Material removal rate of double-faced mechanical polishing of 4H-SiC substrate

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Abstract
Silicon carbide (SiC) has been a promising third-generation semiconductor power device material for high-power, high-temperature, and substrate applications. However, under certain surface quality requirement, its current processing efficiency is the bottleneck. Therefore, it aims to improve the material removal rate (MRR), on the premise of ensuring the surface roughness requirements. To obtain the relationship between any point on SiC substrate and polishing pads, the model about double-faced mechanical polishing has been established, and the kinematics equations have been created. Best optimized material removal rate parameters were obtained. MRR reached the maximum when speed rate of the outside ring gear to the inside sun gear \( m = -1 \), speed rate of lower plate to the inside sun gear \( n = 5 \), and SiC substrate distribution radius \( RB = 75 \). The primary and secondary order of MRR \((n>m>RB)\) was obtained. An accurate mathematical model of orthogonal rotary regression test of Tri-factor quadratic of MRR was established, and the regression model was significant. Surface quality of SiC substrate was observed and characterized with SEM and AFM. It greatly provides a key guarantee for the next process of CMP, confirms the importance of MRR to ultra-smooth polishing, and provides a guarantee for its application in semiconductor equipment and technology.

Keywords Material removal rate · Polishing · Orthogonal · Kinematic · Regression analysis

1 Introduction

Development of semiconductor industry has been closely related to the national defense, military, aerospace, energy, and other important areas of science and technology [1, 2]. Silicon carbide (SiC) is a typical representative of wide-band gap semiconductor materials, which can be used as a substrate for growing gallium nitride (GaN) and graphene [3–5]. It also has become an ideal semiconductor material for producing high-temperature, high-frequency, and high-power electric power devices [6, 7].

Ultra-smooth polishing of the SiC substrate was required atomic surface roughness [8–10]. At present, the biggest problem was that the processing efficiency was too low on the premise of ensuring the surface quality. However, the double-faced mechanical polishing (MP) process was the key to ensure a certain surface roughness (Ra) and the high efficient material removal rate (MRR). At the same time, it was the crux of chemical mechanical polishing (CMP) in the next step. Michio et al. [11] reported that when the ozone gas bubbles are applied to the conventional slurry, surface reaction products can be produced to obtain higher MRR than dedicated slurry. Pan et al. [12] found that the MRR could reach 45nm/h, when polished with H2O2 and silica slurry. Meanwhile, MRR could increase to 105nm/h in CMP of SiC. Many researchers have analyzed the relationship between MRR and surface roughness[13–15].

In this paper, kinematic equations of SiC substrate during double-faced polishing were analyzed. The accurate mathematical model of orthogonal rotary regression test of Tri-factor quadratic of MRR was established, and the parameters affecting MRR were studied.
2 Materials and methods

Experimental materials were used 6 inch N type 4H-SiC. Structure model of double-faced MP was as shown in Fig. 1. The lower plate 1, the upper plate 4, the inside sun gear 5, and the outside ring gear 7 were, respectively, driven by four servo motors. SiC substrates 8 were distributed at the center of five middle planetary gears 6. The five middle planetary gears were caught between the lower pad 2 and the upper pad 3. The upper and the lower pads were, respectively, adhered to each surface of corresponding polishing disk. The five middle planetary gears were meshed with the inside sun gear 5 and the outside ring gear 7 were, respectively, driven by four servo motors. SiC substrates 8 were distributed at the center and the outside ring gear, driving the SiC substrates to realize the motion of revolution and rotation [16, 17].

Kinematic equations of any point on SiC substrate relative to the lower pad during double-faced MP were analyzed. Theoretical model of MRR and the influence of various parameters on the processing efficiency were studied.

Radius of five middle planetary gears represented as $R_1$. Similarly, the inside sun gear radius was $R_2$. Rotational speed of the inside sun gear, the outside ring gear, and lower disk was $\omega_s$, $\omega_r$, and $\omega_p$, respectively. Speed of the five middle planetary gears was $\omega_h$. Furthermore, it was equivalent to that the five middle planetary gears only just revolved on its axis with an angular velocity $\omega_s$ when $-\omega_h$ added to the whole model. We selected certain point $B$ ($R_B$, $\varphi$) on the substrate in the coordinate system $X_1O_1Y_1$ and established kinematic equations of the point $B$ relative to lower pad in $X_2O_2Y_2$. Among them, SiC substrate distribution radius $RB=|O_1B|$, $RB\in[0, R_M]$. $R_M$ was the maximum radius of SiC substrate. Besides, $\varphi$ was the angle between $O_1B$ and $O_1X_1$. $\varphi\in[0, 2\pi]$. $\theta_1=\omega_s t$, $\theta_2=\omega_h t$, $\theta_3=\omega_p t$. Kinematic equations have been hold follows:

