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Using Inverse Method to Establish Simulation Calculation Method of Surface Morphology of the Polished Silicon Wafer and Experimental Verification

Zone-Ching Lin*, Yih-Lin Cheng **, Yan-Yu Chen **,
Bei-Chen Kuo **and You-Cheng Lin **

Keywords: silicon wafer, abrasive removal depth, inverse method surface morphology, chemical mechanical polishing

ABSTRACT

The paper proposes using the specific downward force energy ($SDFE_{reaction}$) value of silicon wafer soaked in room-temperature slurry. After CMP machine performs CMP of silicon wafer at room temperature, the paper combines gravimetric method with conjugate foci method of laser scanning confocal microscope (LSCM) to measure the total abrasive removal depths at different positions on the cross-section of silicon wafer surface and the average abrasive removal depth per minute at different positions on the cross- section of silicon wafer surface. With the data obtained above, the paper further proposes using the innovative inverse method to calculate the downward force borne by different element positions on the cross-section of silicon wafer surface. Furthermore, the paper employs the downward force at each element position obtained by inverse method to derive the abrasive removal depth per minute at each element position on the axis of the cross-section of silicon wafer surface at different rotational speeds, and can obtain the simulation polished surface morphology of silicon wafer surface. Finally, the paper conducts another experiment with total downward force 3psi and rotational speed 40rpm, makes comparison between the experimental results and simulation results of total abrasive removal depth and surface morphology, so as to prove the rationality of this paper's theoretical simulation model.

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* *Professor, Opto-Mechatronics Technology Center (OMTC), National Taiwan University of Science and Technology, No.43, Keelung Rd., Sec.4, Da'an Dist., Taipei City 10607, Taiwan, email: zclin@mail.ntust.edu.tw*

** *Professor, Department of Mechanical Engineering, National Taiwan University of Science and Technology, No.43, Keelung Rd., Sec.4, Da'an Dist., Taipei City 10607, Taiwan, email: ylcheng@mail.ntust.edu.tw*

** *Graduated Student, Department of Mechanical Engineering, National Taiwan University of Science and Technology, No.43, Keelung Rd., Sec.4, Da'an Dist., Taipei City 10607, Taiwan, email: x26520941@gmail.com*

** *Graduated Student, Department of Mechanical Engineering, National Taiwan University of Science and Technology, No.43, Keelung Rd., Sec.4, Da'an Dist., Taipei City 10607, Taiwan, email: M11203238@ntust.edu.tw*

** *Graduated Student, Department of Mechanical Engineering, National Taiwan University of Science and Technology, No.43, Keelung Rd., Sec.4, Da'an Dist., Taipei City 10607, Taiwan, email: M11303236@ntust.edu.tw*

INTRODUCTION

Chemical mechanical polishing (CMP) is a machining behavior with very complicated operations. Preston (1927) proposed the first theoretical model of CMP material removal, which was expressed as MRR = KPV, with MRR denoting the material removal rate, P denoting the applied pressure, and V denoting the relative velocity of wafer to polishing pad, and K denoting the Preston constant. 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. Lin et al. (2012) studied the use of CMP of sapphire wafer as well as wafer removal by chemical reaction caused by the contact of slurry containing SiO_2 with the substrate, to observe the change in removal amount and surface morphology of wafer when there are different downward forces, rotational polishing speeds, polishing pads with different morphologies, such as hole-pattern polishing pad and pattern-free polishing pad, sizes of abrasive particles and volume concentrations of slurry. 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 wafer to polishing pad, and derived the relative abrasive length at each position on wafer to polishing pad. Lin et al. (2022) once conducted CMP experiment of sapphire wafer, and from the experimental results, analyzed the results of surface morphology of different surface cross-sections of sapphire wafer polished by CMP machine at different total downward forces and different rotational speeds. Most of the results show that the thickness of wafer at its center point on the cross-section of sapphire wafer surface is the smallest, and the thickness towards the outer edge of wafer in radial direction appears to be increasing gradually.

According to the user manual of Olympus Corporation's OLS5000 laser scanning conjugate microscopy (LSCM) equipment (2023), it is introduced that this LSCM equipment can measure the distance between positions of two points, and can also measure the heights at the positions of two points to a set reference line. The study once used the LSCM equipment of National Taiwan University of Science and Technology to take measurement test of silicon wafer surface, and also found that the LSCM had the abovementioned functions. Therefore, through LSCM, the study can obtain the measurement data of relative height of the morphology of the wafer surface at different points. Huy et al. (2023) analyzed the surface properties and microstructure of the polishing pad being used in the CMP process. They used LSCM (OLS5000) to scan the surface topology of the cross-section of an IC1000 polishing pad, and divided it into holes by controlling the threshold and using the watershed algorithm, and then analyzed the distribution of holes in size according to the results of image processing.

EXPERIMENTAL METHOD

CMP Experiments

The slurry used in the experiments of the paper is a product of Allied High Tech Products, with the diameter of abrasive particle being 50nm and volume concentration of slurry being 50%. 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. The polishing pad used is the pattern-free Rodel IC-1000. The slurry used is the one produced by San Chun Scientific Co., Ltd. In the slurry there are SiO_2 abrasive particles, with diameter being 50nm; the slurry temperature is room temperature; and the volume concentration of the slurry is 50%. The total downward force and rotational speed of the CMP machine can be adjusted and set.

Measurement Method of Relative Height of Wafer Surface Using LSCM.

The paper uses the Olympus OLS5000 Laser Scanning Confocal Microscope (LSCM) to measure the relative height of surface morphology of the polished wafer. The steps of measurement are shown as follows:

(1) The theoretical simulation of the paper is to divide the silicon wafer surface into multiple elements, with each element being 1mm × 1mm in size. Therefore, the polished silicon wafer is firstly placed on the circular outer surface of the silicon wafer with a 90-degree steel square. Then a horizontal ruler is placed at a position perpendicular to the 90-degree steel square, and the center position of the 2-inch silicon wafer with a radius of 25.4mm can be measured.

