Title
Material Removal Regions in Chemical Mechanical Polishing: Coupling Effects of Slurry Chemicals, Abrasive Size Distribution and Wafer-Pad Contact Area, Part 1

Permalink
https://escholarship.org/uc/item/0n2575s1

Authors
Luo, Jianfeng
Dornfeld, David

Publication Date
2003

Peer reviewed
Abstract—A material removal rate (MRR) model as a function of abrasive weight concentration has been proposed by extending a material removal model developed earlier [1-2]. With an increase of the weight concentration of abrasives/MRR, three regions of material removal exist: first, a chemically dominant and rapid increasing region, whose range is determined by the generation/passivation rate and hardness of the surface passivation layer; second, a mechanically dominant linear region, where the material removal is proportional to the weight concentration; and third, a mechanical dominant saturation region, where the material removal saturates because the total contact area is fully occupied by the abrasives. The passive layer of the wafer surface is proposed to be a bi-layer structure. In the first part of this paper, a detailed model is proposed to explain that the transition from the first to the second region is due to a transition from a wafer surface covered with a single soft material to a surface covered with both soft and hard materials. The chemicals contribute to the material removal through the generation rate of the upper softer layer of the passive films. The slope of the linear region is a function of abrasive size distribution, and the saturation removal rate is a function of abrasive size distribution and wafer-pad contact area. These are supported by experimental results to be discussed in the second part of this paper [39]. The model can help to clarify the roles of chemicals, wafer-pad contact area and abrasive size distribution in chemical mechanical polishing.

Keywords: abrasive weight concentration, abrasive size distribution, chemical-mechanical polishing, hardness, material removal rate, pad, passivation, wafer.

1. Introduction

The material removal rate in the solid-solid contact mode of chemical mechanical polishing (CMP) usually increases linearly with the abrasive weight concentration. This is observed experimentally [3-6] [37]. However, this linear increase only holds for a limited range of abrasive weight concentrations, as shown in Figure 1. Two exceptions exist. First, when there are few or no abrasives in the slurry, the material removal is
usually close to zero [8-11]. This has been observed for various wafer materials including copper [8], aluminum [9], tungsten [10], silicon [11], and slurry recipes. This material removal, mainly due to the chemical erosion and dissolution, is much smaller than that due to chemical-mechanical removal with abrasives. This is reasonable. Otherwise, both high and low features on the wafer surface will be removed aggressively as observed in isotropic wet etching, and therefore no “planarization” can be realized. A small increase of the abrasive concentration in this region close to the pure chemical removal without abrasives usually leads to a rapid increase of the material removal, Figure 1. The observed linear increase is much slower than this rapid increase, and usually does not cross zero at zero weight concentration, Figure 1. Second, when the concentration of abrasives is larger than a certain value, say, $C_s$, the material removal rate will stop increasing but keep constant [3], [6-7]. This phenomenon is called material removal saturation. A qualitative explanation of this is that the total contact area between the wafer and pad surface is occupied by the active abrasives when saturation occurs, and a further increase in concentration cannot increase the number of abrasives on the contact area. This leads to the material removal saturation since MRR is supposed to be proportional to the active abrasive number [1-2]. This qualitative explanation is shown schematically in Figure 2.

Therefore, there are two transitions of material removal regions with the increase of the abrasive weight concentration. First, a transition from a rapid increase region at small abrasive concentrations to a slower linear increase region. And second, a transition from the linear increase region to the saturation region at large abrasive concentrations. In this paper, we discuss the extension of the material removal model proposed by Luo and
Dornfeld [1] to explain these transitions quantitatively. Three regions of material removal are proposed. First, a chemically dominant and rapid increasing region, whose range is determined by the generation/passivation rate and hardness of the surface passivation layer. Second, a mechanically dominant linear region, where material removal increases proportionally with the weight concentration of abrasives. The material removal in both of the above regions increases linearly with abrasive weight concentrations, although with different slopes. We propose that this transition is due to a transition from a wafer surface covered with a single softer material to a surface covered with both softer and harder materials. And, third, a mechanically dominant saturation region, where the material removal saturates because the total contact area is fully occupied by the abrasives. The range of the first region, slopes of the rapid increasing and slower linear increasing region, the two transition concentrations and the saturation material removal rate are proposed to be functions of the chemicals, abrasive size distribution and wafer-pad contact area. Formulations of material removal rate as a function of the abrasive weight concentration are proposed for the above three regions. They agree with the previous model [1-2]. Experimental evidences supporting these regions are presented in the second part of this paper. The understanding of the proposed coupling effects of slurry chemicals, abrasive weight concentration, abrasive size distribution and wafer-pad contact area may help to understand the fundamental mechanism in CMP and optimize the process in the future.

