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Mathematical Modeling of Material Removal Rate in Sapphire CMP using Silica Particle

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Abstract **-** In this research, we aim to define a mathematical model for the material removal rate (MRR) in the chemical mechanical polishing (CMP) of sapphire. Silica slurries with particle sizes of 4, 20, 55, and 105 nm were used as abrasives in the polishing tests. The results showed that the material removal rate increased with abrasive particle size from 20 to 105 nm. However, we found that 4 nm silica particles produced a remarkably high removal rate, comparable to that achieved using 105 nm silica particles. These results indicated that the MRR is governed by dominant factors related to the abrasive particle size. To further investigate this relationship, the chemical and mechanical contributions of silica particles were analyzed based on the experimental data. A predictive model for the material removal rate in sapphire CMP was then derived. The comparison between the predicted MRR values and experimental results showed that the maximum error decreased from 20% to 3.33% as the abrasive size increased from 4 nm to 105 nm. The results in this research may indicate the MRR of sapphire CMP.

Keywords**:** Sapphire, Chemical mechanical polishing, Silica, Mathematical model, Material removal rate

1. Introduction

Sapphire (α-Al_2O_3 single crystal) has become a crucial material widely utilized in various fields, including optical devices, visual windows, and as a substrate material in light-emitting diode (LED) fabrication [1]. The performance of these devices is significantly influenced by the surface quality of the sapphire substrate. Therefore, a key requirement in these applications is achieving an ultra-smooth, planar surface free from subsurface damage in sapphire wafers [2, 3]. However, sapphire is classified as a hard-to-process material due to its extreme hardness and brittleness, making it challenging to achieve the desired surface characteristics through conventional machining techniques [4, 5]. Chemical mechanical polishing (CMP) is recognized as a critical technique for manufacturing highly smooth and planarized sapphire wafers [6]. CMP combines both chemical and mechanical effects to achieve a damage-free, ultra-smooth sur-face. Colloidal silica particles are widely used as abrasives in sapphire CMP because they provide an optimal material removal rate (MRR). This is attributed to their ability to chemically react with the sapphire surface, forming a reacted layer, which is subsequently removed through mechanical abrasion [7,8]. The interplay between these chemical and mechanical interactions determines the effectiveness of the CMP process in achieving the required surface quality.

Although CMP is a critical manufacturing process for achieving high planarization and meeting the stringent surface quality requirements of sapphire wafers, the underlying mechanisms of the CMP process remain unclear [9]. Additionally, several theoretical and technical challenges persist [10]. The first mathematical model of CMP was proposed by Preston [11], which predicted that the material removal rate (MRR) is dependent on the applied pressure and the relative velocity during the polishing process. In recent years, numerous researchers have investigated and refined CMP modeling to enhance prediction accuracy. Hyunjin et al. [12] developed a mathematical model based on the contact mode between a patterned wafer and a polishing pad. Similarly, Hyunseop et al. [13] introduced a semi-empirical MRR model based on contact mechanics to predict the polishing time required for film material removal.

However, our previous research [14] revealed that silica particles larger than 10 nm primarily contribute to the mechanical action during the sapphire polishing process, suggesting that abrasive particle size plays a crucial role in determining the dominant material removal mechanism. In contrast, when using 4 nm silica particles, chemical reactivity becomes the dominant factor in the sapphire polishing process. Furthermore, the threshold particle size that distinguishes the dominant mechanism between mechanical and chemical effects is approximately 10 nm. As a result, planning the polishing time and estimating consumable costs remain challenging.

The primary contribution of this study is the development of a mathematical model for MRR based on both mechanical and chemical factors as a function of particle size. To achieve this, the material removal rates (MRRs) in sapphire CMP were analyzed using experimental data. Subsequently, a mathematical model for MRR was derived. Additionally, the effects of mechanical and chemical interactions on the polishing process were further examined. Finally, the discrepancy between the MRR values predicted by the model and those obtained from experiments was evaluated and discussed.

2. Research Methodology

2.1. Polishing Test

Colloidal silica particles with sizes of 4 nm (NALCO 1115), 20 nm (NALCO 1040), 55 nm (NALCO TX15582), and 105 nm (NALCO 2329 Plus) were used as abrasive particles in the slurry for sapphire CMP experiments. The polishing pro-cess was performed using a CMP machine (IMT Rana-30) with a slurry reuse system that operated without a filtration unit, as illustrated in Fig 1. The detailed polishing conditions are presented in Table 1.

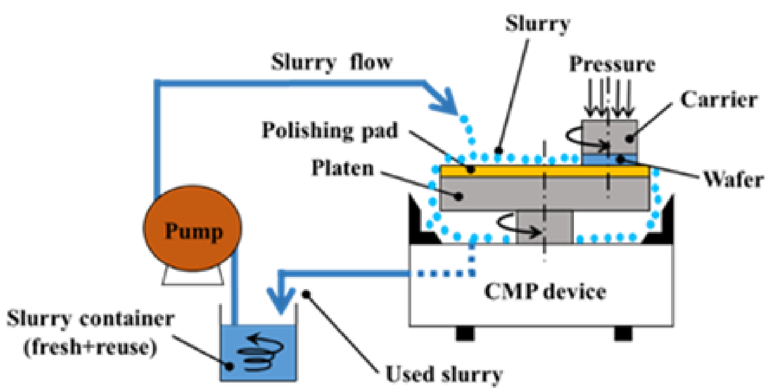

Fig. 1: Schematic of chemical mechanical polishing device with reuse slurry system.