(2) After measuring the center position of circle, move the horizontal line that passes through the center of circle to the left for 4mm, 8mm and 12mm from the center of circle, and use a stylus pen with a tip less than 0.5mm to mark the positions of the three points, as shown in Figure 1.

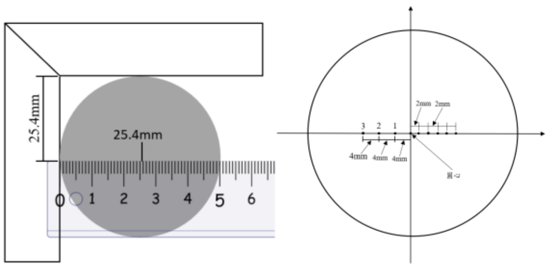

Fig. 1 Measurement of the center position of circle and various positions of element i

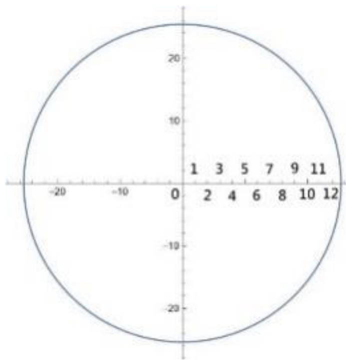

Fig. 2 Schematic diagram of the positions of height measurement points of silicon wafer on the radius line on silicon wafer surface

(3) Placing the silicon wafer on the measuring desk of LSCM can more accurately connect the three points that pass through the center of circle to the

left for 4mm, 8mm and 12mm to form a horizontal line passing through the center of circle, and fix the center point's position of circle.

(4) After that, set a horizontal reference baseline, and move it to the right from the center of circle for 2mm to various positions of element i, with a total of 13 points set, as shown in Figure 2. Starting from the center position of circle, scan with LSCM to measure the relative height of the center of circle and each point element i to the reference line.

Experimental Method of Combining Gravimetric Method with LSCM Adopting Conjugate Foci Method for Measuring the Surface Morphology of Silicon Wafer

The paper further proposes combining gravimetric method that measures the average abrasive removal depth of silicon wafer being polished for 20 minutes, with LSCM adopting conjugate foci method to measure the relative height value of the surface being polishing for 20 minutes at the position of each point element i in radial direction starting from the center of circle. Furthermore, the experimental results obtained by combining gravimetric method with conjugate foci method are used to calculate the total abrasive removal depth value at the center of silicon wafer and at the element i position of each measuring point being polished for 20 minutes. The calculation method is shown below.

(1) The paper's use of gravimetric method is to firstly measure the weight of the unpolished silicon wafer using a precision balance, use a CMP machine with its total downward force known to polish silicon wafer for 20 minutes in a room-temperature slurry with volume concentration 50%, and then use a precision balance to measure its weight. Then the abraded and removed weight of silicon wafer being polished for 20 minutes can be calculated. Divide the abrasive removal weight by the density of silicon wafer to obtain the abrasive removal volume. Divide the obtained abrasive removal volume by the area of silicon wafer to obtain the average abrasive removal depth of silicon wafer being polished for 20 minutes.

(2) Place the silicon wafer being polished for 20 minutes on a LSCM. First of all, calculate the average height value of the relative surface height of each element i position point measured by conjugate foci method to the reference line. After that, from the average height value, subtract the relative height values of the reference line of the center of circle and each element i position point. Then a +/- relative height values of the center of circle and each element i position point to the average height value can be obtained.

(3) Let the average abrasive removal depth of wafer being polished for 20 minutes calculated by gravimetric method, add to the +/- relative height values of the center of circle and each element i position measured and calculated by conjugate foci method in step (2) above to the average height value. Then, the total abrasive remove of depths of the center of circle and each element i position moving to the right for 2mm each time start from center position of circle on wafer being polished for 20 minutes can be obtained.

CALCULATION METHOD OF SPECIFIC DOWNWARD FORCE ENERGY

The paper refers to the thesis of Jhang (2015) who set downward force for atomic force microscopy (AFM) to perform nanocutting and machining of silicon wafer soaked in slurry at room temperature, and uses the data obtained in experiment to calculate the specific downward force energy ($SDFE_{reaction}$) value of silicon wafer soaked in slurry at room temperature. The distance d is multiplied by the probe's forward elasticity coefficient kr to obtain the downward force F_d (μN) (Lin and Hsu, 2012).

$$F_d = k_r d \tag{1}$$

The mechanism for silicon wafer to be machined is the moving and removal of atomic particles, and this is a model of volume change (Lin and Hsu, 2012). Therefore, the specific downward force energy ($SDFE_{reaction}$) in the chemical reaction layer of silicon wafer soaked in a slurry with volume concentration 50% at room temperature is defined as the product after multiplying the downward force that the cutting tool of probe applies onto the workpiece by the cutting depth. Thus, $SDEF_{reaction}$ as shown in equation (2):

$$SDFE_{reaction}(\text{specific downward force energy}) = \frac{F_d \times \Delta d}{\Delta V} \tag{2}$$

where:

F_d denotes the downward force of cutting tool applied onto the workpiece of silicon wafer.

Δd denotes the cutting depth.

ΔV denotes the workpiece volume removed by the downward force of cutting tool.

Since the AFM probe tip is just like a semispherical cutting tool, the volume of silicon wafer removed by cutting tool can be obtained by the geometric equation of the sphere. Therefore, the removed volume at this time is half of the spherical crown volume under the cutting depth, and the removed volume is expressed as equation (3):

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

where:

R denotes the tip radius of the cutting tool of probe.

$\triangle d$ denotes the cutting depth

Referring to the thesis of Jhang (2015), the specific downward force energy value ($SDFE_{reaction}$) in the chemical reaction layer of silicon wafer soaked in room-temperature slurry with volume concentration 50% for 60 minutes is obtained to be $0.016208(\mu N \cdot nm/nm^3)$.

