Modeling CMP - Investigation of the Mechanical Removal Mechanism

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Abstract: Chemical mechanical polishing (CMP) is a hybrid polishing process aimed at planarizing wafer surfaces which features a base material (e.g. SiO_2) in which structures made out of another material (e.g. Cu leads) are embedded. Since the two materials differ in the *Young's* Modulus and in hardness, a mere mechanical machining process would result in steps at the border between these materials. A typical example for a material combination in MEMS is a magnetic structure of poles and yokes (NiFe alloys), conductive coil material (Cu), and insulator (photoresist). The motivation of this work is to develop a reliable model which will describe the entire CMP-process combining existing models with own results. Considering Hertzian elastic penetration of the abrasive particles and the micro friction model of *Bowden* and *Tabor* a model can be derived to correlate material removal rate (MRR) with wafer rotational speed, down pressure, and *Young's* modulus of pad and wafer. According to the model, MRR is proportional to the rotational velocity, but pressure yields a nonlinear, asymptotic increase of the MRR.

1. Introduction

CMP accomplishes a high degree of planarization by balancing chemical and mechanical material removal mechanisms. Derived from semiconductor processes, CMP is increasingly used in manufacturing multilayer MEMS structures with different materials. These materials differ in mechanical properties (hardness and stiffness) as well as in the chemical reaction ability. In previous works, we presented work on the planarization of copper embedded in photoresist with a minimal step height at the material boundaries [1]. Applying CMP to high aspect ratio SU-8/permalloy structures showed that CMP is well suited for this material combination [2]. Material removal rates (MRR) of metals (NiFe and Cu) are lower than those of insulators (photoresist). In contrast to metals, which are chemically more active materials, organic insulators are nearly chemically inert. Optimal balancing the MRR of two or more materials needs a profound understanding of the changes in material properties caused by the chemical attack in correlation with the mechanical removal during CMP.

There are three CMP scales, the particle scale, the scale regarding „with-in die non-uniformity“ (WIDNU, also called “local planarization”), and wafer scale regarding „with-in wafer non-uniformity“ (WIWNU, also called “global planarization”). It is desirable to develop models for all three scales. The most challenging ones are on the first two scales, whereas global planarization usually depends on constant wafer wide pressure controlled by tooling. The models at the particle scale are needed to address the roles and interactions of slurry particles, slurry chemicals, polishing pad, and wafer materials. The material removal process in CMP can be considered as a sliding of slurry particles over a chemically influenced thin film layer on the wafer surface. The models at the die scale are required to address the topography evolution of single structural parts as a function of pattern density, line width, pitch width, and polishing time [3].

The most common model for material removal is *Preston's* equation, where removal rate r is related to pressure P and relative velocity v_{rel} between the pad and wafer as:

$$r = k_r * P * v_{rel} \tag{1}$$

where k_r is the *Preston's* coefficient related to chemical erosion processes and material characteristics [4].

Various adaptations of the *Preston's* law have been proposed and a generalized relationship may be written as:

$$r = k_e * P^{\alpha} * v^{\beta} \tag{2}$$

where α, β and k_e are experimental constants. Quantities α and β are considered adjustable parameters and are used to account for nonlinear variation of rate with kinetics or other factors [5].

For glass polishing, *Preston* established a relationship between the removal rate and friction. *Preston's* definition of glass polishing describes the work W_p accomplished in time t as a product of the friction coefficient μ, area A in contact, pressure P and relative velocity v_{rel}:

$$W_p = \mu * A * P * v_{rel} * t \tag{3}$$

$\mu * A * P$ equals the friction force F_{μ}. A well known empirical equation for removal rate r is proposed (eq. 1), where all the other active parameter are related to *Preston's* coefficient k_r [6].

Only a few theories for modeling chemical effects exist. One reason for the difficulty in describing chemical reactions is their strong material dependence. This effect is determined by balancing the content and concentration of the slurry chemicals, anti-agglomerates, and viscosity. Although significant advances in CMP slurry technologies have been achieved over the last decade, the fundamental science underlying slurry formulation and the mechanisms that control various interactions during the polishing process are poorly understood [7]. A holistic model of CMP including chemical influences has been proposed by *Paul* for Tungsten CMP and later advanced for all CMP-processes. While *Preston* describes the linear influence of pressure and relative velocity to the MRR, the approach of *Paul* portraits the material removal as a process governed by several chemical and mechanical effects [8]. Nevertheless, no existing model covers the interaction between chemical attack and changes in material properties.

