta_{aw}\cdot 2r_a \approx \delta_{aw}\sqrt{\delta_{aw}D} \tag{9}$$

Besides, if N_e is the number of effective abrasive particles of each element of wafer, and the unit volume concentration of the number of particles in slurry is supposed to be χ and the average diameter of abrasive particles is D, then $(\frac{6\chi}{\pi D^3})^{2/3}$ is the number of particles per unit volume in slurry. Since the length of each element of wafer is 1mm, the number of effective abrasive particles of effective contact area of a single element is (Zhao and Chang,2002):

$$N_e = A_{rs}\cdot\left(\frac{6\chi}{\pi D^3}\right)^{2/3} = C^{-1}\left(\frac{\beta}{\alpha}\right)^{\frac{1}{2}}\frac{F}{E^*}\left(\frac{6\chi}{\pi D^3}\right)^{2/3} \tag{10}$$

where A_{rs} is the effective contact area of each element, which is for the interface between single element of wafer surface and the asperity peak of polishing pad. In this paper, the contact between the asperity peak of polishing pad and wafer is of Gaussian distribution, which derives equation (5) of A_r for application to calculation.

The paper proposes a supposition that the downward force borne by each element of wafer is: $F=F_{total}/n$. Here, F_{total} is the total downward force of CMP machine for polishing pad to press down to wafer; n is the number of the cut elements of wafer on the contact between wafer and polishing pad. Furthermore, the paper derives a new equation of downward force F_{aw} of a single abrasive particle in polishing the wafer:

$$F_{aw} = \frac{F_{total}}{n\times N_e} \tag{11}$$

where N_e is the number of effective abrasive particles of each element on the effective contact area. The total downward force F_{total} of polishing pad in pressing down to wafer can be measured and known by experimental CMP machine. Besides, the number n of elements of wafer on the contact between wafer and polishing pad is the number of the elements of wafer. From the catalog provided by the manufacturer, the volume concentration (χ) of abrasive particles in slurry can be known. Equation (10) can be used to obtain N, and hence, F_{aw} can also be subsequently obtained.

Substituting the contact force F_{aw} between a single abrasive particle and wafer surface in the SDFE equation (1) of silicon wafer dipped in slurry at different volume concentrations can achieve the abrasive removal depth Δd on wafer surface by a single abrasive particle:

$$\Delta d = \frac{\Delta V\times SDFE_{reaction}}{F_{aw}} \tag{12}$$

$$\Delta d = \frac{\frac{1}{2}\pi\times\Delta d^2\times(R-\frac{\Delta d}{3})\times SDFE_{reaction}}{F_{aw}} \tag{13}$$

where R is the radius of abrasive particle.

After rearranging equation (13), a quadratic equation in one variable that takes Δd as a single variable can be obtained.

$$\frac{1}{6}\pi\times SDFE_{reaction}\times\Delta d^2 - \frac{1}{2}\pi\times R\times SDFE_{reaction}\times\Delta d + F_{aw} = 0 \tag{14}$$

Using equation (14) can solve the quadratic equation in one variable that takes Δd as a single variable.

$$\Delta d = \frac{3R-\sqrt{9R^2-\frac{24F_{aw}}{\pi\times SDFE_{reaction}}}}{2} = \delta_{aw} \tag{15}$$

The paper further substitutes equation (11) in equation (15) to find the innovative polishing depth δ_{aw} of a single abrasive particle on wafer surface:

$$\Delta d = \frac{3R-\left(9R^2-\frac{24\times\frac{F_{total}}{n\times N_e}}{\pi\times SDFE_{reaction}}\right)^{\frac{1}{2}}}{2} = \delta_{aw} \tag{16}$$

Substitute the obtained δaw in equatio (9) and equation (7) to acquire the effective removal volume per unit time of a single abrasive particle of a single element on wafer surface: $\mathrm{Vol} = \delta_{aw}\sqrt{\delta_{aw}D}\times l$. Besides, based on equation (8), $\ell = \omega_p D_{wp}$, and hence $\mathrm{Vol} = \delta_{aw}\sqrt{\delta_{aw}D}\times\omega_p D_{wp}$.