![Figure 2. Material removal saturation due to the limitation of contact area.](image)

2. Transition from the first region to the second region: effects of bilayer properties of the passive film

It is clear that the slurry chemicals must play an important role in the rapid increase of material removal illustrated in Figure 1. The role of chemicals in CMP may be attributed to a wear-accelerated corrosion [12], or a combined corrosion-wear [13], depending on the polished materials, slurry composition/environment, and the applied mechanical load. If this understanding is correct, CMP is basically a chemical process,
which is enhanced by mechanical elements including abrasion. Another understanding of
the roles of chemicals, however, is based on Kaufman’s model for tungsten CMP [10].
Since oxidants such as H₂O₂, KMnO₄, KIO₃, NH₄OH, and K₃Fe(CN)₆ are frequently
used in CMP slurries, Kaufman et al. [10] proposed that chemical action of the slurry is
responsible for continuously oxidizing the metal surface to form a thin passive layer
(usually several to ten nanometers thick) which is immediately removed by the slurry
abrasives. The fresh metal surface exposed due to the abrasion is then rapidly
repassivated and removed. This passivation-abrasion-repassivation process continues
until that the desired metal thickness is realized. Kaufman’s model implies that the CMP
is basically a mechanical process enhanced by chemical actions, whose effects on MRR
are attributed to the material and mechanical properties of this passive surface layer, such
as the hardness value, and its generation rate. This passivation-abrasion-repassivation
mechanism of material removal has also been applied to explain the metal removal and
planarization in copper and aluminum CMP [14-17]. For silicon and silicon oxide CMP,
a near surface change was observed [11] [18-19]. Cook [20] proposed that a surface
hydrated softer layer (≡SiOH) is formed under chemical attack for silica CMP and it is
this layer that is removed. Therefore, a similar mechanism of surface modification,
abrasion and then re-modification seems to be at work for silicon and silicon oxide CMP
as well.

Based on the use of different slurry chemicals, Carpio [21] pointed out that both
dissolution-type chemistry and passivation-type chemistry may exist in CMP, specially,
in copper CMP. For example, while ammonium hydroxide (NH₄OH) based slurry
passivates the copper surface, nitric acid (HNO₃) may dissolve it easily with the aid of
abrasion to expose the copper surface [21]. A corrosion inhibitor such as BTA has to be
used to protect the recessed areas on the wafer surface from the dissolution. In this paper,
we extend Kaufman’s model to explain that the rapid increase of material removal in the
region of small abrasive weight concentration is due to a bilayer property of the passive
films. The phenomena that occur in the dissolution-based CMP may not be able to be
explained by the model proposed herein.

![Figure 3. The bilayer-structure of the passive layers (from [22-24]).](image-url)
Various micrographic and microchemical examinations of passive films on many metals and alloys have shown that they form as bilayers, consisting of a compact, harder barrier layer underlying a porous, precipitated, hydrated and softer upper layer [22-24], Figure 3. Recently, X-ray photoelectron spectroscopy (XPS) analysis has demonstrated that in the slurry modified copper surface, a Cu(OH) and CuO bilayer may exist [25]. The formation mechanism of the passive layer can be attributed to the diffusion of the metal cation and oxygen anions through the passive films and the generation and annihilation of vacancies (chemical reactions) at the metal/bottom film and upper film/bottom film interfaces, Figure 3. The growth rate of the bilayer on the metal surface including the upper and bottom layers, may be either diffusion-controlled when the films are thick or reaction-controlled when the films are thin. This property of bilayer structures with different microstructures and hardnesses has also been observed in near surface modification of the silicon and silica structure in CMP [18-19]. Trogolo and Rajan [18] found in silica CMP the existence of a 2 nm surface layer with lower density than the bulk, below of which the density increases to a value greater than the bulk, gradually returning to the bulk density at a depth of 15-20 nm below the silica surface. Although Trogolo and Rajan [18] explain the formation of the bilayer structure from a materials science viewpoint, a similar diffusion and reaction mechanism, as it is observed in metals, however, may underlie this phenomenon. The detailed discussion on the dynamical film growth mechanism is beyond the scope of this paper. Here, a parameter GR is simply introduced to represent the generation/growth rate of the upper and bottom layers. It may be a coupling function of slurry chemical and mechanical elements. Two hardness parameters, \( H_{w1} \) and \( H_{w2} \), are used to represent the different material properties of the upper and bottom layers, respectively.