2. Modeling the Removal Rate (Model Description)

Starting point for our model is *Preston's* model for glass polishing outlined above. Furthermore, we are assuming that the main chemical contribution in CMP is to change the material's resistance against indentations through the abrasive grain. Compared to this effect, pure etching is negligible, as experimental results show [9]. Therefore, the change in material hardness may be used as the main factor to describe the chemical impact. Derived from *Luo's* and *Dornfeld's* theory of the indentation depth we suggest an indirect proportional correlation between MRR and hardness. Therefore, in this paper, we are focusing on studying the mechanical effect, particularly the abrasion and evolution of the contact surface due to the abrasive-wafer contact.

According to the *Preston's* model (Equ. 3), the removal rate r can be described as a function of the friction force F_μ:

$$r = k_\mu * F_\mu \tag{4}$$

k_μ: proportionality coefficient

Understanding the deformation mode over the whole particle-wafer interface is important to determine the material removal. If the deformation is elastic (*Hertz*ian elastic deformation) the real contact surface A_{ri} depends on the polishing pressure P, the radius of abrasives d and the equivalent *Young's* modulus E^* [10],

$$A_{ri} = \frac{\pi}{2} * p^{\frac{2}{3}} * \left(\frac{3}{4} * d * \frac{1}{E^*} \right) \tag{5}$$

where the equivalent *Young's* modulus E^* is a function of the elastic properties of the two materials involved in contact, *Young's* modulus and *Poisson's* number of wafer (E_1, ν_1) and abrasive (E_2, ν_2) material:

$$\frac{1}{E^*} = \frac{1-\nu_1^{\,2}}{E_1} + \frac{1-\nu_2^{\,2}}{E_2} \tag{6}$$

From the initial hypothesis (eq. 4), the removal rate in single abrasive-wafer contact r_E may be further developed for an elastic deformation in wafer-abrasive contact:

$$r_E = k * \mu * P * A_{r_i} = k_1 * \mu * P^{\frac{5}{3}} * \left(\frac{E_1 + E_2}{E_1 * E_2}\right)^{\frac{2}{3}} \tag{7}$$

All the constants are in combination with or correlated to the proportionality coefficient k_1.

The two typical contact modes in CMP are the hydro-dynamical contact mode and the solid-solid contact mode or a mixture of both. When the pressure applied to the wafer surface is small and the relative velocity of the wafer is large, a thin fluid with "microscale" thickness will be formed between the wafer and the pad surface. A typical property of CMP is the size of abrasives (nanoscale) being much smaller than the thickness of the slurry film (microscale). Therefore, a lot of abrasives are inactive. Almost the complete material removal is due to three-body abrasion by parts of abrasives in the slurry and the chemical etching by slurry chemicals. When the down pressure applied to the wafer surface is large and the relative velocity of the wafer is small, the wafer and pad asperity contact each other and two-body and three-body abrasion occurs. If the transfer from hydro-dynamical to contact-contact mode occurs during the CMP-process, the friction state will also vary.

Bowden and *Tabor* described the friction coefficient μ as the ratio between the shear strength of the softer material ε and maximal normal strain (yield stress) σ_N [11]. Following this model, the coefficient of friction by CMP could be expressed as follows:

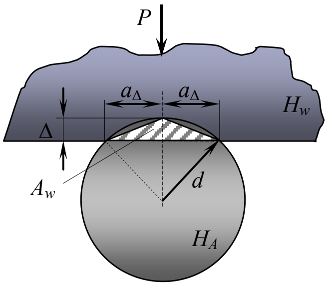
$$\mu = \mu_w \frac{\tau}{\sigma_N} \tag{8}$$

The state of friction (hydro-dynamical or contact-contact) is defined by the shear-pressure ratio (τ/σ_N) and material properties. Shear strain τ is equivalent to the sliding velocity v_{rel} and proportional to the rotational speed ω of pad and wafer. On the other hand, normal strain σ_N is a function of polishing pressure P on the wafer. Friction also depends on material properties which are expressed by a friction coefficient μ_w of surfaces in contact. Therefore, the equation for a material removal rate r_E including the friction state could be further revised:

$$r_E = k_1 * \mu_w * \frac{k_\omega * \varpi}{k_p * P} * P^{\frac{5}{3}} * \left(\frac{E_1 + E_2}{E_1 * E_2}\right)^{\frac{2}{3}} = k_2 * \varpi * P^{\frac{2}{3}} * \left(\frac{E_1 + E_2}{E_1 * E_2}\right)^{\frac{2}{3}} \tag{9}$$

The proportionality coefficient k_1 includes all the constants.

