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Simulation and Single Regression Models of Average Abrasive Removal Depth Being Close to Experimental Value of CMP with Different Volume Concentrations and Diameters of Abrasive Particles of Slurry and Experiments

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ABSTRACT

The paper establishes a theoretical simulation model of abrasive removal depths of silicon wafer under chemical mechanical polishing (CMP) by a pattern-free polishing pad with different volume concentrations of slurry and different diameters of abrasive particles. The paper firstly obtains specific downward force energy ($SDFE_{reaction}$) values of silicon wafer under different volume concentrations of slurry. Furthermore, the paper uses the $SDFE_{reaction}$ value to obtain the theoretical simulation value of the abrasive removal depths per minute of silicon wafer obtained under different volume concentrations of slurry, different diameters of abrasive particles, different downward forces and different rotational velocities. The paper compares the theoretical simulation values of the respective abrasive removal depth per minute of silicon wafer under CMP with the results of 8 experiments under different volume concentrations of slurry at room temperature and different diameters of abrasive particles, and then calculates the ratio of mean difference, which is found to be around 4.2%. Then the value of the ratio of mean difference is used to obtain the average abrasive removal depths per minute being close to the experimental values, under different volume concentrations of slurry, different diameters of abrasive particles, different downward forces and different rotational velocities, and uses these values as the input values, to establish a regression equation $MRR_e = k_{p_e} P^{\alpha_e} V^{\beta_e}$ where α_e and β_e are different constants. This paper uses the different k_{p_e} values as the input values for regression, obtaining the regression equation of $k_{p_e}(x, y)$, where x denotes the volume concentration of slurry, and y denotes the diameter of abrasive particles. Therefore, the paper establishes a regression equation of the average abrasive removal depth per minute $MRR_e = k_{p_e}(x, y) P^{\alpha_e} V^{\beta_e}$ being close to the experimental value. Finally, the paper carries out a new experiment to prove that the regression equation $MRR_e = k_{p_e}(x, y) P^{\alpha_e} V^{\beta_e}$ is reasonable and practical.

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INTRODUCTION

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. 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. 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. Kim and Jeong (2004) studied and analyzed the relative velocity of polishing velocity, and derived the relative abrasive length at each position on wafer to polishing pad. Lin et al. (2008) established a new theoretical model of abrasive removal depth of the sapphire wafer abraded and cut by CMP when the polishing pad had a checkered pattern. 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. Finally, they used statistical concept to develop a description way of the surface contact mechanics of the contact situation between two surfaces, being geographically-weighted/GW model; and this was the foundation of contact mechanics for development in the later days. In 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 in the reference 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. Lin et al. (2022) developed the regression equations of the abrasive removal depth of silicon wafer of different temperature and volume concentrations of slurry for CMP. Their k_p in the regression equation did not show as the function of temperature and volume concentration of slurry.

In the above literature, there is no in-depth exploration for establishment of theoretical model, experiment, regression equation $\mathrm{MRR_e} = \mathrm{k_{p_e}}(x,y)\mathrm{P}^{\alpha_e}\mathrm{V}^{\beta_e}$ of the average abrasive removal depth per minute being close to the experimental value of silicon wafer with different volume concentrations of slurry, x, and different diameters of abrasive particles , y, during CMP by a pattern-free polishing pad.

EXPERIMENTAL PRINCIPLES

The paper conducts a conventional CMP experiment that uses SiO_2 abrasive particles to polish 2-inch silicon wafers. The machine used is Logitech Company's PM-5 polisher, which is located in the Precision Manufacturing Laboratory of the National Taiwan University of Science and Technology, Taiwan. The polishing pad used is the pattern-free Rodel IC-1000. The slurry used is the one produced by Ellipsiz Inetest Co., Ltd. In the slurry there are SiO_2 abrasive particles provided by Sun Chion Co., Led., with their diameters being 50nm and 20nm; and the volume concentration of the slurry is 50%.

The paper uses electronic precision balance to measure the weight of wafer before polishing, and then deducts the weight before polishing from the weight after polishing in order to obtain the experimental value of abrasive removal weight. After dividing the abrasive removal weight by the density of silicon wafer, the abrasive removal volume can be known. Then, after dividing the abrasive removal volume by the area of silicon wafer, the average abrasive removal depth can be acquired. In each experiment, polishing is carried out for 20 minutes, and then the paper finds the experimental value of average abrasive removal depth per minute.

THEORETICAL SIMULATION AND EXPERIMENTAL METHOD OF SPECIFIC DOWNWARD FORCE ENERGY OF SILICON WAFER UNDER DIFFERENT VOLUME CONCENTRATIONS OF SLURRY

First of all, the paper soaks the silicon wafer in slurry with different volume concentrations at room temperature for 30 minutes to make silicon wafer produce a chemical reaction layer. This study uses a smaller downward force to make the cutting depth of the V-shaped groove smaller than 0.09nm, then be calculates the $\mathrm{SDFE_{reaction}}$ value inside the chemical reaction layer of silicon wafer soaked in slurry with different volume concentrations.