Due to the bilayer nature of the metal passive film, two regions of different materials removed with the increase of abrasive weight concentrations, are proposed as follows. When the weight concentration of slurry abrasives is small, the material removal rate (MRR) is close to zero as mentioned before and probably smaller than the growth rate (GR) of the upper porous layer. This implies that the wafer surface is fully covered with the upper porous softer layer during the polishing, as shown in Figure 4 (a). Based on this understanding, and the material removal model proposed by Luo and Dornfeld [1-2], the material removal rate can be written as a function of the abrasive size distribution, down pressure and the hardness \( H_{w1} \) of the upper layer:

\[
MRR = \frac{kC}{H_{w1}^{3/2} x_{ag}^3} \left( 1 - \Phi \left( 3 - C_6 \left[ \frac{x_{ag} + 3\sigma}{\sigma} \right] P_{0}^{1/3} \right) \right) \left[ \Phi \left( 3 - C_6 \left[ \frac{x_{ag} + 3\sigma}{\sigma} \right] P_{0}^{1/3} \right) \right] \left( x_{ag} + \frac{\sigma}{\sigma} \right) P_{0}^{1/2}
\]

(1)
where $x_{\text{avg}}$ is the average size of the abrasives, $\sigma$ the standard deviation of the size distribution function, $C$ the weight concentration of abrasives, $k$ a constant accounting for other factors including relative velocity $V$, and other consumable parameters, and $C_6$ a function of the pad hardness and pad topography [1-2].

Figure 4. Different layer removed with increase of abrasive weight concentration/material removal rate. (a) Small MRR < GR of upper layer (removed material is upper layer). (b) MRR= GR of upper layer (upper layer is removed as formed). (c) MRR> GR (part of removed materials is the upper softer layer which is removed as formed, and part of removed materials is the bottom harder layer).

Considering that the active abrasive size is approximately equal to $x_{\text{avg}}+3\sigma$ [1-2], we can obtain the following simplified material removal rate formulation:

$$MRR= k_1 C/H_{w1}^{3/2}\left[(x_{\text{avg}}+3\sigma)^2/x_{\text{avg}}^3\right]P_0^{1/2},$$

(2)

where $k_1$ includes the portion of the active abrasives (part 2 in Equation (1)). Note that if $x_{\text{avg}}+3\sigma/\sigma$ in part 2 of Equation (1) is approximately constant, the portion of active abrasive number is almost independent of abrasive size distribution, which is the case for the experimental data from [3] to be used in the second part of this paper. From Equation (2), the slope of the material removal as a function of abrasive weight concentration is inversely proportional to the hardness $H_{w1}$ of the upper film. Therefore, the material
removal increases rapidly with abrasive weight concentration when the upper layer composed of softer hydrated materials is removed (region 1 in Figure 1).

With the increase of the weight concentration $C$ of abrasives, the material removal rate increases. At a certain concentration $C_1$, Figure 1, the material removal rate $MRR_1$ will be equal to the generation rate $GR_1$ of the upper softer layer. Then the softer upper layer will be removed as soon as generated, Figure 4(b). This soft layer is thin and its generation is expected to be reaction controlled. With a continued increase of the abrasive weight concentration, the material removal rate $MRR$ becomes larger than the generation rate $GR_1$ of the upper layer materials. Under this larger material removal rate, the upper layer material is generated slower than removed and part of the harder bottom layer is exposed. Therefore, instead of a single upper layer of materials, a layer of bi-material composed of both the upper softer materials and the bottom harder materials on the wafer surface (see Figure 4(c)) will be continuously formed and removed. The ratio of the area of softer materials to the harder materials is determined by the ratio of $MRR_1$ to $MRR-MRR_1$. It is proposed that of all the active abrasives, part of the abrasives with a number proportional to $C_1/x_{avg}^3$ is removing the softer upper layer with an in-situ generation rate $GR_1$, while the other part with a number proportional to $(C-C_1)/x_{avg}^3$ is removing the exposed harder bottom layer. Considering that the material removal rate at concentration $C_1$ is $MRR_1$ and material removal increases linearly with the active abrasive number, we can write the material removal rate with concentration larger than $C_1$ as:

