Tribology International 93 (2016) 11–16

Contents lists available at ScienceDirect

Tribology International

journal homepage: www.elsevier.com/locate/triboint

A material removal model for silicon oxide layers in chemical mechanical planarization considering the promoted chemical reaction by the down pressure

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ARTICLE INFO

Article history:
Received 13 February 2015
Received in revised form
20 August 2015
Accepted 3 September 2015
Available online 12 September 2015

Keywords:
CMP
Model
Promoted reaction
Chemical mechanical synergy

ABSTRACT

This paper proposes a material removal rate model for silicon oxide layers in a chemical mechanical planarization (CMP) process based upon micro-contact force equilibrium theory and chemical mechanical synergistic effects, in which considers the promoted chemical reaction of the slurry with the wafer surface by the polishing pressure rarely investigated by previous models. The present model clarifies the contradictory relationships between the abrasive concentration and removal rate. Furthermore, the nonlinear dependences of removal rate on polishing pressure and abrasive size are addressed as well. The current theoretical predictions are in good qualitative agreement with the published experimental data.

1. Introduction

The chemical–mechanical polishing (CMP) technology is critical to the development of the integrated circuits (IC) industry due to its capacity in wafer planarization [1,2]. In a CMP process, a rotating wafer is pressed against a rotating polishing pad while slurry, comprising some chemical agents and abrasive particles, is fed into the wafer-pad interaction zone. The combined chemical and mechanical interactions are believed to be responsible for the material removal. Nevertheless, the effect of chemical mechanical synergy (CMS) on the material removal in a CMP process remains unclear and ambiguous [3,4].

Investigations of the effect of CMS on the material removal rate (*MRR*) in the CMP process appear to have taken three different approaches. One approach focuses on the mechanical aspect, and the chemical effect was normally considered through a dynamical hardness value of the wafer surface [5–8]. The other approach is based on the mechanist-assisted chemical effect, which takes into account the surface reaction kinetics in the CMP process [9–11]. However, the properties of the wafer and polishing pad were not included in these models despite their significant influences on the polishing results. In our previous work, a mathematical model was proposed to fully describe the influence of CMS on material removal during CMP based on the molecular scale removal mechanism [12]. Another related model was an extension to the modeling of CMS [13], which in further isolated each of the contribution of the CMS to the *MRR* based on the corrosion-wear mechanism. However, these previous models ignored the acceleration of the chemical reaction of the slurry with the wafer surface by the polishing pressure.

Some static chemical reaction rate is so slow that one may not detect the change of reaction. Several researchers reported that the reaction between H_2O_2 and silicon under normal temperature is slow, and the thickness of oxide chemical layer is around 2–3 Å after a 10 min etching process [14–16]. Concurrently, Hickenboth et al. [17] concluded that the chemical reaction will be accelerated by physical factors, such as pressure and temperature. Therefore, one can speculates that the pressure may play a dominant role to control the chemical reactions of the slurry with the wafer surface, which would change the subsurface structure of silicon wafer in a CMP process.

Additionally, contradictory results had been reported for the effect of abrasive concentration on the *MRR*. Tamboli and Zhang [18,19] reported that the increase in abrasive concentration leads to the non-linear increase in the *MRR*. In contrast, Choi et al. [20] stated that the *MRR* increases initially with the abrasive concentration at low abrasive concentrations. Conversely, the *MRR* decreases at high abrasive concentrations with the increasing in the abrasive concentration. Several researchers have independently investigated the dependence of material removal rate on the abrasive concentration [21,22], which predicted that the increase in the abrasive concentration leads to the nonlinear increase in the *MRR*. Most recently, Wang et al. [23] attempted to

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http://dx.doi.org/10.1016/j.triboint.2015.09.008
0301-679X/

establish a model to correlate the relationship between abrasive concentration and *MRR*. Nevertheless, the experimental results of Choi et al. [20] could not be explained by the above models yet.

The objective of the present paper is to develop a mathematical model considering the promoted chemical reaction by the polishing pressure in the CMP process of silicon oxide wafers, which is applied to investigate the effect of the abrasive concentration and size on the *MRR*.

2. Modeling

2.1. Assumptions

The following assumptions are made to develop the present model, which have also been adopted by several researchers [24,25]. Various parameters considered in the present analysis and the underlying assumptions are described in details as the model develops.

(i) Pad/wafer contact was regarded as the contact between a rough surface and a smooth surface.
(ii) For simplicity, the chemical diffusion of the oxidizer into the wafer surface is assumed to be accelerated by the polishing pressure and temperature of the slurry.