THEORETICAL MODEL AND EQUATION OF INVERSE METHOD FOR CALCULATION DOWNWARD FORCE BORNE BY DIFFERENT ELEMENT POSITIONS ON THE SURFACE CROSS-SECTION OF SILICON WAFER UNDERGOING CMP

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

In reference (Greenwood and Williamson, 1966), 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 made a supposition in the paper that abrasive particles were embedded in the polishing pad only on the contact area between the asperity peak of polishing pad and wafer, and performed polishing of wafer. In order to use pattern-free polishing pad under this model, this paper divides the silicon wafer into multiple elements, with each element in the size of 1mm*1mm. When the silicon wafer is rotating, each element will have continuous and relative rotational contacts with the pattern-free polishing pad.

For the equations of contact area and contact load indicated in reference [15], the paper further modifies the equations, and innovatively proposes the equation of effective contact area A_{rsi} between asperity peak of polishing pad and each element i of silicon wafer, as well as the downward force F_{awei} borne by each element i calculated using inverse method. It is supposed that only on the effective contact area A_{rsi} between the asperity peak of polishing pad and element i of wafer, there are abrasive particles embedded on the polishing pad, and these abrasive particles are used to polish the silicon wafer.

According to reference (Qin et al., 2004), the effective contact area A_{rsi} of element i and the downward force F_{awei} borne by the element i are shown in equation (4) and equation (5) respectively. In this paper the effective contact area of each element i of silicon wafer is A_{rsi}, and the downward force borne by each element i is F_{awei}. The paper uses combining gravimetric method and LSCM adopting conjugate foci method to obtain the total abrasive removal depth at center of circle and different element positions of silicon wafer being polished for 20 minutes. Then, the paper divides the total abrasive removal depth after polishing for 20 minutes by 20 to obtain the experimental result of abrasive removal depth per minute $\delta_{\Delta tei}$ at center of circle and different element positions. The paper uses the experimental result of abrasive removal depth per minute at room temperature of slurry and applies the equation for the theoretical model derived from the inverse method innovatively established by the paper to calculate the downward force (F_{awei}) borne by center of circle and different element i positions on the cross-section of silicon wafer surface.

$$A_{rsi} = \eta A_0 \pi \beta \int_h^{\infty} (z-h)\, \varphi(z) dz \tag{4}$$

$$F_{awei} = \frac{4}{3} \eta A_0 E^* \sqrt{\beta} \int_h^{\infty} (z-h)^{\frac{3}{2}} \varphi(z) dz \tag{5}$$

$$\varphi(z) = \frac{1}{\sigma\sqrt{2\pi}} exp(-\frac{z^2}{2\times\sigma^2}) \tag{6}$$

A_0 : area of each element of silicon wafer

η : areal density of the asperity peak of polishing pad

E^* : equivalent Young's modulus

$$E^* = \frac{1-\nu_p{}^2}{E_p} + \frac{1-\nu_w{}^2}{E_w} \tag{7}$$

E_p : Young's modulus of polishing pad

E_w : Young's modulus of silicon wafer

V_p : Poisson's ratio of polishing pad

V_w : Poisson's ratio of silicon wafer

Regarding the statistical numerical values of the related parameters, such as Poisson's ratio of silicon wafer and asperity peak of polishing pad, etc., the paper refers to the values in different references, as shown in Table 1.

Table 1. Statistical numerical values of the related parameters of asperity peak (Greenwood and Williamson, 1966)

Parameter	Description	Value
E_p	Young's modulus of polishing pad	100 (Mpa)
σ	Standard deviation of height distribution for asperity peak of polishing pad	25 (μm)
β	Average radius for asperity peak of polishing pad	30 (μm)
v_p	Poisson's ratio of polishing pad	0.3
E_w	Young's modulus of silicon wafer	161.12 (GPa)
V_w	Poisson's ratio of silicon wafer	0.27
η	Areal density for asperity peak of polishing pad	$2*10^8$ (m^{-2})

Using equation (4) and equation (5), the paper obtains:

$$\frac{A_{rsi}}{F_{awei}} = \frac{3\pi\sqrt{\beta}}{4E^*} \frac{\int_h^{\infty}(z-h)\varphi(z)dz}{\int_h^{\infty}(z-h)^{\frac{3}{2}}\varphi(z)dz} \tag{8}$$

Numerical integration in reference (Johson, 1985) is employed to integrate equation (8). Since the ratio of two integrals is approximately a constant for h/σ within a range, equation (9) can be obtained as follows:

$$A_{rsi} = C^{-1}\sqrt{\frac{\beta}{\sigma}} \frac{F_{awei}}{E^*} \tag{9}$$

In equation (9), C is a constant. In reference (Yu and Orlowski, 1993), the constant C was derived and calculated. As known from reference (Johson, 1985), the ratio $h/_\sigma$ of polishing pad is generally between 0.5 and 3.0. When $h/_\sigma$ 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 reference (Johson, 1985) are made by the same company and of similar model number. Therefore, for the variables of equation (9), the paper refers to the β and σ values in reference (Johson, 1985), and the numerical statistical values of the parameters in different references that the paper refers to are shown in Table 1. Besides, since the size of each wafer element used in this paper is greater than β and σ values, it is feasible for the paper to consider the effective contact area A_{rsi} between the asperity peak of polishing pad and each silicon wafer element i, as well as the contact downward force F_{awei} at the element i position. As for E*, it can be calculated by substituting equation (7) into the numerical values of the related parameters shown in Table 1. Therefore, $C^{-1}\sqrt{\frac{\beta}{\sigma}}/E^*$ can be calculated, and its value is a fixed value. The paper sets $\frac{C^{-1}\sqrt{\frac{\beta}{\sigma}}}{E^*} = k_{rs}$, where k_{rs} is a fixed value, thus obtaining equation (10) as follows:

$$A_{rsi} = k_{rs} * F_{awei} \tag{10}$$

Then the paper uses equation (10) to calculate the effective contact area (A_{rsi}) between the asperity peak of polishing pad and each silicon wafer element i.

