Research Article

Influence of the Molecular Adhesion Force on the Indentation Depth of a Particle into the Wafer Surface in the CMP Process

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By theoretical calculation, the external force on the particle conveyed by pad asperities and the molecular adhesion force between particle and wafer are compared and analyzed quantitatively. It is confirmed that the molecular adhesion force between particle and wafer has a great influence on the chemical mechanical polishing (CMP) material removal process. Considering the molecular adhesion force between particle and wafer, a more precise model for the indentation of a particle into the wafer surface is developed in this paper, and the new model is compared with the former model which neglected the molecular adhesion force. Through theoretical analyses, an approach and corresponding critical values are applied to estimate whether the molecular adhesion force in CMP can be neglected. These methods can improve the precision of the material removal model of CMP.

1. Introduction

During the course of chemical mechanical polishing (CMP) process and as the particle's diameter gets close to the nm scale and the particle's indentation depth into wafer's surface is around 0.01–1 nm, the attractive intermolecular forces acting at the particle/wafer interface and the external force applied on the particle may be close in magnitude. Ignoring the molecular forces will influence the accuracy of the model of CMP process and leads to errors. Therefore, in this paper in-depth study was conducted on the influential law of the molecular forces between particle and wafer surface on CMP process, and a more complete particle indentation depth model considering the effect of the molecular forces between particle and wafer surface is established. Several important modeling assumptions are as follows.

In the CMP process, the abrasive particles are in the liquid environment. According to DLVO theory [1], the molecular forces between particle and wafer surface are mainly the electric double-layer repulsion and van der Waals attraction; other intermolecular forces are smaller than them in the order of magnitude and therefore can be ignored.

DLVO theory also shows that double-layer repulsion is major, and van der Waals attraction can be ignored at large particle/wafer surface approaching distance. van der Waals attraction is dominant and electrical double-layer repulsion can be neglected, when the approaching distance is less than the critical value of 3 nm. In the CMP process, the indentation depth of particle into wafer surface is about 0.01–1 nm, so just van der Waals attraction is considered.

There will be molecular force between particle and polishing pad surface. Igor Sokolov found that in liquid environment the magnitude of the Hamaker constant of the particle/pad system is about $0.1 \times 10^{-20}$ J, while the magnitude of the Hamaker constant of the particle/wafer system is about $1 \times 10^{-20}$ J [2]. van der Waals attraction is proportional to Hamaker constant, so the van der Waals attraction between particle and wafer is ten times the magnitude of that between particle and pad. Hence, the van der Waals attraction between particle and pad can be neglected [3].

It is assumed that the particle and wafer surface is completely smooth; therefore, the molecular force between the particle and the asperities of wafer surface is negligible.
2. Applied Forces Exerted on a Particle

2.1. Force Balance Equation of a Particle. In the CMP process, the abrasive particle is pressed into the contact area of pad/wafer under the external force, which forms a three-body contact. Pad is so soft that after wafer is pressed to contact pad asperities, pad asperities will wrap abrasive particles. In this case, the working pressure \( p \) is sustained by the pad asperities and the abrasive particle together [4]. The schematic diagram of a three-body contact of pad/wafer/particle is shown in Figure 1.

The applied forces exerted on abrasive particle include the external force \( F_Z \) conveyed by pad asperities, antiforce \( F_h \) by wafer surface, the molecular adhesion force \( F_a \) between particle and wafer surface, and abrasive particle gravity. As the abrasive particle diameter is in nanometer scale, taking Al\(_2\)O\(_3\) abrasive whose density is larger in CMP as an example to calculate its gravity gives \( 1.88 \times 10^{-3} \) nN, while the magnitude of the external force acting on abrasive particle generally can reach tens to hundreds of nN [5], and the abrasive gravity can be ignored. Small deformation takes place in the contact area between wafer surface and particle, as its indentation depth into wafer surface \( \delta_W \) is far less than the particle diameter \( D \); the whole process is considered as a completely plastic deformation [4], and the total plastic contact stress between wafer and particle, that is, antiforce by wafer surface \( F_h \), is given as

\[
F_h = H_W \pi D \delta_W. \tag{1}
\]

When a particle is in equilibrium state, the force balance equation is shown as follows:

\[
F_h = F_Z + F_a. \tag{2}
\]

The schematic diagram of the force applied on the particle is shown in Figure 2.