Regarding the control of volume concentration of slurry, since the volume concentration of slurry is defined as the ratio of the volume of the slurry to the volume of all abrasive particles contained in a unit slurry, this definition can be used to calculate how much deionized water has to be added to prepare a slurry with the specified volume concentration. Hence, the paper adds deionized water to the slurry with volume concentration 50%, achieving 3 kinds of prepared slurry with volume concentrations 40%, 30% and 20%.

Therefore, the paper's $\mathrm{SDFE_{reaction}}$ inside the chemical reaction layer of silicon wafer soaked in slurry with different volume concentrations is defined by the product of multiplying the cutting depth by the downward force of the cutting tool of probe applied onto the silicon wafer workpiece being soaked in slurry with different volume concentrations. It refers to the quotient after dividing the energy produced in the machining process by the volume of the workpiece removed by the downward force of the cutting tool, as shown in equation (1):(Lin et al., 2018)

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

where $\mathrm{F_d}$ denotes the downward force of cutting tool applied onto the workpiece; Δd denotes the cutting depth; and ΔV denotes the workpiece volume removed by the downward press of cutting tool.

From moving of cutting tool to machining of groove, the depth in the middle area gradually inclines to be a fixed cutting depth. As to the volume removed by the moving cutting tool with downward force, due to machining in the aforesaid process, the volume of the distance of the radius R behind the cap of workpiece being cutted 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:

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

where R denotes the tip radius of the cutting tool of probe, and Δd denotes the cutting depth. The diameter of tip of probe is 150nm in this study

After referring to the paper of Jhang (2015), and after soaking the single-crystal silicon wafer substrate in slurry with different volume concentrations, the paper obtains the $SDFE_{reaction}$ values inside the thickness of the layer under chemical reaction of slurry. It obtains that when the slurry temperature is 23℃, volume concentrations 20%, 30%, 40% and 50% of slurry, $SDFE_{reaction}$ are 0.016772 $\mu N \cdot nm / nm^3$, 0.016438 $\mu N \cdot nm / nm^3$, 0.016352 $\mu N \cdot nm / nm^3$ and 0.016208 $\mu N \cdot nm / nm^3$ respectively.

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

In the research 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. In order to use pattern-free polishing pad under this model, this paper divides the silicon wafer into 2,029 elements, with each element in the size of 1mm*1mm. When the silicon wafer is rotating, each element will have continuous relative turning contacts with the pattern-free polishing pad. The 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 silicon wafer.

According to the paper of Qina et al. (2004), the effective contact area A_{rs} and the downward force F are shown in equation (3) and equation (4) respectively. In this paper the effective contact area of each element of silicon wafer is A_{rs}, and the downward force F borne by each element is $F = \frac{F_{total}}{n}$, where F_{total} denotes the total downward force of CMP machine, and n denotes the number of the divided elements of silicon wafer.

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

$$F = \frac{4}{3}\eta A_0 E^* \beta^{\frac{1}{2}} \int_h^\infty (z-h)^{\frac{3}{2}}\phi(z)dz \quad (4)$$

$$\phi(z) = \frac{1}{\sigma\sqrt{2\pi}}\exp(-\frac{z^2}{2\times\sigma^2}) \quad (5)$$

A_0: area of each element of silicon wafer

η: areal density of the asperity peak of polishing pad

E^*: equivalent Young's modulus

$$E^* = \frac{1-\nu_p{}^2}{E_p} + \frac{1-\nu_w{}^2}{E_w} \quad (6)$$

E_p: Young's modulus of polishing pad

E_w: Young's modulus of silicon wafer

ν_p: Poisson's ratio of polishing pad

ν_w: Poisson's ratio of silicon wafer

Using equations (3) and (4), the paper obtains the following equation:

$$\frac{A_{rs}}{F} = \frac{3\pi\beta^{\frac{1}{2}}}{4E^*}\frac{\int_h^\infty (z-h)\phi(z)dz}{\int_h^\infty (z-h)^{\frac{3}{2}}\phi(z)dz} \quad (7)$$

The function for the height distribution of asperity peak is equation (5), which is substituted in equation (7). Numerical integration, as shown in Johnson's paper (1985), is employed to integrate equation (7). Since the ratio of two integrals is approximately a constant for h/σ within a range, equation (8) can be obtained as follows:

$$A_{rs} = C^{-1}(\frac{\beta}{\sigma})^{\frac{1}{2}}\frac{F}{E^*} \quad (8)$$

In equation (8), C is a constant. In the paper of Yu et al. (1993), the constant was derived and calculated. As known from Johnson's paper (1985), the ratio h/σ of polishing pad is generally between 0.5 and 3.0. 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's paper (1985) are made by the same company and of similar model number. Therefore, for the variables of equation (8), the paper refers to the β and σ values in Johnson's paper (1985).