When using inverse method to deduce a equation for the theoretical model of contact force F_{awei} borne by silicon wafer element i, the paper considers the Gaussian distribution of the asperity peaks of polishing pad, total downward force and rotational speed of the equipment of CMP machine, properties of silicon wafer material, volume concentration of slurry at room temperature, as well as the diameter of abrasive particles.

Through the total downward force of CMP machine, the downward force borne by the element i position of silicon wafer is F_{awei}. From the downward force borne by each abrasive particle of element i as well as the SDFE$_{reaction}$ value in the chemical reaction layer of silicon wafer soaked in slurry at room temperature, the paper divides the total abrasive removal depth at element i position of wafer being polished for 20 minutes which measured using gravimetric method combined with LSCM adopting conjugate foci method, by 20, obtaining the abrasive removal depth per minute at center of circle and element i position. Then inverse method can be used to derive the equation for calculating the downward force F_{awei} borne by center of circle and the element i position.

Theoretical Model and Equation for Inverse Calculation of Downward Force Borne by a Certain Element of Silicon Wafer with Consideration for Room-temperature Slurry and Total Downward Force of CMP Machine.

In reference (Kim and Jeong, 2004) a pattern-free polishing pad was used to polish wafer. It mentioned that the position of any single point P on silicon wafer, the relative speed $V_{w/p}$ of polishing pad is expressed as equation (11):

$$V_{w/p} = \omega_p D_{wp}\sqrt{(\rho\zeta)^2 + 2\rho\zeta\cos\varphi + 1} \tag{11}$$

Here, $\rho = \frac{r}{R_W}$ ， $\zeta = \frac{R_W}{D_{WP}}(1-R)$ ， $R = \frac{\omega_w}{\omega_p}$ ， $\varphi = \omega_W t$, where R_W denotes the radius of wafer, ω_w denotes the rotational speed of wafer, ω_p denotes the rotational speed of polishing pad, and D_{WP} denotes the distance between the center of wafer and the center of polishing pad, as shown in Fig 1. Therefore, when the silicon wafer and the polishing pad are at the same rotational speed, i.e. $\omega_w = \omega_p$ ， $\zeta = 0$, then $V_{W/P} = \omega_p D_{WP}$. And it is also mentioned in this reference that when $\omega_w = \omega_p$, and after a period of time t, the actual relative abrasive length of wafer and polishing pad 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 $\omega_p D_{WP}$. Since the rotational speed ω_p of polishing pad is a set value and D_{WP} is a fixed value of the equipment of CMP machine, $\omega_p D_{WP}$ will be a set value that will not be changed with any position on the wafer. Thus, if there are abrasive particles at a point P to polish wafer, the relative moving length of wafer polishing for the unit time per minute of wafer polishing is $\omega_p D_{WP}$.

In this paper, we set the central position of each element of silicon wafer to be at the above 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 obtain the relative number of polishing times FF per unit time for the contact between each element and polishing pad. Therefore, FF $= \omega_p D_{wp}$. The paper lets the size of each element of silicon wafer be 1mm×1mm; and hence, FF $= \omega_p D_{wp}$.

Right now, the element i on the wafer's surface volume $Vo\ell_i$ that can be removed by each abrasive particle per unit time is shown in Figure 3, and expressed as the following equation:

$$Vo\ell_i = A_{pi} * \ell \tag{12}$$

$Vo\ell_i$: volume of wafer removed by a single abrasive particle per unit number of polishing times

A_{pi} : 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 A_{rsi} in each element i divided from silicon wafer are distributed evenly. Therefore, the moving length ℓ of a single abrasive particle per unit time of per minute in each divided element i of silicon wafer is expressed as equation (13):

$$\ell = \omega_p D_{wp} \tag{13}$$

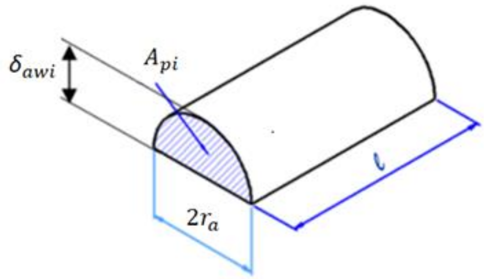

Fig 3. Relative abrasive removal volume of element i's single abrasive particle during polishing of silicon wafer

where:

$$A_{pi} \approx \frac{1}{2} \cdot \delta_{awi} \cdot 2r_a \approx \delta_{awi}\sqrt{\delta_{awi}D} \tag{14}$$

D : average diameter of abrasive particles

δ_{awi} : abrasive removal depth of element i's single abrasive particle on silicon wafer surface

Besides, if N_{ei} denotes the number of effective abrasive particles at each element i of silicon wafer, and the unit volume concentration of abrasive particles in slurry is supposed to be χ, and the average diameter of abrasive particles is D, then $\left(\frac{6\chi}{\pi D^3}\right)^{2/3}$ is the number of abrasive particles in slurry per unit volume. Since the length of each silicon wafer element is 1mm, the number of effective abrasive particles in the effective contact area A_{rsi} of a single element i is expressed as equation (15) (Zhao and Chang, 2002):

$$N_{ei} = A_{rsi} \cdot \left(\frac{6\chi}{\pi D^3}\right)^{\frac{2}{3}} = k_{rs} * F_{awei}\left(\frac{6X}{\pi D^3}\right)^{2/3} \tag{15}$$

where A_{rsi} denotes the effective contact area between the asperity peak of polishing pad and element i on wafer surface, being the interface between element i position and polishing pad. In this paper, the contact between the asperity peak of polishing pad and wafer is of Gaussian distribution, which can be applied to derive equations (10) of A_{rsi} for calculation.