Multiply Vol by the number N_e of effective abrasive particles of each element. Therefore, the effective abrasive removal volume $V_{\Delta t}$ per unit time of each element is expressed as the following equation:

$$V_{\Delta t} = Vol\times N_e \tag{17}$$

The paper proposes dividing $V_{\Delta t}$ by the area A_0 at the position of a single element of wafer, to obtain the average abrasive removal depth $\delta_{\Delta t}$ per unit time at the position of each element:

$$\delta_{\Delta t} = \frac{V_{\Delta t}}{A_0} \tag{18}$$

Theoretical Equation for Calculation of Abrasive Removal Depth in CMP of Silicon Wafer by Pattern-Free Polishing Pad

Therefore, after multiplying the effective removal volume per unit time of a single element by the number n of the cut elements of wafer contacting the polishing pad, the effective removal volume per unit time can be obtained. After dividing the effective removal volume of wafer per unit time by the area A_w of wafer, the average abrasive removal depth of wafer per unit time can be obtained.

Based on the above, the effective abrasive removal volume V_{Vol} of wafer per unit time is expressed as the following equation:

$$V_{Vol} = V_{\Delta t} \times n = Vol \times N_e \times n \tag{19}$$

Therefore, the equation of abrasive removal depth d_{ab} of silicon wafer per unit time is expressed as follows:

$$d_{ab} = \frac{V_{Vol}}{A_w} = \frac{Vol \times N_e \times n}{\pi {R_w}^2} \tag{20}$$

where R_w is the radius of silicon wafer.

After rearranging the above equation, the following is obtained:

$$d_{ab} = \frac{\delta_{aw}\sqrt{\delta_{aw}D} \times \omega_p D_{wp} \times A_{rs} \cdot \left(\frac{6\chi}{\pi D^3}\right)^{2/3} \times n}{\pi {R_w}^2} \tag{21}$$

And

δ_{aw} and A_{rs} are shown in equation (16) and equation (5), respectively.

In equation (21), F_{total} can be known from measurement by CMP machine. The $SDFE_{reaction}$ value of the chemical reaction layer of silicon wafer dipped in slurry at different volume concentrations can be known from calculation in AFM experiment. The rotational velocity ω_p of polishing pad is a set value; and D_{wp} is known. By the time the slurry is purchased, the diameter D of abrasive particles is known to be 50mmm, so that the radius R of abrasive particles is 25mm. The number n of the cut elements of silicon wafer can be known; and the volume concentration χ of slurry can be known as well. Therefore, the abrasive removal depth d_{ab} of silicon wafer per unit time of minute can be calculated and known. As seen from d_{ab} of equation (21), the paper can derive an innovative theoretical equation of abrasive removal depth per unit time of minute of silicon wafer polishing of CMP with pattern-free polishing pad and being affected by slurry at different volume concentrations, as shown in equation (21), which is of academic innovativeness.

REGRESSION MODEL OF CMP BY PATTERN-FREE POLISHING PAD DIPPED IN SLURRY AT DIRRERENT VOLUME CONCERTRATIONS

The paper also considers the regression equation of abrasive removal depth with slurry at different volume concentrations at room temperature, different down forces and rotational velocities**,** and also probably considers the compensatory regression equation of the effects of slurry at different volume concentrations at room temperature. Since right now there are affecting parameters of slurry at different volume concentrations, downward forces and different rotational velocities, there have to be quite a lot of simulation cases before the regression equation can be obtained.

First of all, the paper performs CMP experiment, with the radius of abrasive particle in slurry at 50nm, rotational velocity of wafer and polishing pad at both 60rpm, slurry's volume concentrations at 20%, 30%, 40% and 50% at room temperature and different downward forces. After that, we substitute in equation (16) the already obtained $SDFE_{reaction}$ value of the chemical reaction layer of silicon wafer dipped in slurry at 4 different volume concentrations at room temperature in order to find δ_{aw}. Furthermore, from equation (21), and through simulation for 4 kinds of volume concentrations of slurry with different downward forces, the abrasive removal depth d_{ab} of silicon wafer per minute can be calculated. Subsequently, the paper compares the CMP experimental results with pattern-free polishing pad and slurry at different volume concentrations at room temperature, with the simulation calculated results of abrasive removal depth value per minute of silicon wafer dipped in slurry at different volume concentrations at room temperature. Then the paper finds the equation of difference ratio of experimental result to simulation result, as shown in the following equation:

$$\text{Difference ratio} = \frac{\begin{array}{c}(\text{Simulation calculated abrasive removal depth per minute} - \\ \text{Experimental average abrasive removal depth per minute})\end{array}}{\text{Simulation calculated abrasive removal depth per minute}} \tag{22}$$