$$MRR = MRR_1 + k_1(C-C_1)/H_{w2}^{3/2}[(x_{avg}+3)^2/x_{avg}^3]P_0^{1/2} \quad C > C_1 \quad (3)$$

This transition of material removal rate from region 1 to region 2 is shown schematically in Figure 5. $H_{w2}$ is larger than $H_{w1}$. Therefore, the material removal in region 2 increases proportionally with the weight concentration but more slowly. The possibility that two different materials, one, the metal substrate, and the other, the metal oxide, are removed simultaneously with the increase of material removal has been noted by Kuo and Tsai [26], although they did not notice that a transition may occur on the interface of this bi-layer structure of passive films, instead of the metal/oxide interface. The transition on the metal/oxide interface, however, is possible with a further increase of the material removal rate, which is not covered in this paper.

From the above discussion, the chemicals influence the material removal in region 2 from two aspects: the generation rate of the upper softer layer, and the hardness value of the upper and bottom layers. The generation rate $GR_1$ is a function of mechanical elements including abrasive size and down pressure, and the chemical elements, including oxidizer concentrations. The addition of oxidation reagents increasing the passivation or growth rate of the upper soft layer, will lead to a higher portion of soft materials on the wafer surface, and therefore, an increase of material removal. That the material removal increases with the addition of oxidation reagents has been observed in experiments for various wafer materials including tungsten [4] [10] [27] and copper [5] [14] [28]. Aluminum can be passivated easily even with exposure to DI water and ambient air. Therefore, the generation rate $GR_1$ may saturate easily. This explains why $MRR$ in
Figure 5. The transition from rapid increase region 1 to slower linear increase region 2.

aluminum CMP does not change much with the increase of oxidizer concentrations [9]. A change of applied potential on the aluminum CMP in phosphoric acid based slurry, however, reveals that the passivation rate and material removal rate may increase simultaneously with a high anodic polarization [26]. The increases of oxidizer concentrations do not change the basic micrographic structure of passive layers. This implies that their hardness values do not change much with concentrations. Therefore, the lines in the second region should move up and down parallel with each other only with changes of the oxidizer concentration. Figure 6(a) shows this idea schematically. In the second part of the paper, experimental results that support this concept will be presented.

Figure 6(a). The transition from rapid increase region 1 to slower linear increase region 2 under different generation rates of upper hydrated softer film but the same hardness A.
Changing the type of oxidizers, however, may lead to a change of the hardness. If the metal oxide is too hard, MRR may be small even with a high generation rate. This idea is shown schematically in Figure 6(b). Therefore, a proper oxidizer for CMP should satisfy two conditions simultaneously: first, high oxidization rate, and second, soft enough metal oxide after the passivation. The hydration of the passive film might be indispensable for CMP in consideration of the softness requirement.

![Figure 6 (b). The transition from rapid increase region 1 to slower linear increase region 2 under the same generation rates but different hardness of upper hydrated softer film.](image)

However, it is also noteworthy that in the first region, the chemicals contribute to the material removal through the hardness value of the upper, softer layer only. The passivation rate of the upper softer layer does not contribute to the material removal rate. This implies that an increase in oxidizer concentration does not necessarily increase the material removal rate, if the material removal is in the first region. Gutmann [38] noted that in copper CMP, when the material removal is large, an increase of oxidizer concentration yields an apparent increase of material removal rate. When the material removal is small, however, the material removal rate does not change much. An explanation of this phenomenon is that when the material removal is large, the material removal lies in the second region, where the passivation rate contributes to the material removal; when the material removal is small, the material removal lies in the first region, where the passivation rate does not contribute to the material removal. This can be seen schematically in Figure 6(a).