Divide the downward force F_{awei} borne by the element i by the number of abrasive particles N_{ei} borne by the effective contact area A_{rsi} of element i, the downward force F_{awi} of element i's single abrasive particle of wafer can be obtained, and expressed as equation (16):

$$F_{awi} = \frac{F_{awei}}{N_{ei}} = \frac{1}{k_{rs}*\left(\frac{6X}{\pi D^3}\right)^{2/3}} \tag{16}$$

After substituting the downward force F_{awi} of a single abrasive particle on element i of the polished silicon wafer into the $SDFE_{reaction}$ equation (2) of silicon wafer soaked in slurry at room temperature, the abrasive removal depth Δd_i of element i's single abrasive particle on wafer surface can be obtained, and expressed as equation (17):

$$\Delta d_i = \frac{\Delta V_i \times SDFE_{reaction}}{F_{awi}} \tag{17}$$

Substituting equation (3)'s $\Delta V_i = \frac{1}{2}\pi \times (\Delta d_i)^2 \times \left(R - \frac{\Delta d_i}{3}\right)$ into equation (17), equation (18) can be obtained:

$$\Delta d_i = \frac{\frac{1}{2}\pi \times (\Delta d_i)^2 \times \left(R - \frac{\Delta d_i}{3}\right) \times SDFE_{reaction}}{F_{awi}} \tag{18}$$

where R denotes the radius of abrasive particle.

After rearrangement of equation (17), a quadratic equation in one variable that takes Δd_i as a single variable can be obtained, and expressed as equation (19):

$$\frac{1}{6}\pi \times SDFE_{reaction} \times (\Delta d_i)^2 - \frac{1}{2}\pi \times R \times SDFE_{reaction} \times \Delta d_i + F_{awi} = 0 \tag{19}$$

Using equation (19), the paper obtains Δd_i, which is just the abrasive removal depth δ_{awi} of element i's single abrasive particle on wafer surface, and can be expressed as equation (20):

$$\Delta d_i = \frac{3R - \sqrt{9R^2 - \frac{24F_{awi}}{\pi \times SDFE_{reaction}}}}{2} = \delta_{awi} \tag{20}$$

Then, from equation (12) and equation (14), the effective removal volume per unit time (per minute) of element i's single abrasive particle on wafer surface is $Vo\ell_i = A_{pi} * \ell = \delta_{awi}\sqrt{\delta_{awi}D} \times \ell$. From equation (13), $\ell = \omega_p D_{wp}$, so equation (21) can be obtained:

$$Vo\ell_i = \delta_{awi}\sqrt{\delta_{awi}D} \times \omega_p D_{wp} \tag{21}$$

Multiply $Vo\ell_i$ by the number N_{ei} of effective abrasive particles of element i. Then the effective abrasive removal volume $V_{\Delta tei}$ of element i per unit time can be obtained and expressed as equation (22):

$$V_{\Delta tei} = Vol_i \times N_{ei} = \delta_{awi}\sqrt{\delta_{awi}D} \times \omega_p D_{wp} \times k_{rs} \times F_{awei}\left(\frac{6X}{\pi D^3}\right)^{2/3} \tag{22}$$

The paper proposes dividing $V_{\Delta tei}$ by the area A_0 at the single element position of silicon wafer to obtain the average abrasive removal depth per minute $\delta_{\Delta tei}$ at the element i position. Besides, since the area of each element in this paper is $A_0 = 1mm^2$, $\delta_{\Delta tei}$ can be obtained and expressed as equation (23):

$$\delta_{\Delta tei} = \frac{V_{\Delta tei}}{A_0} = V_{\Delta tei} = \delta_{awi}\sqrt{\delta_{awi}D} \times \omega_p D_{wp} \times k_{rs} \times F_{awei}\left(\frac{6X}{\pi D^3}\right)^{2/3} \tag{23}$$

Since the paper employs inverse method to calculate the downward force F_{awei} borne by the element i of silicon wafer undergoing CMP, and the abovementioned way of combining gravimetric method with conjugate foci method can be used to measure the total abrasive removal depth at different element i position, then divide 20 to obtain the abrasive removal depth per minute at different element i positions on the cross-section of silicon wafer surface, the abrasive removal depth per minute $\delta_{\Delta tei}$ at the element i position can be obtained. Therefore, from equation (23), equation (24) can be derived:

$$F_{awei} = \delta_{\Delta tei} / \left[\delta_{awi}\sqrt{\delta_{awi}D} \times \omega_p D_{wp} \times k_{rs} \times \left(\frac{6X}{\pi D^3}\right)^{\frac{2}{3}}\right] \tag{24}$$

In the calculation process of equation (24), since the rotational speed ω_p, diameter D of abrasive particle, $SDFE_{reaction}$ value of slurry at room temperature and volume concentration x of slurry are all known, equation (16) can be used to calculate F_{awi}. Then equation (20) can be used to calculate δ_{awi}. Since $\delta_{\Delta tei}$ is the abrasive removal depth per minute at the element i position can be obtained, the downward force F_{awei} borne by the element i can be calculated. The above shows the paper's use of inverse method to establish the theoretical model and equation for simulated calculation of the downward force borne by different elements i on the surface cross-section of silicon wafer undergoing CMP.

REGRESSION MODEL AND EQUATION FOR CALCULATION OF DOWNWARD FORCE BORNE BY DIFFERENT ELEMENT POSITIONS ON THE CROSS-SECTION OF SILICON WAFER SURFACE

As seen from the schematic diagram of the positions of measurement points of silicon wafer on the zero-degree cross-section of silicon wafer surface in Fig 2. Therefore, the 13 values of F_{awei} calculated at the center point of silicon wafer and at the 12 measured points on the right, as shown in the schematic diagram, can only be used to make regression analysis, and then the regression equation F_{awei} for different element i positions can be obtained. The regression model of F_{awei} in this paper adopts a third-order regression equation, which is expressed as equation (25):

$$\hat{y}_F = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 \quad (25)$$

Here, $\hat{y}_F = F_{awei}$, where x denotes the length value from the element i position to the center of silicon wafer, as shown in Fig 2.

The closer to 1 for the R^2 value, the better the explanatory ability of the model.

Besides, the closer to 0 for the average residual value, the better it is.