After dividing the total downward force F_{total} of CMP machine by the number of silicon wafer elements, n, the downward force borne by each element is $F=F_{total}/n$. Then the paper uses equation (8) to calculate the contact area (A_{rs}) between the asperity of polishing pad and each silicon wafer element.

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

$$V_{w/p} = \omega_p D_{wp}\sqrt{(\rho\zeta)^2 + 2\rho\zeta\cos\phi + 1} \quad (9)$$

Here, $\rho = \frac{r}{R_w}$, $\zeta = \frac{R_w}{D_{wp}}(1-R)$, $R = \frac{\omega_w}{\omega_p}$, $\phi = \omega_w t$, where R_w denotes the radius of wafer, ω_w denotes the rotational velocity of wafer, ω_p denotes the rotational velocity of polishing pad, and D_{wp} denotes the distance between the center of wafer and the center of polishing pad. Therefore, when the silicon wafer and the polishing are at the same rotational velocity, $\omega_w = \omega_p$, $\zeta = 0$; and then $V_{w/p} = \omega_p D_{wp}$. And as mentioned in the paper of Kim and Jeong (2004), when $\omega_w = \omega_p$, and after a period of time t, the actual relative abrasive length of wafer and polishing at each position P is $\omega_p D_{wp} t$. Therefore, if t is one minute, the actual relative abrasive length per minute at each position P on wafer surface is $\omega_p D_{wp}$.

In this paper, we set the central position of each element of silicon wafer to be at the aforesaid 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 can achieve the relative number of polishing times FF per unit time for the contact between each element and polishing pad. Therefore, $FF = \frac{\omega_p D_{wp}}{L_e}$.

The paper lets the size of each element of silicon wafer be 1mm*1mm; and hence, L_e = 1mm.

Right now, the wafer's surface volume (Vol) that can be removed by each abrasive particle per unit time is expressed as the following equation:

$$Vol = A_p * \ell \tag{10}$$

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

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

$$\ell = \omega_p D_{wp} \tag{11}$$

where

$$A_p \approx \frac{1}{2} \cdot \delta_{aw} \cdot 2r_a \approx \delta_{aw}\sqrt{\delta_{aw} D} \tag{12}$$

D denotes the average diameter of abrasive particles.

Besides, if N_e denotes the number of effective abrasive particles of each wafer element, and the unit volume concentration of the 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 in slurry per unit volume. Since the length of each wafer element is 1mm, the number of effective abrasive particles of effective contact area of a single element is (Zhao and Chang, 2002):

$$N_e = A_{rs} \cdot \left(\frac{6\chi}{\pi D^3}\right)^{2/3} = C^{-1}(\frac{\beta}{\alpha})^{\frac{1}{2}} \frac{F}{E^*} (\frac{6\chi}{\pi D^3})^{2/3} \tag{13}$$

where A_{rs} denotes the effective contact area between the asperity peak of polishing pad and the surface of each wafer element, being the interface between single element's position and polishing pad.

The paper proposes a supposition that the downward force borne by each wafer element is: $F = F_{total}/n$. Here, F_{total} denotes the total downward force for the polishing pad of CMP machine; n denotes the number of the divided wafer elements on the contact surface 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:

$$F_{aw} = \frac{F_{total}}{n \times N_e} \tag{14}$$

The total downward force F_{total} of polishing pad in pressing downward to wafer can be measured and known by the CMP machine for experiments. Equation (13) can be used to obtain N_e, and hence, F_{aw} can also be subsequently obtained. After substituting the downward force F_{aw} between a single abrasive particle and wafer surface in the $SDFE_{reaction}$ equation (1) of silicon wafer soaked in slurry with different volume concentrations, the abrasive removal depth Δd of a single abrasive particle on wafer surface can be achieved:

$$\Delta d = \frac{\Delta V \times SDFE_{reaction}}{F_{aw}} \tag{15}$$

Substitute equation (2)'s $\Delta V = \frac{1}{2}\pi \times (\Delta d)^2 \times (R - \frac{\Delta d}{3})$ in equation (15) to obtain equation (16):

$$\Delta d = \frac{\frac{1}{2}\pi \times (\Delta d)^2 \times (R - \frac{\Delta d}{3}) \times SDFE_{reaction}}{F_{aw}} \tag{16}$$

where R denotes the radius of abrasive particle.