A better understanding of the generation/growth mechanism of the passive films is needed to exactly evaluate the transition concentration and growth rate. An exact evaluation of this value is beyond the scope of this paper. Here, we propose that the value of transition concentration $C_1$ is independent of the abrasive size distribution and the down pressure $P_0$ applied on the wafer top surface. This could be based on the following understanding on the coupling effects of mechanical and chemical elements. At the transition concentration $C_1$, the material removal rate is equal to the generation rate of the upper porous film, therefore, from Equation. 2,
The abrasives are indented into the upper layer surface under force $F$, Figure 4. (The details on the indentation model can be found in [1] and [2].) The polishing consists of the passage of abrasive particles under load across the wafer surface. The area of the leading edge between a single abrasive and the surface layer is equal to the radius $a_2$ of the projected indentation circle times the indentation depth $d_2$ [1], as seen in Figure 4, and is proportional to $(x_{avg} + 3s)^2 P_0^{1/2}$ [1]. The active abrasive number $N \mu C_1 / x_{avg}^3$ [1-2]. Therefore, the total area of leading edge at the transition concentration $C_1$ is proportional to $k_1 C_1 (x_{avg} + 3s)^2 / x_{avg}^3 P_0^{1/2}$. Cook [20] proposed that the temperature at the leading edge is much higher due to the bonding breakage. Therefore, the chemical reactions that take place are more intensive than those on the other areas at the wafer surface. Furthermore, due to the high-energy state of the stressed metal, a higher intensity of broken bonds in the neighborhood of the leading edge, may lower the energy barrier to oxidation [29]. Hence, it is reasonable to assume that the generation rate of the upper layer is proportional to this direct contact-leading edge area. This relationship can be simply written as

\[
GR_1 = k_1 C_1 / H_{w_1}^{3/2} \left[ (x_{avg} + 3s)^2 / x_{avg}^3 \right] P_0^{1/2}
\]  

(4)

This function decouples the effects of the mechanical elements, including down pressure and abrasive size distribution, from other elements. The function $f(C_1, j)$ is introduced here to account for the effects of other chemical and mechanical factors $j$, such as the applied potential, chemical concentration, ion diffusion constant, slurry PH value and temperature. The $C_1$ may influence the generation rate through other elements except the leading edge area and this is accounted for in function $f(C_1, j)$. An assumption in Equation (5) is that the abrasive size distribution and down pressure affect the generation rate through the leading edge area only. Substitution of Equation 4 into Equation 5 yields

\[
GR_1 = k_1 (x_{avg} + 3s)^2 / x_{avg}^3 P_0^{1/2} f(C_1, j)
\]

(5)

\[
GR_1 = k_1 (x_{avg} + 3s)^2 / x_{avg}^3 P_0^{1/2} f(C_1, j) = \text{const}
\]

independent of abrasive size distribution and down pressure $\square$ transition concentration

\[
C_1 = \text{const independent of abrasive size distribution and down pressure.}
\]

For convenience, Equation 3 can be written in another form:

\[
MRR = k_1 (C + b) / H_{w_2}^{3/2} \left[ (x_{avg} + 3s)^2 / x_{avg}^3 \right] P_0^{1/2}
\]

(6-a)

where $-b$ is the intercept of the $MRR$ line with the concentration axis, Figure 5, representing the effects of passivation rate of the upper softer layer on the total material removal rate. It is easy to realize that $b = C_1 (H_{w_2} / H_{w_1})^{3/2}$ from Figure 5. Since $C_1$ is
independent of the abrasive size distribution and down pressure, $b$ should be independent of the abrasive size distribution and down pressure as well. The prediction of the transition under different abrasive size distribution based on this model is shown in Figure 7. Separating the portion of active abrasive from $k_1$ we obtain the material removal as a function of slurry chemicals, abrasive size distribution and down pressure as follows:

\[
MRR = \frac{k(C+b)}{H_{w2}^{3/2}} \left( 1 - \Phi \left( 3 - C_3 \frac{x_{avg} + 3\sigma}{\sigma} \right) P_0^{1/3} \right) \left( \frac{x_{avg} + 3\sigma}{\sigma} \right) P_0^{1/2}, \quad \forall C > C_1
\]