Table 1. Polishing conditions.

Slurry type	Colloidal silica, pH 11 adjusted using KOH
Ceoncentration	5 wt%
Particle size	4, 20, 55 and 105 nm
Wafer size	φ25.4×1 mm
Polishing pad	SUBA 600
Polishing time	180 min
Polishing pad seasoning	Nylon brushing
Conditioning time	5 min
Polishing pressure	0.1 MPa
Platen/carrier speed	60/60 rpm
Slurry flow rate	60 ml/min

2.2. Mathematical Modeling Method

The material removal rate (MRR) can be divided into two components. The first component is governed by chemical reactivity as the dominant factor. In this case, the MRR decreases as the abrasive particle size increases. Therefore, the removal rate is inversely proportional to the abrasive particle size and can be expressed as

$$MRR_{chemical} = \frac{k_1}{d} \tag{1}$$

The other part, which is the mechanical action as dominant factor. The mate-rial removal rate increased with the increasing of abrasive size. Therefore, the removal rate is the direct proportion of abrasive size, can be expressed by

$$MRR_{mechanical} = k_2 d \tag{2}$$

Hence, the totally material removal rate of sapphire CMP is calculated by sum of Eq. (1) and (2), can be expressed by

$$MRR = \frac{k_1}{d} + k_2 d \tag{3}$$

Where k_1 is chemical factor, k_2 is mechanical factor, and d is diameter of silica particles.

3. Results and discussion

3.1. Material removal rate

The results showed that the material removal rates (MRRs) of sapphire in-creased with the particle size of colloidal silica, from 20 nm to 55 nm to 105 nm. However, the ultrafine silica particles (4 nm) produced a remarkably high MRR, comparable to that achieved with the 105 nm silica particles.

3.2. Mathematical Modeling of Material Removal Rates

After taking the polishing results of sapphire and diameter size of silica particles to calculate the chemical and mechanical factors (k_1 = 1.9981, k_2 = 0.0029). We then plot the curve fitting by using Eq. (3) compared to the experiment results as shown in Fig. 2.

The material removal rates (MRRs) obtained from the fitting curve closely matched those obtained from the polishing experiments. The MRRs derived from both the model and experimental results are presented in Table 2. These results demonstrate that the MRRs predicted by the model exhibit high accuracy, particularly when larger abrasive particle sizes are used. Additionally, the mathematical model for the material removal rate in sapphire CMP can be defined by both the mechanical and chemical factors of silica particles, as a function of abrasive size. We expect that the mathematical model we have developed will be capable of accurately predicting the MRR for sapphire CMP across a range of abrasive (silica) sizes.

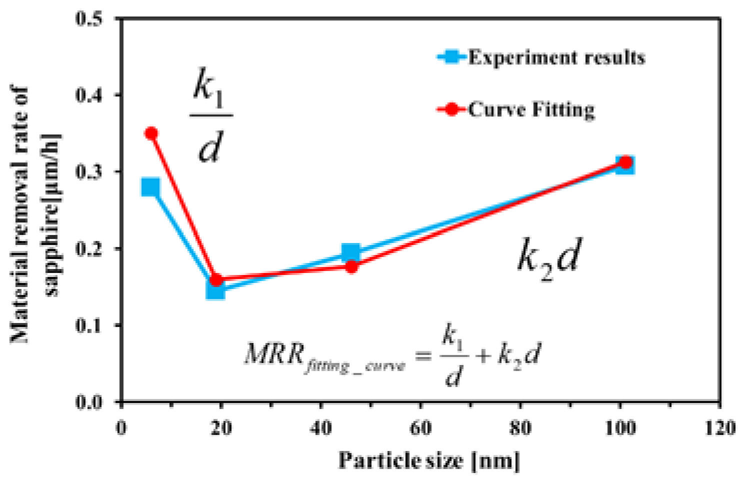

Fig. 2: A comparison of the material removal rate (MRR) for sapphire CMP, obtained from polishing experiments and the fitting curve.

Table 2. MRRs obtained by modeling and experimental results.

Particle size (nm)	MRR_{Model} (µm/h)	$MRR_{Experiment}$ (µm/h)	Error (%)
4	0.35	0.28	20
20	0.16	0.15	6.25
55	0.17	0.19	11.76
105	0.30	0.31	3.33

4. Conclusion and Future Work

4.1. Conclusion

We proposed a mathematical model based on CMP experimental results to predict the material removal rate (MRR) of sapphire. The model considers both mechanical and chemical factors, which depend on particle size. The comparison between the MRRs obtained from the polishing tests and the model revealed that the error decreased as the particle size increased. We found the error of MRRs decreased from 20% to 3.33% from the silica particle sizes of 4 nm to 105 nm respectively.

4.2. Future work

To enhance the accuracy of MRR predictions, the mathematical model should incorporate additional experimental results. Therefore, silica particles with sizes of 150 nm and 200 nm should be used in polishing tests to refine the model. Additionally, a case study using silica particles of varying sizes from the model's database should be conducted to validate the accuracy of the model.

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