The paper further substitutes equation (14) in equation (16) to find the innovative abrasive depth δ_{aw} removed by a single abrasive particle from the wafer surface:

$$\Delta d = \frac{3R - (9R^2 - \frac{24 \times \frac{F_{total}}{n \times N_e}}{\pi \times SDFE_{reaction}})^{\frac{1}{2}}}{2} = \delta_{aw} \tag{17}$$

Substitute the obtained δ_{aw} in equatio (12) and equation (10) to acquire the effective removal volume of a single abrasive particle of a single element from the wafer surface per unit time: $Vol = \delta_{aw}\sqrt{\delta_{aw} D} \times \ell$.

Besides, based on equation (11), $\ell = \omega_p D_{wp}$, the following is achieved:

$$Vol = \delta_{aw}\sqrt{\delta_{aw} D} \times \omega_p D_{wp} \tag{18}$$

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

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

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

$$\delta_{\Delta t} = \frac{V_{\Delta t}}{A_0} \tag{20}$$

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

$$V_{Vol} = V_{\Delta t} \times n = Vol \times N_e \times n \tag{21}$$

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

$$d_{ab} = \frac{V_{Vol}}{A_w} = \frac{Vol \times N_e \times n}{\pi R_w^2} \quad (22)$$

where A_w is the area of wafer and R_w denotes the radius of silicon wafer. After rearrangement the above equations, the following equation is obtained:

$$d_{ab} = \frac{\delta_{aw}\sqrt{\delta_{aw}D} \times \omega_p D_{wp} \times A_{rs} \cdot \left(\frac{6\chi}{\pi D^3}\right)^{2/3} \times n}{\pi R_w^2} \quad (23)$$

In equation (23), F_{total} can be known from measurement by CMP machine. The $SDFE_{reaction}$ value of the chemical reaction layer of silicon wafer soaked in slurry with 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 diameters D of abrasive particles are known to be 50mnm and 20nm, so that the radiuses R of abrasive particles are 25nm and 10nm. The number n of the divided 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 (23), the paper can derive an innovative theoretical equation of abrasive removal depth per unit time of minute of silicon wafer under CMP by a pattern-free polishing pad and being affected by slurry with different volume concentrations and different diameters of abrasive particles, as shown in equation (23), which is of academic innovativeness.

In the experiment, CMP of silicon wafer is performed repeatedly for 5 times. For the experiment performed each time, silicon wafer is polished for 20 minutes, achieving the average abrasive removal depth of silicon wafer per minute of the experiments done for 5 times. Under the same conditions, and using the foregoing already derived theoretical equation of abrasive removal depth of silicon wafer per unit time of minute, the paper simulates calculation of the abrasive removal depth d_{ab} per minute.

REGRESSION EQUATION OF AVERAGE ABRASIVE REMOVAL DEPTH PER MINUTE BEING CLOSE TO THE EXPERIMENTAL VALUE OF SILICON WAFER UNDER CMP WITH DIFFERENT VOLUME CONCENTRATIONS AND DIFFERENT DIAMETERS OF ABRASIVE PARTICLES OF SLURRY

The paper substitutes the $SDFE_{reaction}$ value of the chemical reaction layer of silicon wafer obtained from soaking silicon wafer in slurry with different volume concentrations, and the diameter of abrasive particles in slurry in equation (17), to obtain δ_{aw}. Furthermore, using equation (23), the paper can obtain the simulation calculated abrasive removal depth per minute d_{ab} of silicon wafer. After that, the paper compares the simulation calculated results under CMP by a pattern-free polishing pad with different volume concentrations of slurry at room temperature, different diameters of abrasive particles in slurry, different downward forces and different rotational velocities, with the experimental results of abrasive removal depth per minute of silicon wafer under different volume concentrations of slurry at room temperature, different diameters of abrasive particles in slurry, different downward forces and different rotational velocities, thus acquiring the equation of the ratio of difference between simulation and experimental results, as shown in the following equation:

$$\text{Ratio of differnece} = \frac{\text{Simulation calculated abrasive removal depth per minute} - \text{Experiment calculated abrasive removal depth per minute}}{\text{Simulation calculated abrasive removal depth per minute}} \quad (24)$$

The paper finds that the value of such a ratio of difference is within a certain range, and the change is not too great. Therefore, using the value of individual ratio of difference of silicon wafer under polishing with different volume concentrations of slurry at room temperature and different diameters of abrasive particles in slurry, the paper obtains the ratio of mean difference. Therefore, using this value of ratio of mean difference, it can make compensatory modification of the simulation calculated abrasive removal depth per minute of silicon wafer under CMP by a pattern-free polishing pad with different volume concentrations of slurry and different diameters of abrasive particles, and achieve the average abrasive removal depth per minute that is close to the experimental value. Therefore, from equation (24), it can derive an equation for calculation of the average abrasive removal depth per minute being close to the experimental value, as shown in equation (25).