(6-b)

$c+b$ and $H_{w2}$ in Equation (6-b) are taking place of $C$ and $H_{w1}$ in Equation 1 for the range of $C > C_1$. $c+b$ can be taken as an effective concentration, and the wafer surface can be taken as covered with a single material with an effective hardness $H_{w2}$. The independence of $b$ on the down pressure guarantees the validity of the previous model [1] on the down pressure dependency of material removal rate in the range of $C > C_1$, which can be written as:

\[
MRR = h_1 \left[ 1 - \Phi \left( 3 - h_2 P_0^{1/3} \right) \right] P_0^{1/2},
\]

(6-c)

where

\[
h_1 = k(C+b) \frac{(x_{avg} + 3\sigma)^2}{(H_{w2})^{3/2} x_{avg}^3}
\]

(6-d)

is dependent on the chemicals, abrasives and pad, and

\[
h_2 = C_3 \frac{(x_{avg} + 3\sigma)}{\sigma}
\]

(6-e)
is dependent on the pad topography \((C_3)\), pad materials \((C_3)\), and abrasive size distribution but independent of chemicals. Note that \(h_2\) reflects the sensitivity of material removal on the down pressure distribution and can be used to optimize the non-uniformity from the viewpoint of consumable effects [31]. In the second part of the paper [39], we will present experimental evidence to support the down pressure dependency of material removal rate, Equations (6-c)-(6-e).

![Figure 8. Typical polishing characteristics for TEOS blanket wafer (from [32]).](image)

In summary, the rapid increase of material removal with a small increase of the abrasive concentration in the first region, is due to the nature of low hardness of the upper porous softer layer. The exponent 3/2 of the hardness term in the material removal rate function accelerates this change. The transition is due to a transition from a region where a single softer material is removed to a region where softer and harder materials are removed simultaneously. This transition may not be a function only of the abrasive weight concentration. Based on the same reasoning, it may be a function of other mechanical elements such as down pressure and velocity as well. When the material removal is small at small down pressure and velocity, the material removal increase may be much faster since the material removed is the softer upper layer. Typical polishing data for TEOS blanket wafers from Ouma [32] supports this, Figure 8. The dashed line in Figure 8 represents the change of the down pressure dependency of material removal rate with the wafer hardness \((H_{w1} \text{ to } H_{w2})\) based on Luo and Dornfeld’s model [1]. The CMP usually works in the second region. This transition may explain why the linear fit for
CMP MRR data as a function of down pressure and velocity usually intercept with the MRR axis with a non-zero value, Figure 8.

2. Transition from the second to the third region: effects of abrasiv size distribution and wafer-pad contact area.

The second transition is the transition of the material removal rate from the linear, slower increase region 2, to a saturation region 3, where material removal stops increasing with the weight concentration of abrasives. We propose that this transition is because the contact area between wafer and pad is completely occupied by active abrasives.

Before the material removal saturates, the material removal formulation as a function of abrasive size distribution in region 2 has been developed in last section as:

\[ MRR = k_1(C+b)/H_w^{3/2}[(x_{avg}^3+3D^2)/x_{avg}^3]P_0^{1/2} \]  

\[ (7) \]

The value of \( k_1(C+b)/x_{avg}^3 \) is proportional to the number \( N \) of abrasives on the contact area \( A \) between wafer and pad [2]. When the weight concentration is small, most of the contact is direct contact between the wafer and pad asperities. The contact area \( A \) is dependent on the down pressure, pad material and pad topography but independent of the abrasive geometry and abrasive size [1], Figure 9(a). When the area is totally occupied by abrasives, however, the abrasives behave as an interfacial layer between the wafer and pad asperities, Figure 9(b). In this case, the pad asperities are considered to have a higher effective Young’s modulus. With larger abrasives, the effective Young’s modulus of the pad is larger. This changes the contact area \( A' \). When saturation occurs, this contact area will be totally occupied by active abrasives and therefore the number of abrasives will not increase with concentration any more.

\[ (a) \text{ slow linear region} \quad (b) \text{ saturation region} \]