According to our past experience, such a difference ratio value is approximately within a certain range, and the change would not be too great. Therefore, using the 4 difference ratio values of silicon wafer dipped in slurry at 4 different volume concentrations at room temperature, we can obtain the average difference ratio value. Therefore, using this average difference ratio value, we can make compensatory correction of the simulation calculated abrasive removal depth per minute, thus achieving an average abrasive removal depth value per minute that is close to the experimental value.

Therefore,

Average abrasive removal depth value per minute being close to experimental value.= Simulation calculated abrasive removal depth per minute − (Simulation calculated abrasive removal depth per minute × Average difference ratio value) (23)

Hence, we can use this method to simulate calculation of the abrasive removal depth per minute of silicon wafer dipped in slurry at different volume concentrations at room temperature. After that, using the calculation method of average difference ratio value, the paper finds an average abrasive removal depth per minute being close to the experimental result. Therefore, we can use this method to decrease the number of times of experiment before finding through simulation calculation the result of abrasive removal depth per minute of silicon wafer dipped in slurry at different volume concentrations at different downward forces and different rotational velocities and different room temperatures. Then we can find the abrasive removal depth per minute being close to the experimental value.

In this study, we also select different downward forces, different rotational velocities at room temperatures for conducting CMP experiment of silicon wafer dipped in slurry at different volume concentrations, so as to find the experimental result of average abrasive removal depth per minute. Through simulation, the abrasive removal depth per minute is also calculated. The simulation calculated result is applied to the calculation method of average different ratio, and the calculated average abrasive removal depth per minute is close to the experimental result. This result is compared with the average abrasive removal depth per minute obtained from experiment, thus proving the feasibility of using the average difference ratio method to find an average abrasive removal depth per minute that is close to the experimental result.

After that, for the simulation calculated abrasive removal depths per minute of silicon wafer dipped in slurry at different volume concentrations at room temperature at multiple different downward forces and different rotational velocities, we use average difference ratio method to find an average abrasive removal depth per minute that is close to the experimental result. For the simulation obtained multiple average abrasive removal depths per minute that are close to the experimental result, we use them as input values for regression analysis so as to perform regression analysis and find the regression equation.

In general, Preston's volumetric material removal equation is commonly used in CMP, and is expressed as MRR = KPV, where K is a constant; P is downward force; and V is rotational velocity. However, in order to calculate the abrasive removal depth, a new regression equation is used. Focusing on the regression equation of average abrasive removal depth per minute to be close to the experimental result and with consideration for difference ratio value, the paper firstly supposes that the abrasive removal depth per minute is MRR_e. Then the paper makes regression calculation of the equation $\mathrm{MRR}_e = \mathrm{k}_{pe}\mathrm{P}^{\alpha_{de}}\mathrm{V}^{\beta_{de}}$, where k_{pe} is a constant; P is downward force; and V is rotational velocity of wafer and polishing pad. The values of k_{pe}, α_e and β_e can be acquired by the following method and equation:

$$\mathrm{MRR}_e = \mathrm{k}_{pe}\mathrm{P}^{\alpha_e}\mathrm{V}^{\beta_e} \quad (24)$$

We can write a natural logarithm (El-Kareh,1995), so that equation (24) can be changed as $\ln MRR_e = \ln k_{pe} + \alpha_e \ln P + \beta_e \ln V$.

This equation is equivalent to $\mathrm{y} = \beta_{0e} + \beta_{1e}\chi_1 + \beta_{2e}\chi_2$ (25)

$\mathrm{y} = \ln MRR_e$, $\beta_0 = \ln k_{pe}$, $\chi_1 = lnP$, $\chi_2 = lnV$, $\beta_{1e} = \alpha_e$, $\beta_{2e} = \beta_e$,

Therefore, $\mathrm{Y} = \hat{\beta}X$.