Average abrasive removal depth per minute being close to the experimental value
= Simulation calculated abrasive removal depth per minute – (Simulation calculated abrasive removal depth per minute × Ratio of mean difference) (25)

For the simulation calculated abrasive removal depth per minute of silicon wafer under different downward forces, different rotational velocities, different volume concentrations of slurry at room temperature and different diameters of abrasive particles, the paper further uses the method of the ratio of mean difference to find the average abrasive removal depth per minute being close to the experimental value. Furthermore, the paper takes the average abrasive removal depth per minute being close to the experimental value, obtained by using the method of the ratio of mean difference, under different downward forces, different rotational velocities, different volume concentrations of slurry at room temperature and different diameters of abrasive particles in slurry, as the input value for regression analysis, so as to conduct regression analysis, and find the regression equations of the average abrasive removal depth per minute being close to the experimental value, $\mathrm{MRR_e} = \mathrm{k_{p_e}} \mathrm{P}^{\alpha_e} \mathrm{V}^{\beta_e}$. Because the obtained regression equations $\mathrm{MRR_e} = \mathrm{k_{p_e}} \mathrm{P}^{\alpha_e} \mathrm{V}^{\beta_e}$, the α_e in a constant and β_e is a another constant, only $\mathrm{k_{p_e}}$ is change. Therefore, if x is the volume concentration of slurry and y is the diameter of abrasive particle, the study uses obtained different $\mathrm{k_{p_e}}$ values as the input data to obtains the regression equation of $\mathrm{k_{p_e}}(x, y)$, and get $\mathrm{MRR_e} = \mathrm{k_{p_e}}(x, y) \mathrm{P}^{\alpha_e} \mathrm{V}^{\beta_e}$.

SIMULATION RESULTS AND EXPERIMENTAL RESULT OF SILICON WAFER UNDER CMP, AS WELL AS REGRESSION ANALYSIS RESULTS AND DISCUSSION OF AVERAGE ABRASIVE REMOVAL DEPTH PER MINUTE BEING CLOSE TO EXPERIMENTAL VALUE

The paper substitutes the parameters of different volume concentrations 20%, 30%, 40% and 50% of slurry and different diameters of abrasive particles 20nm, 30nm, 40nm and 50nm in the theoretical simulation equation for calculation. Such simulation calculation is made under different downward forces 3 psi, 2.5 psi, 2 psi, 1.5 psi and 1 psi, as well as different rotational velocities 20rpm, 30rpm, 40rpm, 50rpm and 60rpm. Then the paper achieves the simulation calculated results of abrasive removal depth per minute d_{ab} of the theoretical model in combination of different parameters, including the aforesaid room-temperature slurry, different volume concentrations of slurry, different diameters of abrasive particles in slurry, different downward forces and different rotational velocities.

The paper uses the theoretical simulation equation to calculate the abrasive removal depth per minute d_{ab}. With the results calculated from the theoretical simulation and with the experimental results, the paper uses the method of analyzing the equation of the ratio of difference between the theoretical simulation results and the experimental results, to find the ratio of mean difference. With this ratio of mean difference, the paper uses the theoretical simulation results to calculate the abrasive removal depth per minute being close to the experimental value. Therefore, we can use this method to decrease the number of times of experiment, and then find the simulation calculated abrasive removal depth per minute under different downward forces, different rotational velocities, different volume concentrations of slurry at room temperature and different diameters of abrasive particles in slurry.

The paper takes 8 groups of experiments of silicon wafer under CMP by a pattern-free polishing pad with slurry at room temperature, different diameters of abrasive particles and different volume concentrations, different downward forces and different rotational velocities: (1) 50nm, 20%, 3psi, 60rpm; (2) 50nm, 30%, 3psi, 60rpm; (3) 50nm, 40%, 2psi, 40rpm; (4) 50nm, 50%, 2psi, 40rpm; (5) 20nm, 20%, 3psi, 60rpm; (6) 20nm, 20%, 3psi, 60rpm; (7) 20nm, 30%, 3psi, 60rpm; and (8) 20nm, 40%, 2psi, 40rpm. The paper compares the theoretical simulation results of abrasive removal depth d_{ab} of silicon wafer under CMP by a pattern-free polishing pad with different diameters of abrasive particles in slurry at room temperature and different volume concentrations of slurry, with the results of abrasive removal depth of the 8 groups of CMP experiments aforesaid.The paper calculates the theoretical simulation value of the respective abrasive removal depth per minute of silicon wafer under CMP in the aforesaid 8 groups of experiments .