*Figure 9. Schematic of two contact modes with different abrasive weight concentrations.*
Now, let us estimate the relationship between the contact area and the abrasive size distribution. As shown in Figure 10, the abrasives, which are closely packed together, are taken as an interfacial layer between the wafer and pad asperities with effective Young’s modulus $E_a^*$ and thickness $x_{avg-a}$. The pad asperities are assumed to have a spherical tip with radius $R$ and Young’s modulus $E_p$, as used in [1]. The pad asperity and the interfacial layer are modeled as two springs in series, so the effective Young’s modulus of the pad asperity $E_p^*$, considering the interfacial abrasive layer, can be approximated as

$$E_p^* = E_a^* E_p \left( \frac{R + x_{avg}}{E_a^* R + E_p x_{avg}} \right).$$

Since not all of the interfacial space between the dashed curve in Figure 10 (b) and the pad asperity is occupied by abrasives, the effective Young’s modulus $E_a^*$ of the interfacial layer of abrasives is much smaller than the real Young’s modulus $E_a$ of the abrasive materials. This $E_a^*$ can be estimated as $E_a^* = E_a A' / A$ where $A'$ is the real contact area between the abrasives and the wafer, and $A$ the contact area occupied by the abrasives, as shown in Figure 10 (b). The $A'$ is equal to the number of active abrasives times the projected area of the indentation of a single abrasive into the wafer. $A$ is equal to the
number of abrasives times the area occupied by a single abrasive. Therefore, the ratio between \(A''\) and \(A'\) can be estimated as \(A''/A' = P/H_w\) based on Equation (4) in [1], where \(P\) is the contact pressure and \(H_w\), the effective wafer hardness. Therefore, \(E_a^* = E_a P/H_w\).

Since the contact pressure \(P\) (around \(10^6\) Pa [1]) is much smaller than the wafer hardness (around \(10^9\) Pa for tungsten and \(10^{10}\) Pa for silicon oxide and silicon [34]), the effective \(E_a^*\) is much smaller than the real \(E_a\). For alumina abrasives, the real \(E_a\) is around 500 GPa [5]. Therefore, the effective \(E_a^*\) is around 500 GPa/(1000 ~ 10,000) = 0.05 ~ 0.5 GPa.

The effective radius \(R^*\) of the asperity considering the interfacial abrasive layer is \(R+x_{avg-a}\). Figure 10. Based on contact mechanics ([33] & Equation 2 in [1]), an approximate relationship between the abrasive size \(x_{avg-a}\) and the contact area \(A\) under force \(F\) can be obtained as

\[
\left(\frac{R}{E_p^*}\right)^{2/3} = \frac{A \mu}{E_a^* R + E_{p^*} x_{avg-a}} \left(\frac{E_{a^*}}{E_p}\right)^{2/3}
\]

\[
= \frac{R}{E_p^*} \left[1 + \frac{E_p}{RE_a^*} x_{avg-a}\right]^{2/3}
\]

\[
\mu (1+m_1 x_{avg-a})^{2/3},
\]

where \(m_1 = E_p/(RE_a^*)\) is a constant related to the pad topography, pad material and abrasive material. Polymers used here usually have Young’s modulus around 1 GPa [34]. The value of \(E_a^*\) has been estimated earlier as 0.05 ~ 0.5 GPa. The radius \(R\) of the pad asperity should be around 10 ~100 \(\mu\)m. Therefore \(m_1\) can be estimated to be around 0.02 ~ 2 \(\mu\)m\(^{-1}\).

Once the contact area is known, the relationship between the contact pressure \(P\) and the active abrasive size can be estimated as:

\[
P \mu = P_0/A \mu (1+m_1 x_{avg-a})^{2/3}.
\]

The force applied on a single active abrasive is

\[
F = 0.25 \sqrt{2} P_0 x_{avg-a} \mu (1+m_1 x_{avg-a})^{2/3}
\]

It is noteworthy that the contact area at saturation increases with the abrasive size while the contact pressure decreases with the abrasive size.