$$
\begin{align*}
\begin{bmatrix}
X_B \\
Y_B
\end{bmatrix} &= \begin{bmatrix}
\cos \theta_3 & -\sin \theta_3 \\
\sin \theta_3 & \cos \theta_3
\end{bmatrix} \cdot \begin{bmatrix}
\cos (-\theta_2) & \sin (-\theta_2) \\
-\sin (-\theta_2) & \cos (-\theta_2)
\end{bmatrix} \cdot \begin{bmatrix}
(R + r) \\
0
\end{bmatrix} + \begin{bmatrix}
\cos \theta_1 \\
\sin \theta_1
\end{bmatrix} \cdot \begin{bmatrix}
RB \cos \varphi \\
RB \sin \varphi
\end{bmatrix} \\
\begin{bmatrix}
X_B \\
Y_B
\end{bmatrix} &= \begin{bmatrix}
RB \cos (\theta_1 + \theta_2 + \theta_3 + \phi) + (R + r) \cos (\theta_2 + \theta_3) \\
RB \sin (\theta_1 + \theta_2 + \theta_3 + \phi) + (R + r) \sin (\theta_2 + \theta_1)
\end{bmatrix}
\end{align*}
$$

(1)

Fig. 1. Model of double-faced MP of SiC single crystal substrate. a Structure figure. b Geometric figure
The results expressed by Equations (1)–(7) were shown the kinematics equations of point $B$ on the surface of SiC relative to lower pad during double-faced MP. $XB$, $VXB$, and $AXB$ were, respectively, the components of point $B$ on $X$ axis of the displacement, velocity, and the acceleration. $YB$, $VYB$, and $AYB$ were, respectively, the components of point $B$ on $Y$ axis of the displacement, velocity, and the acceleration.

According to the equation Preston [18]:

$$MRR = K \cdot P \cdot V$$

During the polishing time $t$, the $MRR$ of point $B$ on the SiC substrate surface was as follows:
Substituting Equation (5) into Equation (9), we got:

$$MRR = \frac{K \cdot P \cdot \int_{0}^{t} VBdt}{t}$$  \hspace{1cm} (9)$$

Then substituting Equation (5) into Equation (9), we get:

$$MRR = \frac{K \cdot P \cdot \int_{0}^{t} \left\{ \left[ \left( RB \cdot \left( \omega_c + \omega_h + \omega_p \right) \right] + \left[ \left( R + r \right) \cdot \left( \omega_h + \omega_p \right) \right] + 2RB \cdot \left( R + r \right) \cdot \left( \omega_h + \omega_p \right) \cdot \left( \omega_h + \omega_p \right) \cdot \cos \left( \omega_c t + \phi \right) \right\} \frac{1}{2} dt}{t}$$  \hspace{1cm} (10)$$

According to the transmission ratio relationship of the composite gear train:

$$i_{sr}^h = \frac{\omega_r^h}{\omega_r} = \frac{\omega_s - \omega_r}{\omega_s - \omega_r} = -\frac{Z_r}{Z_s}$$  \hspace{1cm} (11)$$

$$i_{sc}^h = \frac{\omega_c^h}{\omega_c} = \frac{\omega_s - \omega_h}{\omega_s - \omega_h} = -\frac{Z_c}{Z_s}$$  \hspace{1cm} (12)$$
Table 4 Variance analysis of L25

| Index | Source | SS  | DF  | F    | Significance |
|-------|--------|-----|-----|------|--------------|
| MRR   | A      | 0.489 | 4   | 7.562 | **           |
|       | B      | 2.219 | 4   | 34.314| **          |
|       | C      | 0.004 | 4   | 0.062 |             |
|       | Error  | 0.19  | 12  |       |              |

Note: F_{0.01} (4, 12) = 5.410, **means 0.01 levels significant

According to formula (8), it is assumed that the pressure \( P \) in Preston equation is constant pressure.