The contact between the abrasive particles and the wafer is considered to be a sliding indentation of a half-space by a hard indenter and the contact between the polishing pad and abrasive particle is considered to be a quasi-static indentation of a half-space by a hard indenter.



P:	polishing pressure
a_Δ:	radius of the projected circle of contact
Δ:	penetration depth
H_w:	hardness of the wafer surface
H_A:	hardness of abrasive particles
d:	radius of the abrasive
A_w:	chip (cutting) surface

Figure 1: Model of the contact between an abrasive particle and wafer surface used to calculate the deformation and material removed by a single abrasive grain

Luo and *Dornfeld* describe the penetration depth Δ of an abrasive particle into the wafer as follows [12]:

$$\Delta = P * d * \frac{1}{H_w} \tag{10}$$

For typical CMP-processes the radius of the abrasive d is very small in comparison to the penetration depth Δ. Therefore, a proportional relation between the chip surface A_w and penetration depth Δ can be assumed. The volume of the removed material by polishing is a function of the chip surface A_w which is a result of a constant rotatory motion of wafer and pad. As a first approximation (for a triangle chip surface A_w), the hardness H_w of the wafer surface can be described as a function of the chip surface A_w as follows:

$$A_w = f(\Delta) \approx f(H_w) \tag{11}$$

Based on equ. 10 and assuming the proportionality between removal rate r and the removed material volume, the following relationship between the removal rate r_Δ, depth Δ, and the material resistance to penetration H_w could be established:

$$r_\Delta = k_\Delta * d * \frac{1}{H_w} \tag{12}$$

The fraction r_Δ of the removal rate describes the penetration of abrasives in the wafer material and thus the material resistance, defining the chip thickness.

The total removal rate r regarding the influence of stress, friction, and chip thickness can be expressed as follows:

$$r = r_E * r_\Delta k_\Delta * d * \frac{1}{H_w} * k_2 * \omega * P^{\frac{2}{3}} * \left(\frac{E_1 + E_2}{E_1 * E_2}\right)^{\frac{2}{3}} \tag{13}$$

After adding all of the constants in a final coefficient k_3, the following equation for a total removal rate r is obtained:

$$r = k_3 * \mu_w * \frac{1}{H_w} * \omega * P^{\frac{2}{3}} * \left(\frac{E_1 + E_2}{E_1 * E_2}\right)^{\frac{2}{3}} \tag{14}$$

$$k_3 = 1{,}296 * k * k_\Delta * k_\omega * k_p^{-1} * d^{\frac{5}{3}} \tag{15}$$

There is a linear relationship between the removal rate r and friction μ_w as well as rotational velocity ω, an inverse relationship with the material's hardness H_w, and an exponential one with the pressure P. As already mentioned, this model considers chemical influences by a respective change of the wafer surface properties.

3. Experimental Setup and Procedure

To verify the CMP model, experiments with MEMS wafers for a NiFe/SU-8 combination were conducted. For the tests, a Peter Wolters 3R40 polishing machine (adapted for CMP) was used. The plate diameter was 400 mm, the load was applied through weights. In the experiments, a polishing fluid without chemical reactive additives at a flow rate of 15 ml/min and Al_2O_3-abrasives with 40 nm radius was used. The test Al_2O_3 ceramic wafers had a diameter of 4". Two wafers had been structured, one with electroplated NiFe81/19-permalloy and the second with spin-on coated epoxy based photoresist SU-8. Both wafers featured the same patterns with lateral dimensions of 5 mm x 25 mm and a difference in height of 20 µm and both experiments were carried out under the same conditions. A DekTak™ profilometer was used for measuring step heights between structures. The removal rate was established as a middle value of five measured points on the wafer.