From Equation 11 in [1],

\[
\sqrt{\phi_l} = \frac{\sqrt{2}}{4} x_{avg-a} \left(\frac{P}{H_w}\right)^{3/2} V
\]
where $H_w$ is the *effective* hardness of the wafer and $V$ the relative velocity of the wafer, and (10), the material removed by a single active abrasive in the situation of saturation satisfies:

$$\sqrt{\text{Vol}_{\text{removed}}}x_{\text{avg}}^2P^{3/2}\mu x_{\text{avg}}^{-2}(1+m_1x_{\text{avg}})^{-1}$$  \hspace{1cm} (12)

The abrasive size dependence of material removed by a single abrasive in the situation of saturation is different from that without saturation. This is because the contact pressure and contact area are dependent on the *active* abrasive size.

The number of *active* abrasives $N$ in the situation of saturation is:

$$N= A'/\left(0.25\left[\frac{x_{\text{avg}}^2}{x_{\text{avg}}^2+a}\right]\mu (1+m_1x_{\text{avg}})^{2/3}x_{\text{avg}}^{-2}\right)$$  \hspace{1cm} (13)

Therefore, the material removal rate $MRR_s$ at saturation should satisfy

$$MRR_s= N\sqrt{\text{Vol}_{\text{removed}}}\mu (1+m_1x_{\text{avg}})^{1/3}\mu A^{-1/2}$$  \hspace{1cm} (14)

The saturation material removal rate decreases with the increase of the abrasive size. It is a function of abrasive size and wafer-pad topography only.

Based on the above discussions, the material removal rate can be written as a function of abrasive size distribution and concentration as follows:

$$MRR\mu k_1(C+b)\left(x_{\text{avg}}+3\sqrt{\mu}\right)^2/x_{\text{avg}}^3$$  \hspace{1cm} (15)

when $C<C_s$, which is a function of weight concentration, and

$$MRR\mu(1+m_1x_{\text{avg}})^{-1/3}=[1+m_1(x_{\text{avg}}+3\sqrt{\mu})]^{1/3}\mu A^{-1/2}$$  \hspace{1cm} (16)

when $C\geq C_s$, which is independent of weight concentration. If the slope of the linear region is $S$, which satisfies

$$S\mu k_1(x_{\text{avg}}+3\sqrt{\mu})/x_{\text{avg}}^3$$  \hspace{1cm} (17)

as shown in (15), then the relationship between $C_s$ and abrasive size can be written as

$$C_s=MRR_s/S-b\mu [1+m_1(x_{\text{avg}}+3\sqrt{\mu})]^{1/3}/x_{\text{avg}}^3/(x_{\text{avg}}+3\sqrt{\mu})-\text{const},$$  \hspace{1cm} (18)

where $\text{const}$ is independent of abrasive size distribution.

In summary, when $C_1<C<C_s$, the material removal is mainly mechanical removal. A linear relationship between the concentration and the material removal rate exists in this region. The contact mode in this region could be described schematically as in Figure 9(a). When $C>C_s$, the material removal saturates since the contact area has been totally
occupied by the abrasives [3], [7]. The contact mode in this region is shown in Figure 9(b), schematically. The contact area in the saturation region is larger than that in the linear region. It is noteworthy that this second transition of material removal regions was also modeled by Fu. et al. [34] and Paul [35-36] using different approaches.

3. Conclusion

A material removal rate (MRR) model as a function of abrasive weight concentration has been proposed by extending a material removal model developed earlier [1-2]. With an increase of the weight concentration of abrasives/MRR, three regions of material removal exist: first, a chemically dominant and rapid increasing region, whose range is determined by the generation/passivation rate and hardness of the surface passivation layer; second, a mechanically dominant linear region, where the material removal is proportional to the weight concentration; and third, a mechanical dominant saturation region, where the material removal saturates because the total contact area is fully occupied by the abrasives. The passive layer of the wafer surface is proposed to be a bi-layer structure. In the first part of this paper, a detailed model is proposed to explain that the transition from the first to the second region is due to a transition from a wafer surface covered with a single soft material to a surface covered with both soft and hard materials. The chemicals contribute to the material removal through the generation rate of the upper softer layer of the passive films. The slope of the linear region is a function of abrasive size distribution, and the saturation removal rate is a function of abrasive size distribution and wafer-pad contact area. These are supported by experimental results to be discussed in the second part of this paper. The model can help to clarify the role of chemicals, wafer-pad contact area and abrasive size distribution in chemical mechanical polishing.

References