2.2. Tensile stress

According to the Ref. [26], a corresponding tensile stress is responsible for the traveling contact problem of a single abrasive particle with the wafer surface, which is given by

$$\sigma_t = \frac{1}{2} P_s (1 - 2\upsilon_1)(1 + C\mu) \tag{1}$$

where $P_s = F_s / A_c$ is the mean contact pressure between the abrasive particle and wafer surface, F_s is the force of a single abrasive particle, and A_c is the contact area between the abrasive particle and wafer surface. μ is the coefficient of friction between the particle and wafer surface, υ_1 is the Poisson's ratio for the wafer, and C is a dimensionless parameter calculated by $C = 3\pi(4 + \upsilon_1)/8(1 - 2\upsilon_1)$.

Based on the Amontons law [27], the coefficient of friction between the particle and wafer μ is expressed as

$$\mu = \frac{F}{F_s} = \frac{F}{P_s A_c} \tag{2}$$

At the scale of interaction under discussion, an operational definition of the friction force is written as [25]

$$F = \frac{A_c f_b E_1}{10} \tag{3}$$

where f_b is the fraction of the contact area in which bonding occurs ($\sim 1\%$) and E_1, Young's modulus of wafer.

Submitting Eqs. (2) and (3) into Eq. (1) yields

$$\sigma_t = \frac{1}{2}(1 - 2\upsilon_1)(P_s + C f_b E_1 / 10) \tag{4}$$

2.3. The mean contact pressure

On the basis of Hertzian contact theory [28], the contact area A_c is given by

$$A_c = \pi \left(\frac{2DC_2 F_s}{3E} \right)^{2/3} \tag{5}$$

where D is the abrasive diameter.

The dimensionless value of C_2 can be calculated by

$$C_2 = \frac{9}{16} \left[(1 - \upsilon_1^2) + (1 - \upsilon_2^2) \frac{E_1}{E_2} \right] \tag{6}$$

in which E_2, υ_2 are the Young's modulus and Poisson's ratio of abrasive particle, respectively.

Submitting Eq. (5) into Eq. (2) yields

$$P_s = \frac{F_s^{1/3}}{\pi} \left(\frac{2DC_2}{3E} \right)^{-2/3} \tag{7}$$

2.4. The force of single particle

In a CMP process, the applied down force on the wafer surface balances the force at the polishing interface provided by the abrasive/wafer contact force and the pad asperity/wafer contact force [7]. It was assumed that the ratio of abrasive/wafer contact force to the total contact force is Ψ. Then, the following equation is obtained

$$NF_s = \Psi P A_p \tag{8}$$

where P is the polishing pressure, and N is the number of the effective slurry particles.

The number of the effective slurry particles is an important variable influencing the material removal. Following the force equilibrium analysis of a sandwiched pad/particle/wafer presented by Jeng [7], an equation for the effective abrasive particle number N can be derived by

$$N = A_r (3\omega - d) \frac{6 d_s \rho_s W}{\pi \rho_a D^3} \tag{9}$$

in which A_r is the real contact area between the wafer and pad, ω is the standard deviation of the asperity height, and d is the distance between the wafer and the mean plan of the asperity. The reference plan is assumed to pass through the mean of the asperity height distribution. d_s is the dilution ratio of the slurry, ρ_s is the density of the slurry before dilution, W is the concentration of the slurry before dilution, ρ_a is the density of the abrasive particles and D is the average diameter of the abrasive particles.

Submitting Eq. (9) into Eq. (8) yields

$$F_s = \Psi \frac{\pi \rho_a P A_p D^3}{6 A_r (3\omega - d) d_s \rho_s W} \tag{10}$$

2.5. Pad/wafer contact

The micro-contacts between the pad and the wafer surfaces could be modeled by the GW [29] elastic model. With this model, the contact ratio α is

$$\alpha = \frac{A_r}{A_P} = \pi \eta R \int_d^{+\infty} (z - d) \Phi(z) dz \tag{11}$$

The contact polishing pressure between the wafer surface and the pad is

$$P = \frac{4}{3} \eta E_{pw} R^{1/2} \int_d^{+\infty} (z - d)^{3/2} \Phi(z) dz \tag{12}$$

where $\Phi(z) = \frac{1}{\omega\sqrt{2\pi}} \exp\left(\frac{-z^2}{2\omega^2} \right)$, A_P is the area of wafer, R is the radius of the pad asperity summit, η is the density of the asperity, and z is the height of the asperity. Since the pad is normally much softer than the wafer, $E_{pw} = E_p / (1 - v_p^2)$, where E_p and v_p are, respectively, the Young's modulus and the Poisson's ratio, and the subscript 'p' represents the pad.

Once Eqs. (7), (10)–(12) are derived, the Eq. (4) can be used to calculate the tensile stress.