Use least square method, and then multiply Y by *X'*, achieving $X'Y = (X'X)\hat{\beta}$.

$$\text{Therefore, } \hat{\beta} = (X'X)^{-1}(X'Y') \text{ and } \hat{\beta} = \begin{bmatrix}\beta_{0e}\\ \beta_{1e}\\ \beta_{2e}\end{bmatrix} \quad (26)$$

From the matrix of equation (26) aforesaid, we can calculate $\mathrm{k}_{pe} = e^{\beta_{0e}}$, $\alpha_e = \beta_{1e}$, $\beta_e = \beta_{2e}$, and further find the regression equation of $\mathrm{MRR}_e = \mathrm{k}_{pe}\mathrm{P}^{\alpha_e}\mathrm{V}^{\beta_e}$.

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Furthermore, we test whether the regression result obtained from MRR_e equation with slurry at a certain volume concentration as well as the R-square value of the average abrasive removal depth per minute being close to the experimental result are less than 1 too much, or whether the average residual is greater than 0 too much. If positive, the paper would consider adding to the MRR_e regression equation a compensatory regression equation of S_{vce} with consideration of the effects of slurry at different volume concentrations at room temperature, i.e. $MRR_e = k_{pe}P^{\alpha_e}V^{\beta_e} + S_{vce}$. Here, the paper lets S_{vce} be a quadratic regression model; $S_{vce} = y_{vce}$; and the volume concentration of slurry be x_{vc}.

$$\therefore\ y_{vce} = \beta_{0vce} + \beta_{1vce}x_{vce} + \beta_{2vce}x_{vce}^2 \quad (27)$$

Thus, $Y_{vce} = \hat{\beta}_{vce}X_{vce}$, and

$$\hat{\beta} = (X'_{vce}X_{vce})^{-1}X'_{vce}Y_{vce} \text{, and } \hat{\beta}_{vce} = \begin{bmatrix}\beta_{0vce}\\ \beta_{1vce}\\ \beta_{2vce}\end{bmatrix} \quad (28)$$

X'_{vce} is a transformation matrix.

$$\therefore\ \mathrm{MRR}_e = k_{pe}P^{\alpha_e}V^{\beta_e} + (\beta_{0vce} + \beta_{1vce}x_{vce} + \beta_{2vce}x_{vce}^2) = k_{pe}P^{\alpha_e}V^{\beta_e} + S_{vce} \quad (29)$$

Use the regression equation obtained from the above regression analysis to check whether the R-square value is close to 1, and whether the average residual is close to 0. We also use a different downward force and a different rotational velocity to simulate calculation of the average abrasive removal depth per minute being close the experimental result, with slurry at different volume concentrations at room temperature, and calculate the MRR_e value of the abrasive removal depth per minute obtained from the regression equation under the same condition. The paper makes comparison between these two results, and proves that the regression equation is reasonable.

RESULTS AND CONCLUSIONS

Simulation Result of the Theoretical Model of Silicon Wafer Receiving CMP by Pattern-

Free Polishing pad

From the theoretical model-based simulation result of abrasive removal depth per minute, we find that the abrasive removal depth per minute can be easily affected by the change of volume concentration of slurry, downward force and rotational velocity. First of all, we use downward force 3psi and rotational velocity 60rpm at room temperature, as well as the volume concentration of slurry at 20%, 30%, 40% and 50% successively to analyze the theoretical model-based simulation results of abrasive removal depth per minute. When the volume concentration of slurry is 20%, 30%, 40% and 50%, the simulation results of abrasive removal depth per minute are 23.0627nm/min, 24.8571nm/min, 26.3745nm/min and 28.4015nm/min respectively. Therefore, it is known that when the rotational velocity is fixed and the downward force is great, the abrasive removal depth per minute is great.We also simulate that the downward force is fixed and the rotational velocity is high, it is found that the abrasive removal depth per minute is great.