From the aforesaid 8 experimental values of silicon wafer under CMP with different diameters of abrasive particles in slurry at room temperature, different volume concentrations of slurry, different downward forces and different rotational velocities, the paper finds the ratio of mean difference value between them, which is around 4.2%. Under different volume concentrations of slurry, different diameters of abrasive particles in slurry, different downward forces and different rotational velocities, and according to equation (25) that the average abrasive removal depth per minute being close to the experimental value = simulation calculated abrasive removal depth per minute – (simulation calculated abrasive removal depth per minute × ratio of mean difference), the paper subtracts the “simulation calculated abrasive removal depth per minute × ratio of mean difference 4.2%” from the theoretical simulation result of abrasive removal depth per minute, achieving the average abrasive removal depth per minute being close to the experimental value. For example, Table 1 shows the simulation results of average abrasive removal depth per minute being close to the experimental value of the modified theoretical model under volume concentration 20% of slurry, diameter 20nm of abrasive particles in slurry, different downward forces and different rotational velocities.

The paper takes some conditions for example, including volume concentration 20% of slurry, diameter 20nm of abrasive particles in slurry, different downward forces 1psi, 1.5psi, 2psi, 2.5psi, 3psi, and different rotational velocities 20rpm, 30rpm, 40rpm, 50rpm, 60rpm, and then uses the modified theoretical simulation value of the average abrasive removal

Table 1 Simulation results of average abrasive removal depth per minute (unit: nm/min) being close to the experimental value of the modified theoretical model under volume concentration 20% of slurry, diameter 20nm of abrasive particles in slurry, different downward forces and different rotational velocities

Downward force / Rotational velocity	1 psi	1.5 psi	2 psi	2.5 psi	3 psi
20 rpm	4.1629	6.2866	8.3828	10.4795	12.5753
30 rpm	6.2443	9.4299	12.5742	15.7192	18.8629
40 rpm	8.3257	12.5732	16.7656	20.9590	25.1506
50 rpm	10.4071	15.7165	20.9570	26.1987	31.4382
60 rpm	12.4886	18.8597	25.1485	31.4385	37.7258

depth per minute being close to the experimental value = simulation calculated abrasive removal depth per minute – (simulation calculated abrasive removal depth per minute × ratio of mean difference), and takes the obtained modified new theoretical simulation results of average abrasive removal depth per minute being close to the experimental value, as the input values of the new regression equation, acquiring the regression equation MRR_e=0.1221 $P^{1.0059}V^1$. The unit of abrasive removal depth is nm/min; the R-square value of the regression equation is 0.999992; the average residual is -0.000002; k_{p_e} is 0.1221; and the values of α_e and β_e are 1.0059 and 1 respectively. As shown in Table 2, both the R-square values and the average residuals meet the standards.

The paper uses the least square method to conduct regression analysis of the modified theoretical simulation results of average abrasive removal depth per minute being close to the experimental values under CMP by a pattern-free polishing pad with diameter 20nm of abrasive particles in slurry, different volume concentrations 20%, 30%, 40%, 50% of slurry, different downward forces and different rotational velocities, to conduct regression analysis, obtaining the regression equations shown in Table 2.

Using the equations of $MRR_e = k_{p_e}P^{\alpha_e}V^{\beta_e}$ shown in Table 2, the paper calculates different volume concentrations 20%, 30%, 40%, 50% of slurry to obtain the regression results of $MRR_e = k_{p_e}P^{\alpha_e}V^{\beta_e}$ under the diameter 20nm of abrasive particles in slurry, different volume concentrations 20%, 30%, 40%, 50% of slurry, different downward forces and different rotational velocities.

Not only using the regression analysis method aforesaid, the paper, focusing on different diameters 30nm, 40nm, 50nm of abrasive particles in slurry and different volume concentrations 20%, 30%, 40%, 50% of slurry, also uses the average abrasive removal depths per minute being close to the experimental

Table 2 Regression equations $MRR_e = k_{p_e}P^{\alpha_e}V^{\beta_e}$ under diameter 20nm of abrasive particles in slurry, different volume concentrations of slurry, different downward forces and different rotational velocities

Volume concentration of slurry	Regression equation $MRR_e = k_{p_e}P^{\alpha_e}V^{\beta_e}$
20%	MRR_e=0.2085 $P^{1.0059}V^1$
30%	MRR_e= 0.2247$P^{1.0059}V^1$
40%	MRR_e= 0.2384$P^{1.0059}V^1$
50%	MRR_e= 0.2567$P^{1.0059}V^1$

values, obtained under the conditions of different downward forces and different rotational velocities, and employs the least square method to conduct regression analysis, achieving the regression results of $MRR_e = k_{p_e}P^{\alpha_e}V^{\beta_e}$.