Mean absolute error (MAE) is the average of the absolute values of all predicted differences. It is an indicator for measuring the accuracy of the prediction model. What it calculates is the average of the absolute values of the differences between the predicted values and the actual values. The MAE equation is expressed as equation (26) (Douglas, 2013).

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| \quad (26)$$

where:

y_i denotes the ith actual value observed.

$\hat{y_i}$ denotes the ith predicted value observed.

n denotes the number of samples, referring to the total number of samples in the data set.

The paper uses the MAE to explain the degree of difference between the experimental values or simulation values of the 13 points of element and values in the regression model.

SIMULATED CALCULATION OF SURFACE MORPHOLOGY OF SILICON WAFER HAVING UNDERGONE CMP FOR 20 MINUTES AT DIFFERENT ROTATIONAL SPEEDS

As seen from equation (23) derived by the paper above, if the rotational speed is ω_p, ω_p can be set to be different rotational speeds other than 60rpm, such as 20rpm, 30rpm, 40rpm and 50rpm. Then the abrasive removal depth per minute $[\delta_{\Delta teis}]_{\omega p}$ at element i positions at different rotational speeds can be calculated, as shown in equation (27):

$$[\delta_{\Delta teis}]_{\omega_p} = \delta_{awi}\sqrt{\delta_{awi}D} \times \omega_p D_{wp} \times krs * F_{awei}(\frac{6X}{\pi D^3})^{2/3} \quad (27)$$

If the abrasive removal depth per minute at different element i positions at different rotational speeds calculated by simulation is used, the paper can further obtain the surface morphology of the abrasive removal depth at different element i positions after CMP of silicon wafer for 20 minutes at a certain rotational speed ω_p. What's more, the paper explores the changes in surface morphology of silicon wafer after CMP of silicon wafer for 20 minutes by CMP machine with a set total downward force 3 psi at different rotational speeds.

RESULTS AND DISCUSSION

Experimental Results with Total Downward Force 3psi and Rotational Speed 60rpm

The following items show the detailed experimental and calculation steps in using gravimetric method and conjugate foci method for measuring at the center of circle and at various positions of element i with a total downward force 3psi at rotational speed 60rpm.

(1) In the experiment using the experimental results with fixed total downward force 3psi and rotational speed 60rpm, and also using gravimetric method, the average abrasive removal depth δ_w is calculated, as shown in equation (28).

$$\delta_w = (W_{bef.} - W_{aft.})/\rho_{Si}/A_{wafer} \quad (28)$$

where:

$W_{bef.}$ and $W_{aft.}$ denote the weights before and after polishing of silicon wafer respectively.

ρ_{Si} denotes the density of silicon wafer.

A_{wafer} denotes the area of the polished side of silicon wafer.

The calculation results using gravimetric method are shown in Table 2.

Table 2. Calculation results with fixed total downward force 3psi and rotational speed 60rpm using gravimetric method

$W_{bef.}$ (g)	$W_{aft.}$ (g)	ρ_{Si} (g/nm^3)	A_{wafer}(nm^2)	δ_w (nm)
2.31177	2.30909	2.3290 $\times 10^{21}$	2.0268 $\times 10^{15}$	568.0293

(2) For the fixed total downward force 3psi and rotational speed 60rpm, LSCM employing conjugate foci method is used to measure the relative abrasive removal depth of the relative height values of the reference baseline at the positions of 13 points, including the center of circle and various points of element i. The measurement results are shown in Figure 4.

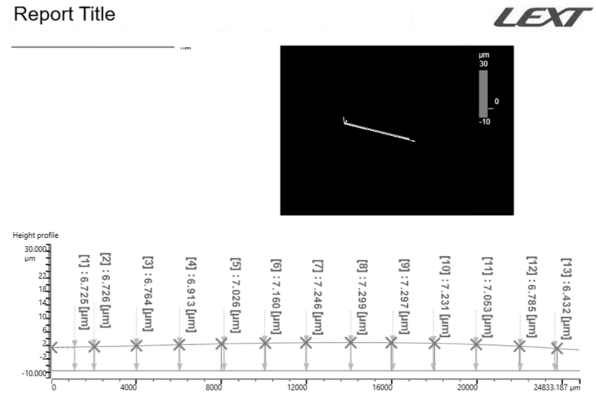

Fig 4. Measurement result of morphology of 13 points of element with fixed total downward force 3psi and rotational speed 60rpm

After using the measurement result of morphology of silicon wafer in Fig. 4 for calculation, the results of experimental value of removal depth, and the experimental values of abrasive removal depth at 13 points of element in total, including the center of circle and 12 points of element i, are shown below.

If $D_1 \sim D_{13}$ are the measured values of the relative reference line measured by conjugate foci method, the average height $\overline{D}$ of the relative reference line at the positions of 13 points in total, including the center of circle and 12 other points of element i, can be firstly calculated, as shown in equation (29).

$$\overline{D} = (\mathrm{D}_1 + \mathrm{D}_2 + \cdots + \mathrm{D}_{13})/13 \tag{29}$$

Find the relative height difference value ΔD_i of the 13 points' positions compared to the average height $\overline{D}$. This relative height difference value ΔD_i is for calculation of the relative removal depth at the 13 points' positions, as shown in equation (30).

$$\Delta D_i = \overline{D} - D_i \tag{30}$$

D_i denotes that $D_i = D_1$ if i = 1, and so on and so forth up to i = 13.

Here, when ΔD_i is a positive value, it refers that the relative removal depth at this point's position is the morphology of abrasive removal depth of the surface being depressed downward. On the contrary, when ΔD_i is a negative value, it refers that the relative removal depth at this point's position is the morphology of abrasive removal depth of the surface being bulging upwards, as shown in Figure 5.

(3) Calculate the total abrasive removal depth $\delta_{totalei}$ at the positions of 13 points in total, including the center of circle and various points of element i, as shown in equation (31).