Regression Analysis of CMP Simulation Result of Silicon Wafer

The paper, using the least square method and focusing on pattern-free polishing pad, makes regression analysis of the theoretical model simulation results being mutually matched with different volume concentrations of slurry at room temperature, different down forces and different rotational velocities. From the $\mathrm{MRR} = k_p P^{\alpha} V^{\beta}$ equation, calculation is made for the volume concentrations of slurry at 20%, 30%, 40% and 50%, thus achieving the regression results of $\mathrm{MRR} = k_p P^{\alpha} V^{\beta}$ at 20%, 30%, 40% and 50%.

Under the simulation results of the theoretical model for multiple conditions that pattern-free polishing pad is used at room temperature, the volume concentrations of slurry are 20%, 30%, 40% and 50%, which are matched with different downward forces of 1psi, 1.5psi, 2psi, 2.5psi and 3psi, as well as different rotational velocities at 20rpm, 30rpm, 40rpm, 50rpm and 60rpm, the paper uses the least square method to perform regression analysis. Under different volume concentrations of slurry, the values of α and β are all 1.0059 and 1 respectively, only that k_p value changes with the change of volume concentration of slurry. When the volume concentrations of slurry are 20%, 30%, 40% and 50%, k_p values are 0.1275, 0.1374, 0.1457 and 0.1569, respectively.

Finally, from the theoretical model-based simulation results as well as the difference value of the regression result of $\mathrm{MRR} = k_p P^{\alpha} V^{\beta}$, it is known that the difference value is all less than 0.3%, which is within an acceptable range since the difference value in practical application is below 1%, and is also a conveniently useable result for calculation with a fixed volume concentration of slurry, different downward forces and different rotational velocities. From here, it is known that the equation $\mathrm{MRR} = k_p P^{\alpha} V^{\beta}$ for slurry at a fixed volume concentration is reasonable and acceptable.

Analysis on the Difference Ratio of CMP Experimental Result and Theoretical Simulation Result of Silicon Wafer

The paper uses 6 groups of CMP experiments of silicon wafer by pattern-free polishing pad at room temperature with different volume concentrations of slurry, different downward forces and different rotational velocities: (1) 20%, 3psi, 60rpm; (2) 30%, 3psi, 60rpm; (3) 50%, 3psi, 60rpm; (4) 40%, 2psi, 40rpm; (5) 50%, 2psi, 40rpm; and (6) 50%, 1psi, 60rpm. Then the paper compares the theoretical simulation result of abrasive removal depth for CMP by pattern-free polishing pad with slurry at different volume concentrations at room temperature, with the above 6 CMP experimental results of abrasive removal depth. The paper calculates the theoretical simulation values of individual abrasive removal depth per minute of the polished wafer dipped in slurry at different volume concentrations at room temperature obtained in the above 6 experiments, as well as the difference ratio values between theoretical simulation results and experimental results, being 4.05%, 4.16%, 4.23%, 4.35%, 4.26% and 4.19% respectively. The paper also calculates the average difference ratio value, which is approximately 4.2%.

The average difference ratio of the simulation results to the experimental results of abrasive removal depth per minute is approximately 4.2%. It can still be proved that the paper's established theoretical model of abrasive removal depth of silicon wafer receiving CMP by pattern-free polishing pad with consideration of the chemical reaction effects of slurry at different volume concentrations is still reasonable.

Corrected Theoretical Model-Based Simulation Result of the Average Abrasive Removal Depth Per Minute Being Close to Experimental Value of Silicon Wafer for CMP with Pattern-Free Polishing Pad.

The paper compares the theoretical simulation result of CMP by pattern-free polishing pad with slurry at different volume concentrations at room temperature, with the 6 groups of CMP experimental results of abrasive removal depth per minute of silicon wafer. From the individual difference ratio value of the polished silicon wafer dipped in slurry at different volume concentrations at room temperature, the paper finds the average difference ratio value, which is approximately 4.2%. After deducting the average difference ratio value of 4.2% from all the theoretical simulation results, the paper obtains a theoretical simulation result of average abrasive removal depth per minute that is close to the experimental result.