Because polishing parameters \( K \) and polishing pressure \( P \) were constants and initial angle \( \phi_0 \) has no effect on \( MRR \), in order to facilitate normalization of simulation analysis, we set \( K = 1 \), \( P = 1 \) Pa, initial angle \( \phi_0 = 0^\circ \), \( \omega_s = -20 \) r/min, \( t = 1 \) s. Influence of the three parameters (speed rate of the outside ring gear to the inside sun gear \( m \), speed rate of lower plate to the inside sun gear \( n \), SiC substrate distribution radius \( RB \)) in formula (15) on \( MRR \) was studied.

\[
MRR = \frac{K \cdot P}{t} \int_0^t \left[ \left( RB \cdot \frac{Z_s \omega_s + Z_r \omega_r}{Z_s + Z_r} + n \cdot w_i \right)^2 + 2RB \cdot (R + r) \cdot \frac{Z_s \omega_s + Z_r \omega_r}{Z_s + Z_r} + n \cdot w_i \right] \cdot \cos \left( \frac{Z_s \omega_s - Z_r \omega_r}{Z_s + Z_r} \cdot t + \phi \right) dt
\]

(15)

Fig. 4. Influence trend of single factor on \( MRR \)

Table 5 Orthogonal rotary regression test of factors and levels design of L23

| Levels | Factors | \( m \) | \( n \) | \( RB \) |
|--------|---------|-------|-------|-------|
| \( +r \) | -1.318  | 4.682 | 70.23 |
| \( +1 \) | -2      | 4     | 60    |
| 0      | -3      | 3     | 45    |
| -1     | -4      | 2     | 30    |
| \( -r \) | -4.682  | 1.318 | 19.77 |

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MRR = 2.3066 × 10^4 occurs at $m = -1$, $n = 5$, $RB = 75$. That is to say, the closer the speed rate of the outside ring gear to the inside sun gear is to 0, and the greater speed rate of lower plate to the inside sun gear, the larger the SiC substrate distribution radius, the higher the MRR it is. The slice figure of the influence of parameters on MRR was shown in Fig. 2.

In Fig. 2, there are one dependent variable and three independent variables ($m$, speed rate of the outside ring gear to the inside sun gear; $n$, speed rate of lower plate to the inside sun gear; $RB$, SiC substrate distribution radius). From the slice diagram, it can be seen the impact of three dimensional parameters on MRR and the effect of three variables on MRR is $n > m > RB$.

### 3 Results and discussion

Polishing disks were made of cast iron, while polishing pads were grooved polyurethane polishing pad IC1400. At $T = 25 \, ^\circ\mathrm{C}$, $\omega_s = -20\, \text{r/min}$, $P = 30 \, \text{kPa}$, diamond powder W2.5. Orthogonal tests of three factors and five levels of $L_{25}$ were carried out. Orthogonal test factors and levels were shown in Table 1, and orthogonal test results were shown in Table 2 as follows:

\[
MRR = \frac{\Delta m}{\rho \cdot \pi r^2 \cdot t}
\]  

(16)

| No. | Factors | $m$ | $n$ | $RB$ | Index |
|-----|---------|-----|-----|------|-------|
| 1   |         | -2  | 4   | 60   | 2.32  |
| 2   |         | -2  | 4   | 30   | 2.32  |
| 3   |         | -2  | 2   | 60   | 1.71  |
| 4   |         | -2  | 2   | 30   | 1.71  |
| 5   |         | -4  | 4   | 60   | 2.10  |
| 6   |         | -4  | 4   | 30   | 2.09  |
| 7   |         | -4  | 2   | 60   | 1.55  |
| 8   |         | -4  | 2   | 30   | 1.53  |
| 9   |         | -1.318 | 3   | 45   | 2.09  |
| 10  |         | -4.682 | 3  | 45   | 1.81  |
| 11  |         | -3   | 4.682 | 45  | 2.42  |
| 12  |         | -3   | 1.318 | 45  | 1.41  |
| 13  |         | -3   | 3    | 70.23| 1.93  |
| 14  |         | -3   | 3    | 19.77| 1.92  |
| 15  |         | -3   | 3    | 45   | 1.93  |
| 16  |         | -3   | 3    | 45   | 1.92  |
| 17  |         | -3   | 3    | 45   | 1.93  |
| 18  |         | -3   | 3    | 45   | 1.93  |
| 19  |         | -3   | 3    | 45   | 1.93  |
| 20  |         | -3   | 3    | 45   | 1.94  |
| 21  |         | -3   | 3    | 45   | 1.92  |
| 22  |         | -3   | 3    | 45   | 1.93  |
| 23  |         | -3   | 3    | 45   | 1.93  |

**Table 6** Orthogonal rotary regression test results of $L_{23}$
$MRR$ was calculated by Equation (16), among them, $\Delta m$ means the difference of quality before and after double-faced mechanical polishing by electronic balance with an accuracy of 0.1 mg, $\rho$ means the SiC substrate density 3.2 g/cm$^3$, and $t$ means polishing time.