4. Model Verification

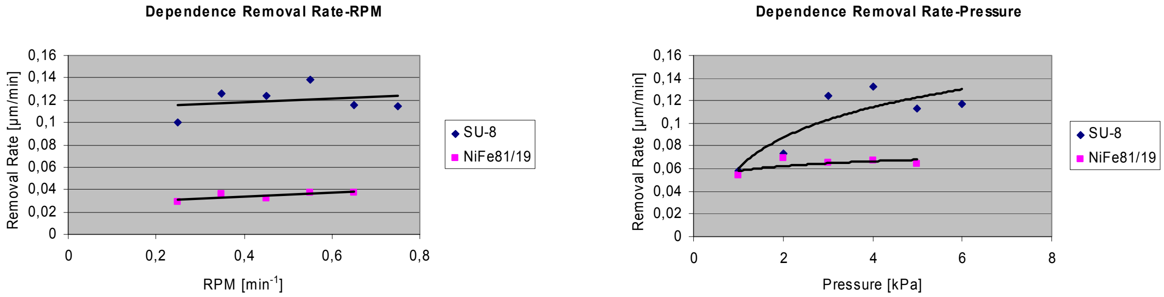


Figure 2: Functional dependence removal rate from RPM (left) and removal rate from pressure (right)

As a result of the experiments, the relationship between the removal rate and the rotational velocity was linear but nonlinear with the pressure. This indicates that the basic model as per equ. 14 seams practical.

5. Conclusion and Outlook

The first experiments indicate that the proposed model offers a satisfying degree of implementation potential. The non-linear dependence between removal rate and pressure shows a crucial influence of pressure on contact circumstances and elastic deformation of the contact area. In contrast, the rotatory speed which defines relative speed in wafer-pad contact influences only the removal speed, which explains its linear proportionality to the removal rate. Further experiments should advance the model and verify additional parameter, taking in account the change of *Young's* modulus and hardness due to the chemical effect in the process.

The next step is to perform further testing to verify the model. However, to come to a practical model for local planarization, (a) an approach has to be developed to equalize the removal rates between the two materials present at the wafer surface, as well as to (b) coming up with a finite element method (FEM) model to properly predict the geometry dependent part of the contact pressure.

References

[1] H.H. Gatzen, C. Morsbach, C. Kourouklis: Chemical-mechanical Planarization of a SU-8/Copper combination for MEMS, Proc. ASPE 18th Ann. Meet. Portland, Oregon, USA, 2003, pp. 575-578

[2] C. Kourouklis, T. Kohlmeier, H.H. Gatzen: The Application of Chemical-Mechanical Polishing for Planarizing a SU-8/Permalloy Combination Used in MEMS Devices, Sensors & Actuators A: Physical, Vol. 106, No. 1-3, 2003, pp. 268-271

[3] Luo J.: Review of Chemical-Mechanical Planarisation Modelling for Integrated Circuit Fabrication: From Particle Scale to Die and Wafer Scales, Laboratory for Manufacturing Automation, eScholarship Repository, Universty of California, 2003

[4] Runnels S. R.: Feature-Scale Fluid-Based Erosion Modeling for Chemical-Mechanical Polishing, Journal of the Electrochemical Society, Vol. 141, No. 7, 1994, pp. 1900-1904

[5] Cooper K., Cooper J., Groschopf J.: Flake J., Solomentsev Y., Farkas J., Effects of Particle Concentration on Chemical-Mechanical Planarisation, Electrochemical and Solid-State Letters, 5 (12), 2002, G109-G112

[6] Preston F. W.: The Theory and Design of Plate Glass Polishing, Society of Glass Technology-Journal, v.11, n.42, 1927, pp.214-256

[7] Bastawros A., Chandra A., Guo Y., Yan B.: Pad Effects on Material-Removal Rate in Chemical-Mechanical Planarization, Journal of Electronic Materials, Vol. 31, No. 10, 2002, pp. 1022-1031

[8] C.J. Evans, E. Paul, D. Dornfeld et al.: Material Removal Mechanisms in Läpping and Polishing, Annals of the CIRP Vol. 52, No. 2, 2003, pp. 611-633

[9] Paul E., Vacassy R.: A Model of Chemical-Mechanical Polishing, III. Inhibitors, Journal of The Electrochemical Society, 150 (12), 2003, G739-G743

[10] Franco G. E., Bagtzolou A. C.: An Elastic Contact Fracture Flow Model, 15th ASCE Engineering Mechanics Conference, 2002, pp.1-7

[11] F. Mugele, B. Person, S. Zilberman, N. Abraham, M. Salmerson: Frictional Properties of the straight-chain alcohols and the Dynamic of layering transitions, Tribology Letters, Vol. 12, No. 2, 2002, pp. 123-129

[12] J. Luo, D.A. Dornfeld: Material Removal Mechanism in Chemical Mechanical Polishing: Theory and Modeling. IEEE Trans. On Semicon. Man., Vol 14, No. 2, 2001, pp. 112-133