From the theoretical simulation values obtained under multiple conditions of pattern-free polishing pad used at room temperature, different volume concentrations of slurry being matched with different downward forces and different rotational velocities, the paper deducts the average difference ratio value of 4.2%. After correction, the paper obtains a new theoretical simulation result of the average abrasive removal depth per minute being close to the experimental result, to serve as the input value of the new regression equation. The volume concentrations of slurry are 20%, 30%, 40% and 50%, which are matched with different downward forces of 1psi, 1.5psi, 2psi, 2.5psi and 3psi, as well as different rotational velocities of 20rpm, 30rpm, 40rpm, 50rpm and 60rpm. The paper uses the least square method to perform regression analysis, and the regression results are shown in Table 1.

Table 1 Regression equation $MRR_e = k_{p_e} P^{\alpha_e} V^{\beta_e}$ of average abrasive removal depth per minute being close to the experimental result with different volume concentrations of slurry at room temperature

Volume concentration	Regression equation $MRR_e = k_{p_e} P^{\alpha_e} V^{\beta_e}$	
50%	$MRR_e=0.1504\ P^{1.0059}\ V^1$	$k_{p_e}=0.1504$ $\alpha_e=1.0059$ $\beta_e=1$ $R^2=0.999992080$ Average residual= -0.00002
40%	$MRR_e=0.1396\ P^{1.0059}\ V^1$	$k_{p_e}=0.1396$ $\alpha_e=1.0059$ $\beta_e=1$ $R^2=0.999992097$ Average residual= -0.00002
30%	$MRR_e=0.1316\ P^{1.0059}\ V^1$	$k_{p_e}=0.1316$ $\alpha_e=1.0059$ $\beta_e=1$ $R^2=0.999992020$ Average residual= 0.000508
20%	$MRR_e=0.1221\ P^{1.0059}\ V^1$	$k_{p_e}=0.1221$ $\alpha_e=1.0059$ $\beta_e=1$ $R^2=0.999999747$ Average residual= -0.000108

Finally, from the new theoretical model-based simulation results of the average abrasive removal depth per minute being close to the experimental result as well as the difference value of the regression result of $MRR_e = k_{p_e} P^{\alpha_e} V^{\beta_e}$, it is known that the difference value is all less than 0.27%, which is within an acceptable range since the difference value in practical application is below 1%, and the difference value is also a conveniently useable result for calculation with a fixed volume concentration of slurry, different downward forces and different rotational velocities. From here, it is known that the equation $MRR_e = k_{p_e} P^{\alpha_e} V^{\beta_e}$ of slurry at a fixed volume concentration in Table 1 is acceptable.

Regression Result of $\mathbf{MRR_e = k_{p_e} P^{\alpha_e} V^{\beta_e} + S_{vc_e}}$ for the Corrected Average Abrasive Removal Depth Per Minute that is Close to the Experimental Result

When making exploration of pattern-free polishing pad focusing on volume concentration of slurry to consider the compensatory regression equation of S_{vc_e}, the paper uses the way of quadratic linear regression to make analysis. We use $S_{vc_e} = (\text{New theoretical simulation value being close to experimental average abrasive removal depth per minute} - k_{p_e} P^{\alpha_e} V^{\beta_e})$ to calculate the difference values for different volume concentrations of slurry, different downward forces and different rotational velocities. The paper also supposes that S_{vc_e} is a quadratic regression model $y = \beta_0 + \beta_1 x + \beta_2 x^2$. We use the calculated difference value to perform quadratic linear regression analysis under the condition of a fixed downward force. The paper once made quadratic linear regression analysis using the two ways of a fixed rotational velocity and a fixed down force, and then compares the R-square values of the regression equations.

We find that for the regressed compensatory equation under the condition of a fixed downward force, its R-square value and compensatory effect are both better than those of the regressed compensatory equation under the condition of a fixed rotational velocity. Therefore, the paper employs the condition of a fixed downward force to make quadratic linear regression analysis of the compensatory equation of S_{vc_e} with consideration of volume concentration of slurry. The regressed S_{vc_e} results are shown in Table 2, and the unit of S_{vc_e} is nm/min.

The purpose of $MRR_e = k_{p_e} P^{\alpha_e} V^{\beta_e} + S_{vc_e}$ equation is to more accurately calculate the average abrasive removal depth per minute of silicon wafer under different volume concentrations of slurry at room temperature, different downward forces and different rotational velocities in order to make it more close to the experimental value.