When the paper uses the least square method to conduct regression analysis of the results of average abrasive removal depth per minute being close to the experimental values of silicon wafer under CMP by a pattern-free polishing pad with different volume concentrations of slurry, different diameters of abrasive particles, different downward forces and different rotational velocities, the paper finds that for the regression equation of the average abrasive removal depth per minute being close to the experimental value under different volume concentrations of slurry, different diameters of abrasive particles, different downward forces and different rotational velocities, the values of α_e and β_e are all 1.0059 and 1 respectively, only that the k_{p_e} values change with different volume concentrations of slurry and different diameters of abrasive particles. For the various equations of $MRR_e = k_{p_e}P^{1.0059}V^1$ obtained from regression, the k_{p_e} values are shown in Table 3 below.

Table 3 k_{p_e} values under different volume concentrations of slurry and different diameters of abrasive particles

Volume Concentration of slurry / Diameter of abrasive particle	20%	30%	40%	50%
20nm	0.2085	0.2247	0.2384	0.2567
30nm	0.1707	0.1839	0.1984	0.2101
40nm	0.1431	0.1535	0.1635	0.1761
50nm	0.1221	0.1316	0.1396	0.1504

Therefore, the paper proposes the regression equation $k_{p_e}(x, y)$ under different volume concentrations of slurry, x, and different diameters of abrasive particles, y. Let $k_{p_e}(x,y)$ be a quadratic regression model $k_{p_e}(x,y) = z = \beta_{0_{kp_e}} + \beta_{1_{kp_e}}x + \beta_{2_{kp_e}}y + \beta_{3_{kp_e}}x^2 + \beta_{4_{kp_e}}y^2 + \beta_{5_{kp_e}}xy$. For these different volume concentrations of slurry that x = 20%, 30%, 40%, 50%, and different diameters of abrasive particles that y = 20nm, 30 nm, 40nm, 50 nm, the paper uses the least square method conducts regression analysis of the various k_{p_e} values in Table 3. The acquired regression equation is $k_{p_e}(x,y) = 0.2742 + 0.1822x - 0.005612y + 0.02562x^2 + 0.00004543y^2 - 0.002199xy$. The R-square value is 0.99965, and the average residual is -0.00006.

The paper also analyzes the percentage difference between the theoretical simulation results of average abrasive removal depth per minute being close to the experimental value after modification and the regression results of $MRR_e = k_{p_e}(x,y)P^{\alpha_e}V^{\beta_e}$, achieving a percentage difference being less than 0.67%. As known from this, the regression equation $MRR_e = (0.2742 + 0.1822x - 0.005612y + 0.02562x^2 + 0.00004543y^2 - 0.002199xy)\mathbf{P}^{1.0059}\mathbf{V}^1$ under different volume concentrations of slurry, different diameters of abrasive particles in slurry, different downward forces and different rotational velocities, is reasonable and acceptable.

Table 4 shows the regression results of average abrasive removal depth per minute, being close to the experimental values, of $MRR_e = (0.2742 + 0.1822x - 0.005612y + 0.02562x^2 + 0.00004543y^2 - 0.002199xy)P^{1.0059}V^1$, under volume concentration 20% of slurry, diameter 20nm of abrasive particles in slurry, different downward forces and different rotational velocities

Table 4 Regression results of average abrasive removal depth per minute (unit: nm/min), being close to the experimental values, of $\mathbf{MRR_e} = (0.2742 + 0.1822x - 0.005612y + 0.02562x^2 + 0.00004543y^2 - 0.002199xy)\mathbf{P}^{1.0059}\mathbf{V}^1$, under volume concentration 20% of slurry, diameter 20nm of abrasive particles in slurry, different downward forces and different rotational velocities

Downward force / Rotational velocity	1 psi	1.5 psi	2 psi	2.5 psi	3 psi
20 rpm	4.1770	6.2805	8.3883	10.4992	12.6125
30 rpm	6.2655	9.4208	12.5824	15.7487	18.9188
40 rpm	8.3540	12.5611	16.7765	20.9983	25.2251
50 rpm	10.4426	15.7013	20.9707	26.2479	31.5314
60 rpm	12.5311	18.8416	25.1648	31.4975	37.8376

Finally, in order to prove the regression equation $MRR_e = k_{p_e}(x,y)P^{\alpha_e}V^{\beta_e}$ of the average abrasive removal depth per minute being close to the experimental value after modification, the paper additionally carries out a new experiment with diameter of abrasive particle 20nm, volume concentration of slurry 20%,downward force 2.5psi and rotational velocity 50rpm at 23°C, which is not in the cases of ratio difference analysis. The paper makes comparison between the values calculated from the regression equation $MRR_e = k_{p_e}(x,y)P^{\alpha_e}V^{\beta_e}$ of the average abrasive removal depth per minute being close to the experimental value after modification and a new experimental result. The percentage difference between the regression results of $MRR_e = k_{p_e}(x,y)P^{\alpha_e}V^{\beta_e}$ and new experimental result is 0.22%, thus proving the rationality and practicality of the regression equation aforesaid.