Optimal level combination can be derived by calculating $K$ value. Range $R$ can be obtained by Equation (17):

$$R = \max K_i - \min K_i (i = 1, 2, 3, 4, 5)$$  \hspace{1cm} (17)

Through range analysis shown in Table 3, the primary and secondary order of $MRR$ was $B > A > C$, at the same time, the corresponding optimal combination was $A_5B_5C_5$. $MRR$ reached the maximum when speed rate of the outside ring gear to the inside sun gear $m = -1$, speed rate of lower plate to the inside sun gear $n = 5$, and SiC substrate distribution

| Source | SS | DF | MS | F | P | Significance |
|--------|----|----|----|---|---|--------------|
| $x_1$  | 0.001761954 | 1  | 0.001761954 | 11.5726150 | 0.004725454 | Yes |
| $x_1^2$ | 0.000336056 | 1  | 0.000336056 | 2.2072385 | 0.161207697 | No |
| $x_2$  | 0.032578451 | 1  | 0.032578451 | 213.9771828 | 0.000000002 | Yes |
| $x_2^2$ | 0.000960483 | 1  | 0.000960483 | 6.3085119 | 0.026009565 | Yes |
| $x_3$  | 0.000099444 | 1  | 0.000099444 | 0.6531524 | 0.433528562 | No |
| $x_3^2$ | 0.000285584 | 1  | 0.000285584 | 1.8757337 | 0.194013919 | No |
| $x_1 \cdot x_2$ | 0.001512500 | 1  | 0.001512500 | 9.9341891 | 0.007644289 | Yes |
| $x_1 \cdot x_3$ | 0.000112500 | 1  | 0.000112500 | 0.7389066 | 0.405584308 | No |
| $x_2 \cdot x_3$ | 0.000012500 | 1  | 0.000012500 | 0.0821007 | 0.77896055 | No |
| Regression | 1.308194637 | 9  | 0.145394960 | 954.6999383 | 1.1E-16 | |
| Lack of Fit | 0.000288889 | 5  | 0.000057780 | 0.2734522 | |
| Residual | 0.001690387 | 8  | 0.000211298 | |
| Total | 1.310173913 | 22 | 0.059553360 | |

Table 7 Variance analysis of L$\text{23}$

![Image](image.png)

Fig. 6. Surface response diagram of $MRR$

| No. | $x_1$ | $x_2$ | $x_3$ | $y$(test) | $y$(model) | Relative error |
|-----|-------|-------|-------|-----------|------------|----------------|
| 2   | -2    | 4     | 30    | 2.32      | 2.324      | 0.0017         |
| 8   | -4    | 2     | 30    | 1.53      | 1.540      | 0.0065         |
| 16  | -3    | 3     | 45    | 1.92      | 1.929      | 0.0047         |
| add1| -3    | 2     | 45    | 1.62      | 1.626      | 0.0037         |
| add2| -2    | 4     | 60    | 2.33      | 2.321      | 0.0039         |
| add3| -1    | 3     | 30    | 2.12      | 2.132      | 0.0056         |

Table 8 Verification of test results

R = max $K_i - \min K_i (i = 1, 2, 3, 4, 5)$
radius \( RB = 75 \). If only the influence of these three factors on \( MRR \) was considered, proportion of the influence of parameters was shown in Fig. 3.

Variance analysis [19] was used to study the significance of the influence of various factors on the index. Analysis of variance was shown in Table 4.

According to the table above, at 99% confidence, \( m \) and \( n \) have a significant effect on \( MRR \) while \( RB \) not. In order to study the influence of factors on index, the trend chart in the intuitive analysis method was used as shown in Fig. 4. Horizontal axis was the five levels of each factor, and the vertical axis was the \( MRR \).

Figure 4 shown that speed rate of lower plate to the inside sun gear \( n \) has the greatest influence on \( MRR \), speed rate of the outside ring gear to the inside sun gear \( m \) has an effect on \( MRR \) while it was approximately linearly correlated, and SiC substrate distribution radius \( RB \) has little influence on \( MRR \).

In order to build an accurate mathematical model and more accurately analyze the relationship between index and factors, orthogonal rotary regression test of Tri-factor quadratic was carried out based on orthogonal test of three factors and five levels of L25. The number of central repeated tests was 9 and asterisk arm length \( \gamma \) was equal to 1.682. Orthogonal rotary regression test of factors and levels design and results were shown in Table 5 and Table 6.