The paper makes calculation for the volume concentrations of slurry at 20%, 30%, 40% and 50%, achieving the regression results of $MRR_e = k_{p_e} P^{\alpha_e} V^{\beta_e} + S_{vc_e}$ as shown in Table 2. From the difference value of the new theoretical simulation results being close to the experimental results to the regression results of $MRR_e = k_{p_e} P^{\alpha_e} V^{\beta_e} + S_{vc_e}$, it is known that the difference value are all less than 0.18%. From here, we can find that the compensatory equation of S_{vc_e} not only can effectively improve calculation of the result to make the difference value at an acceptable range of below 1% for practical application, but also can be conveniently used for calculation with different volume concentrations of slurry, different downward forces and different rotational velocities.

From here, it is known that the $MRR_e =$

${k_p}_e P^{\alpha_e} V^{\beta_e} + S_{{vc}_e}$ equation for slurry at different volume concentrations is acceptable.

Finally, the paper also additionally focuses on the slurry's volume concentration 40%, down force 3psi and rotational velocity 60rpm to conduct CMP experiment, achieving an experimental abrasive removal depth value of 25.3047nm/min, whereas the average abrasive removal depth value per minute being close to the experimental result calculated from the paper's regression equation $MRR_e = {k_p}_e P^{\alpha_e} V^{\beta_e} + S_{{vc}_e}$ is 25.2832 nm/min. These two values of abrasive removal depth are quite close, further proving that the paper's new regression equation with the compensatory equation of $S_{{vc}_e}$ of average abrasive removal depth per minute being close to the experimental result is reasonable and acceptable.

Table 2 Regression equation $MRR_e = {k_p}_e P^{\alpha_e} V^{\beta_e} + S_{{vc}_e}$ of average abrasive removal depth per minute being close to the experimental result with different volume concentrations of slurry at room temperature and with consideration of compensation equation $S_{{vc}_e}$ for volume concentration of slurry

Volume concentration	Downward force	Regression equation $MRR_e = {k_p}_e P^{\alpha_e} V^{\beta_e} + S_{{vc}_e}$
50%	1psi	MRR_e=0.1504 $P^{1.0059}$ V^1 + (15.9796 - 31.9720x - 0.000000000043x^2)
	1.5psi	MRR_e=0.1504 $P^{1.0059}$ V^1 + (-367.6675 + 1419.6408x - 1368.5714x^2)
	2psi	MRR_e=0.1504 $P^{1.0059}$ V^1 + (-9.3762 + 18.7599x - 0.0000000000102x^2)
	2.5psi	MRR_e=0.1504 $P^{1.0059}$ V^1 + (-159.7693 + 661.6724x - 684.2857x^2)
	3psi	MRR_e=0.1504 $P^{1.0059}$ V^1 + (-309.5732 + 1303.4060x - 1368.5714x^2)
40%	1psi	MRR_e=0.1396 $P^{1.0059}$ V^1 + (9.2018 - 23.0160x - 0.0000000064x^2)
	1.5psi	MRR_e=0.1396 $P^{1.0059}$ V^1 + (-241.9450 + 1152.3194x - 1368.5714x^2)
	2psi	MRR_e=0.1396 $P^{1.0059}$ V^1 + (97.3315 - 517.0278x + 684.2857x^2)
	2.5psi	MRR_e=0.1396 $P^{1.0059}$ V^1 + (-217.3746 + 1090.8626x - 1368.5714x^2)
	3psi	MRR_e=0.1396 $P^{1.0059}$ V^1 + (-93.1814 + 506.6473x - 684.2857x^2)
30%	1psi	MRR_e=0.1316 $P^{1.0059}$ V^1 + (7.4536 - 24.8620x - 0.0000000032x^2)
	1.5psi	MRR_e=0.1316 $P^{1.0059}$ V^1 + (-137.9890+ 870.5673x - 1368.5714x^2)
	2psi	MRR_e=0.1316 $P^{1.0059}$ V^1 + (-6.7521 + 22.5222x - 0.0000000000224x^2)
	2.5psi	MRR_e=0.1316 $P^{1.0059}$ V^1 + (-57.9797 + 398.5429x - 684.2857x^2)
	3psi	MRR_e=0.1316 $P^{1.0059}$ V^1 + (1740.3819 - 11549.3075x + 19160x^2)
20%	1psi	MRR_e=0.1221 $P^{1.0059}$ V^1 + (59.9156 - 568.1924x + 1368.5714x^2)
	1.5psi	MRR_e=0.1221 $P^{1.0059}$ V^1 + (-37.3711 + 323.7622x - 684.2857x^2)
	2psi	MRR_e=0.1221 $P^{1.0059}$ V^1 + (1090.9335 - 10928.9257x + 27371.4286x^2)
	2.5psi	MRR_e=0.1221 $P^{1.0059}$ V^1 + (55.6524 - 551.9801x + 1368.5714x^2)
	3psi	MRR_e=0.1221 $P^{1.0059}$ V^1 + (63.8009 - 592.7635x + 1368.5714x^2)