CONCLUSION

The paper establishes a theoretical simulation model of abrasive removal depths of silicon wafer under CMP by a pattern-free polishing pad with different diameters of abrasive particles and different volume concentrations of slurry. $SDFE_{reaction}$ values are substituted in an innovatively established theoretical model of abrasive removal depth per minute of silicon wafer under CMP by a pattern-free polishing pad with different diameters of abrasive particles and different volume concentrations of slurry.

The paper firstly carries out 8 groups of CMP experiments under different volume concentrations of slurry, different downward forces and different rotational velocities, and calculates the theoretical simulation value d_{ab} of the respective abrasive removal depth per minute of silicon wafer under CMP with different volume concentrations of slurry at room temperature as well as the experimental value of average abrasive removal depth per minute, and then calculates the ratio of mean difference between them, which is around 4.2%. After subtracting the theoretical simulation values at the ratio of mean difference 4.2% from all the theoretical simulation values, the paper achieves the values of average abrasive removal depth per minute MRR_e being close to the experimental value. Furthermore, the paper conducts regression analysis of those values to obtain a regression equation $MRR_e = k_{p_e}P^{\alpha_e}V^{\beta_e}$ of the average abrasive removal depth per minute being close to the experimental value under a fixed diameter of abrasive particles and a fixed volume concentration of slurry. As found in the values of k_{p_e}, α_e and β_e of the equation obtained from regression, under different diameters of abrasive particles in slurry and different volume concentrations of slurry, only k_{p_e} is changed, and the values of α_e and β_e are fixed and unchanged. Therefore, the paper further conducts regression analysis of the k_{p_e} value under different volume concentrations x of slurry and different diameters y of abrasive particles, acquiring $k_{p_e}(x, y)$ under different volume concentrations x of slurry and different diameters y of abrasive particles. After substituting, the paper achieves the regression equation $MRR_e = k_{p_e}(x, y)P^{\alpha_e}V^{\beta_e} = (0.2742 + 0.1822x - 0.005612y + 0.02562x^2 + 0.00004543y^2 - 0.002199xy)\mathbf{P}^{1.0059}\mathbf{V}^{1}$.

After comparing the regression results of $MRR_e = k_{p_e}(x, y)P^{\alpha_e}V^{\beta_e}$ with a new experimental result, the paper finds that the difference in between is less than 1%, proving that this regression equation is reasonable and acceptable. Besides, $MRR_e = k_{p_e}(x, y)P^{\alpha_e}V^{\beta_e}$ can be regarded as a better regression equation with high practicality for easier calculation of the experimental value of the abrasive removal depth per minute.

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不同研磨液體積濃度及不同研磨顆粒直徑之化學機械拋光之接近實驗之平均研磨移除深度之模擬及單一迴歸模式和實驗

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摘要

本研究先建立不同研磨液體積濃度及不同研磨顆粒直徑之無花紋研磨墊化學機械拋光矽晶圓的研磨移除深度理論模擬模式。其先求出常溫下不

同體積濃度研磨液之比下壓能值。並建立室溫下不同研磨液體積濃度及不同研磨顆粒直徑之化學機械拋光矽晶圓的各別每分鐘研磨移除深度理論模擬模式，求出理論模擬值與 8 組實驗之平均每分鐘研磨移除深度值，再計算其平均差異比例值約為 4.2%。進一步應用差異比例值計算出不同研磨液體積濃度及不同研磨顆粒，不同下壓力及不同轉速之計算所得之接近實驗之平均每分鐘研磨移除深度，且將其當輸入值，建立$MRR_e = k_{p_e} P^{\alpha_e} V^{\beta_e}$迴歸公式。本研究將室溫下，不同研磨液體積濃度，不同研磨顆粒直徑，不同下壓力及不同轉速所得之不同k_{p_e}值，當輸入值，迴歸出$k_{p_e}(x, y)$的迴歸公式，在此x為研磨液體積濃度，y為研磨顆粒直徑，因此本研究建立接近實驗之平均每分鐘研磨移除深度的迴歸公式$MRR_e = k_{p_e}(x, y) P^{\alpha_e} V^{\beta_e}$，用此單一迴歸公式，可計算出接近實驗之平均每分鐘研磨移除深度實驗值。最後本研究另外進行不在前面做差異比例值分析實驗案例中的新的實驗，將新的實驗所得每分鐘研磨移除深度值與迴歸公式$MRR_e = k_{p_e}(x, y) P^{\alpha_e} V^{\beta_e}$計算所得之接近實驗之每分鐘研磨移除深度值進行比較後，發現其差異很小，由此可驗證迴歸公式$MRR_e = k_{p_e}(x, y) P^{\alpha_e} V^{\beta_e}$為合理且實用。