Table 3. Total abrasive removal depths at 13 points of element with polishing time 20 minutes, total downward force 3psi and rotational speed 60rpm

No.	Measured value D_i (μm)	Difference ΔD_i (nm)	$\delta_{totalei}$ (nm)
1	6.725	248.6154	816.6447
2	6.726	247.8154	815.8447
3	6.764	209.8154	777.8447
4	6.913	61.0154	629.0447
5	7.026	-52.1846	515.8447
6	7.160	-186.1846	381.8447
7	7.246	-272.5846	295.4447
8	7.299	-325.7846	242.2447
9	7.297	-323.7846	244.2447
10	7.231	-257.3846	310.6447
11	7.053	-79.7846	488.2447
12	6.785	189.0154	757.0447
13	6.432	541.4154	1109.4447
$\overline{D}$	7.134	-	-

No. 1 is the center position of circle, There are 13 positions, with each interval of 2mm being the position of an element i.

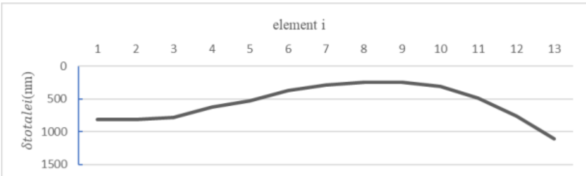

Fig 5. Experimental surface morphology chart of abrasive removal depths at 13 points of element of silicon wafer being polished for 20 minutes, with total downward force 3psi and rotational speed 60rpm

As mentioned above, the paper firstly uses gravimetric method to measure the average abrasive removal depth δ_w of silicon wafer being polished for 20 minutes, and used conjugate foci method to measure and calculate the relative height difference ΔD_i at the positions of 13 points in total, including the center of circle and various points of element i. The two values of δ_w and ΔD_i were added to obtain the total abrasive removal depth $\delta_{totalei}$ at the positions of 13 points in total, including the center of circle and various points of element i of silicon wafer being polished for 20 minutes.

$$\delta_{totalei} = \delta_w + \Delta D_i,\ \mathrm{i=1\sim13} \tag{31}$$

The results of the measured value D_i at 13 points, difference ΔD_i and total abrasive removal depth $\delta_{totalei}$ are shown in Table 3. The total abrasive removal depth is drawn as a morphology chart, as shown in Figure 5, where $\delta_w = 568.0293$(nm).

(4) Calculate the abrasive removal depth per minute $\delta_{\Delta tei}$ at 13 points in total, including the center of circle and various points of element i.

$$\delta_{\Delta tei} = \delta_{totalei}/20 \tag{32}$$

The calculation results of $\delta_{\Delta tei}$ are shown in Table 4.

(4) Calculate the abrasive removal depth per minute $\delta_{\Delta tei}$ at 13 points in total, including the center of circle and various points of element i.

$$\delta_{\Delta tei} = \delta_{totalei}/20 \tag{32}$$

The calculation results of $\delta_{\Delta tei}$ are shown in Table 4.

(5) Substitute the abrasive removal depth per minute $\delta_{\Delta tei}$ at 13 points into equation (24), and F_{awei} can be calculated, with its results shown in Table 4.

(6) Substitute the downward force F_{awei} at the positions of the 13 points of element into equation (28), and the simulated values of abrasive removal depth values per minute $[\delta_{\Delta teis}]_{\omega p}$ can be calculated, with its results shown in Table 4.

(7) Compare the difference between the experimental values $\delta_{\Delta tei}$ and the simulated values $[\delta_{\Delta teis}]_{\omega p}$ at the 13 points, with the results of difference shown in Table 4.

Table 4 Experimental and simulation results with total downward force 3psi and rotational speed 60rpm

No.	D_i (μm)	$\delta_{totalei}$ (nm)	$\delta_{\Delta tei}$ (nm/min)	F_{awei} (N)	$[\delta_{\Delta teis}]_{\omega p}$ (nm/min)	Difference %
1	6.725	816.6447	40.8322	29.7374	39.1989	4.17%
2	6.726	815.8447	40.7922	29.7082	39.1605	4.17%
3	6.764	777.8447	38.8922	28.3245	37.3365	4.17%
4	6.913	629.0447	31.4522	22.9061	30.1941	4.17%
5	7.026	515.8447	25.7922	18.7840	24.7605	4.17%
6	7.160	381.8447	19.0922	13.9045	18.3285	4.17%
7	7.246	295.4447	14.7722	10.7584	14.1813	4.17%
8	7.299	242.2447	12.1122	8.8211	11.6277	4.17%
9	7.297	244.2447	12.2122	8.8939	11.7237	4.17%
10	7.231	310.6447	15.5322	11.3118	14.9109	4.17%
11	7.053	488.2447	24.4122	17.7790	23.4357	4.17%
12	6.785	757.0447	37.8522	27.5671	36.3381	4.17%
13	6.432	1109.4447	55.4722	40.3994	53.2533	4.17%

Experimental Results and Simulation Results with Total Downward Force 3psi and Rotational Speed 40rpm

For the experiment with total downward force 3 psi and rotational speed 60rpm, inverse method is used to calculate the downward force F_{awei} at 13 points in total, including the center of circle and various positions of element i. After substituting the downward force F_{awei} into equation (27), the simulated abrasive removal depth $\delta_{\Delta teis}$ at 13 points in total, including the center of circle and various positions of element i, with rotational speed 40rpm is obtained, with the results shown in Table 5.