CONCLUSION

The theoretical simulation model, regression analysis thory and experimental result analysis established by the paper for abrasive removal depth of silicon wafer of CMP with pattern-free polishing pad can achieve the following conclusions:

1. Regarding the abrasive removal depth of silicon wafer dipped in slurry at different volume concentrations, the greater the volume concentration, the deeper the abrasive removal depth. This is because there are more abrasive particles having polishing effect at the same time, so that the overall average abrasive removal depth of silicon wafer is greater.
2. The theoretical simulation results being close to the experimental result of the experimental average abrasive removal depth per minute are matched with regression analysis theory and the least square method, achieving the new regression equation under the parameters of different downward forces, rotational velocities and volume concentrations of slurry. Through quadratic regression analysis, the paper explores the regression compensation made for the difference caused by change in volume concentration of slurry, and achieves the compensatory parameter $S_{{vc}_e}$ with consideration of the volume concentration of slurry. When the parameter $S_{{vc}_e}$ is not considered, the difference value is quite great; but when consideration of the parameter $S_{{vc}_e}$ is added, the difference value is obviously smaller, and is close to the experimental result. From here, it is proved that the model established by the paper is reasonable.
3. The paper finds that after compensation by $S_{{vc}_e}$, the difference value is smaller, but the shortcoming is that its application needs to be under the condition of a fixed downward force, and hence, it is quite not ideal for use in practical application. As to application by industries, a difference value at below 1% is regarded as reasonable and acceptable. In order to let the result available for use conveniently under the conditions of different volume concentrations of slurry at room temperature, different downward forces and different rotational velocities, the paper suggests neglecting the compensation by $S_{{vc}_e}$, but taking $MRR_e = {k_p}_e P^{\alpha_e} V^{\beta_e}$ as a better regression equation since it is of higher practicality, and is more convenient for calculation of the close experimental value of abrasive removal depth per minute.

ACKNOWLEDGEMENT

The authors would like to thank the support from Ministry of Science and Technology, Taiwan. (MOST 108-2221-E-011-011-121)

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不同體積濃度研磨液之無花紋研磨墊化學機械拋光之研磨移除深度理論模擬及迴歸分析與實驗

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摘要

本研究考慮無花紋研磨墊之粗度峰表面與晶圓接觸面積為高斯分佈，且將矽晶圓浸泡在室溫下不同體積濃度研磨液後，再進行原子力顯微鏡實驗，計算得出浸泡室溫不同體積濃度研磨液的矽晶圓比下壓能值，再將這些值代入創新建立的不同體積濃度之無花紋研磨墊化學機械拋光的研磨移除深度理論模式。將模擬計算所得之每分鐘研磨移除深度值與 用無花紋研磨墊的化學機械拋光(CMP)實驗所得平均每分鐘研磨移除深度的結果相比較最後驗證理論模擬計算所得之結果為合理的。本研究進一步提出模擬與實驗所得結果的平均差異比例的修正觀念，使得補償修正後模擬所得之每分鐘研磨移除深度值將能更接近實驗的結果。本研究也建立室溫下考慮不同體積濃度研磨液，不同下壓力及轉速的不同體積濃度之無花紋研磨墊化學機械拋光的接近實驗的平均每分鐘研磨移除深度新的迴歸模式及公式，並完成加上不同體積濃度研磨液影響的補償迴歸公式與分析。