It was used the STATISTICA 8.0 to analyze the variance of the test results[20, 21], and the regression equation was obtained by fitting the ternary quadratic polynomial. Pareto chart of \( t \) values for coefficients was shown in Fig. 5. The variance analysis of \( MRR \) was shown in Table 7.

Among them, \( x_1 \) stands for speed rate of the outside ring gear to the inside sun gear, \( x_2 \) stands for speed rate of lower plate to the inside sun gear, \( x_3 \) stands for SiC substrate distribution radius. Coefficient of determination was \( R^2 = 0.998 \).

Degree of regression and lack of fit must be tested according the following equation:

\[
F_R = \frac{SS_R/df_R}{SS_Re/df_Re} = 954.69994
\]

\[
F_L = \frac{SS_L/df_L}{SS_Er/df_Er} = 0.27345
\]

Table \( F \) shows that \( F_{0.05} (5, 8) = 3.69, F_{0.05} (9, 13) = 2.71, F_R > F_{0.05} (9,13), F_L < F_{0.05} (5,8) \). Therefore, the regression model was significant, and the lack of fit model was not significant. So as that, the equation fit well. \( MRR \) was derived as (20). After removing the constant term and the insignificant term, the regression model can be simplified as
Surface response diagram of the coupling effect of three factors \( x_1, x_2, \) and \( x_3 \) on \( MRR \) was shown in Fig. 6. The influence and interaction of \( x_1, x_2, \) and \( x_3 \) on \( MRR \) are obtained from Figure 6. Among them, the interaction between \( x_1 \) and \( x_2 \) has a great impact. Meanwhile, an accurate mathematical model is obtained by STATISTICA 8.0 as Equation (20):

\[
MRR = 1.142972 + 0.08991x_1 + 0.004598x_2^2 + 0.386613x_2 - 0.007773x_2^2 + 0.001424x_3 - 0.000019x_2^3 + 0.013750x_1 \cdot x_2 - 0.00025x_1 \cdot x_3 - 0.000083x_2 \cdot x_3
\]

At \( m = -1, n = 5, RB = 75 \), the maximum \( MRR \) was calculated 2.7 \( \mu m/h \). Characterization parameters were calculated as shown in Fig. 7. The total thickness variation (TTV) was within 10 \( \mu m \), bending of wafer (BOW) within 25 \( \mu m \), and Warp within 40 \( \mu m \).

Fig. 9. Surface roughness of C-face and Si-face after MP by AFM at 10um×10um. a C-face 3D, b Si-face 3D, c C-face 2D, d Si-face 2D

In order to verify the applicability of the model, three groups tested in Table 8 and add another three new groups were chosen by formula (20) in Table 8.

In Table 8, it was shown that the test results were closed to the model, and the relative errors were less than 1%. It means that this model can well respond to the changes of the \( MRR \) of the SiC single crystal substrate.
10 um) through AFM (Dimension FastScan) as shown in Fig. 9.

4 Conclusion

The MRR of the double-faced MP of SiC substrate was researched. Based on the coordinate transformation theory, the kinematic equations of SiC substrate relative to lower pad during double-faced MP were analyzed. MRR reached the maximum when speed rate of the outside ring gear to the inside sun gear \( m = -1 \), speed rate of lower plate to the inside sun gear \( n = 5 \), and SiC substrate distribution radius \( RB = 75 \). Through range analysis of orthogonal test factors and levels of L25, the primary and secondary order of MRR \( n > m > RB \) was obtained. An accurate mathematical model of orthogonal rotary regression test of Tri-factor quadratic of MRR was established and the regression model was significant. At \( m = -1, n = 5, RB = 75, TTV < 10 \) um, BOW < 25 um, Warp < 40 um, the maximum MRR was 2.7 um/h, which really improved the processing efficiency. At the same time, \( Ra \) of C-face was \(-6.7 \) nm–7.8 nm (10 um × 10 um), and \( Ra \) of Si-face was \(-4.9 \) nm–4.4 nm (10 um × 10 um) through AFM. This work provided the key for CMP and verified the importance of MRR for ultra-smooth polishing. It has certain guidance for semiconductor equipment and process technology.

Author contribution Peng Zhang: conceptualization, experiments, and writing; Jingfang Yang: data analysis; Huadong Qiu: supervision, investigation.

Data availability All the data have been presented in the manuscript.

Declarations

Ethics approval Not applicable

Consent to participate The authors declare that they all consent to participate in this research.

Consent for publication The authors declare that they all consent to publish the manuscript.

Competing interests The authors declare no competing interests.

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