Table 5. Using the downward force value calculated with total downward force 3 psi and rotational speed 60rpm to calculate the simulation value of abrasive removal depth per minute at rotational speed 40rpm, as well as the experimental value of abrasive removal depth per minute with 3psi and rotational speed 40rpm

No.	60rpm F_{awei} (N)	$[\delta_{\Delta teis}]_{40}$ (nm/min)	40rpm $\delta_{\Delta tei}$ (nm/min)	Difference (%)
1	29.7374	27.2216	27.4913	-0.98%
2	29.7082	27.1949	27.3513	-0.57%
3	28.3245	25.9282	25.4513	1.87%
4	22.9061	20.9682	20.3913	2.83%
5	18.7840	17.1949	16.4913	4.27%
6	13.9045	12.7282	12.3113	3.39%
7	10.7584	9.8482	9.4513	4.20%
8	8.8211	8.0749	7.8313	3.11%
9	8.8939	8.1415	8.2113	-0.85%
10	11.3118	10.3549	10.7113	-3.33%
11	17.7790	16.2749	16.7913	-3.08%
12	27.5671	25.2349	25.7313	-1.93%
13	40.3994	36.9816	37.9313	-2.50%
MAE	-	-	-	2.53%

As seen from the results in Table 5, after substituting the downward forces F_{awei} at various positions of element i inversely calculated with total downward force 3psi and rotational speed 40rpm, into equation (27), the obtained simulation value of abrasive removal depth per minute $[\delta_{\Delta teis}]_{40}$ is compared with the experimental value of abrasive removal depth per minute $\delta_{\Delta tei}$ measured by combining gravimetric method with conjugate foci method with total downward force 3psi and rotational speed 40rpm. As a result, the difference is between -4% and 5%. The mean absolute error (MAE) at 40rpm is 2.53%, indicating that the prediction of the paper's theoretical model is quite accurate. Therefore, it is proved that the downward force F_{awei} at 60rpm obtained from calculation can be used to calculate the simulation values of abrasive removal depth per minute at different rotational speeds through the theoretical model developed by the paper.

Abrasive Removal Depth per Minute and Simulation Result of Surface Morphology with Total Downward Force 3psi and Different Rotational Speeds of 20rpm, 30rpm and 50rpm

Using the way of combining gravimetric method with conjugate foci method to measure the abrasive removal depth per minute $\delta_{\Delta tei}$ at each element i position, with total downward force 3psi and rotational speed 60rpm, the paper substitutes $\delta_{\Delta tei}$ into inverse method to calculate the downward force F_{awei} borne by various positions of element i. After substituting the obtained F_{awei} at rotational speed 60rpm into equation (27), the simulation values of abrasive removal depths per minute, being $[\delta_{\Delta teis}]_{20}$, $[\delta_{\Delta teis}]_{30}$ and $[\delta_{\Delta teis}]_{50}$, at rotational speeds 20rpm, 30rpm and 50rpm respectively can be obtained. After that, $[\delta_{\Delta teis}]_{20}$, $[\delta_{\Delta teis}]_{30}$ and $[\delta_{\Delta teis}]_{50}$ are multiplied by

20 one by one, obtaining the simulated total abrasive removal depths $[\delta_{totaleis}]_{20}$, $[\delta_{totaleis}]_{30}$ and $[\delta_{totaleis}]_{50}$ at each element i position at rotational speeds 20rpm, 30rpm and 50rpm respectively, as well as their surface morphologies, as shown in Figure. 6.

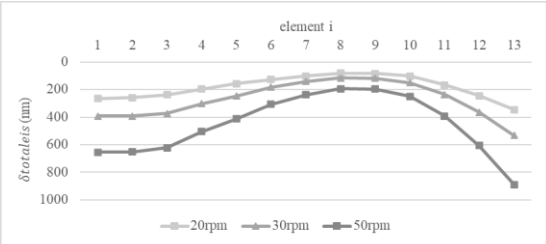

Fig. 6. Surface morphology chart of total abrasive removal depths at various positions of element i of silicon wafer being polished for 20 minutes with total downward force 3psi and different rotational speeds at 20rpm, 30rpm and 50rpm

Establishment of Regression Model of the Inversely Calculated Downward Force at the Positions of 13 Points of Element

The signs in the model of this section is defined as follows:

$\hat{y}_F$ denotes the regression value (N) of downward force F_{awei} .

x denotes the distance from the center of circle. With 0 as the center of circle, a point is set at each interval of 2mm, and there are 13 points positioned.

Conduct regression calculation of downward force F_{awei} at the position of each of the 13 points of element inversely calculated with fixed total downward force 3psi and rotational speed 60rpm, with a third-order regression model attached. Its equation is expressed as equation (33):

$$\hat{y}_F = 28.7632 + 3.0428x - 1.5354x^2 + 0.1057x^3 \quad (33)$$

where

$R^2 = 0.99629$ ◦

Average residual = 0.44095 ◦

CONCLUSION

The paper proposes performing CMP of silicon wafer for 20 minutes with the parameters known, including room temperature, and CMP machine's total downward force and rotational speed, and uses the way of combining gravimetric method with LSCM adopting conjugate foci method to measure the total abrasive removal depths at the center of silicon wafer and at different positions of element i. It can be seen that the abrasive removal depth at the center of circle is the deepest, and then the abrasive removal depth gradually decreases at an interval of 2mm to the right. Therefore, the surface morphology of wafer gradually bulges upward until a wave peak is reached, and then gradually declines to be close to the edge of wafer. In other words, the area between the center of circle and near the edge of wafer is removed more and has greater abrasive removal depth, whereas the area between the center of circle and the middle of wafer's edge has smaller abrasive removal depth. As seen from the downward force at each point calculated by inverse method, the downward force between the center of circle and the position below the edge line of wafer is larger, whereas the downward force between the center of circle and the middle position of wafer's edge is smaller.

The paper develops the inverse method to calculate the downward force borne by different element positions on the cross-section of silicon wafer surface. Then using the obtained downward forces at different element i to derive the abrasive removal depth per minute for different rotational speed, and the surface morphology being polished silicon wafer can be obtained. From the downward force at each point, the simulation value of abrasive removal depth per minute with the same total downward force 3 psi and rotational speed 40rpm can be calculated. The experimental and simulation results of abrasive removal depth per minute at the positions of various points show that the difference in between is within the range of −4% ~ 5%, thus proving that it is feasible to simulate the values of abrasive removal depth per minute with fixed total downward force and different rotational speeds.

The paper uses regression analysis method to obtain regression equation of downward force borne by each element position on the cross-section off silicon wafer surface.

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