2.2. External Force \( F_Z \). Fu and Chandra used a creative equivalent beam bending model to calculate the external force \( F_Z \) conveyed by pad asperities to particle during CMP [10]. In his model, the particles are assumed to be distributed uniformly in the contact area between pad and wafer and the part of the pad between two particles is reduced to a fixed-fixed bending beam. According to beam theory of mechanics of materials, \( F_Z \) can be expressed as

\[
F_Z = \left( \frac{4E}{3\pi} \right)^{1/4} \left[ E_p t_p \frac{D}{2} \left( \frac{A_r}{N} \right)^2 p^3 \right]^{1/4}, \tag{3}
\]

where \( E_p \) is Young’s modulus of pad, \( t_p \) is the equivalent beam thickness, \( A_r \) is the effect contact areas between pad and wafer, and \( N \) is the number of effective particles embedded into the contact areas between pad and wafer.

According to Zhao and Chang [4], the number of effective particles embedded into the contact areas between pad and wafer \( N \) can be calculated by

\[
N = A_r \left( \frac{6\chi}{\pi D^3} \right)^{2/3} = A_r \left( \frac{6C_a \rho_f}{\pi D^3 \rho_s} \right)^{2/3}, \tag{4}
\]

where \( \chi \) is abrasive particle volume concentration, \( C_a \) is abrasive particle mass concentration, \( \rho_f \) is slurry density, and \( \rho_s \) is abrasive particle density.

Factors affecting the thickness of equivalent beam \( t_p \) include particle diameter \( D \), Young’s modulus of pad \( E_p \), and the working pressure \( p \). Based on the theory of dimensionless unit analysis of the four variables, we have

\[
\left( \frac{t_p}{D} \right)^{3/4} = k_2 \left( \frac{E_p}{p} \right)^{k_1}, \tag{5}
\]

where \( k_2, k_1 \) are dimensionless constants.

Substituting (4), (5) into (3), we obtain

\[
F_Z = \left( \frac{4E}{3\pi} \right)^{1/4} k_2 \left( \frac{E_p}{p} \right)^{1/4} \left( \frac{E_p}{p} \right)^{k_1} \left( p \right)^{3/4} D^2 \left( \frac{6C_a \rho_f}{\pi \rho_s} \right)^{-1/3}. \tag{6}
\]

According to Qin’s analysis [11], in the range of the working pressure \( p \) in a typical CMP, the average stress of the actual contact area between pad and wafer \( p_r \) approximately changes very slowly with the increase of the working pressure \( p \). It is reasonable to assume that, with a wafer being pressed onto a polishing pad, \( p_r \) is independent of \( p \), the increment of which is determined by the increase of abrasive particles being embedded into the contact area between pad asperities.

**Figure 1:** Schematic of pad/wafer/particle three-body contact.

**Figure 2:** Applied forces on the particle.
and wafer. Therefore, $p_r$ can be considered as a constant. As a single particle is concerned, the applied force of pad on it $F_Z$ keeps unchanged, so the indentation depth of the particle into the wafer $\delta_W$ is unchanged. This point of view is substantiated by Zhao and Chang [4], Qin et al. [11], and Jeng and Huang [12]. If the working pressure $p$ does not affect the indentation depth $\delta_W$, we can obtain $k_1 = 3/4$ in (6). And then rearranging (6) yields

$$F_Z = 2.48k_2E_pD^2\left(\frac{6C_a\rho_f}{\pi\rho_s}\right)^{-1/3}.$$  

In (7) $k_2$ is a dimensionless constant and has no relation to a variety of the pad/wafer/particle and operating parameters during the course of CMP. Based on the study of Qin et al. [11] and Jiange et al. [9], $k_2$ is 0.078 in a typical CMP, so (7) is rearranged to (8). Equation (8) can be applied to every case of CMP:

$$F_Z = 0.19E_pD^2\left(\frac{6C_a\rho_f}{\pi\rho_s}\right)^{-1/3}.$$  

2.3. Molecular Adhesion Force between Particle and Wafer $F_a$. As shown in Figure 3, during the course of a particle approaching a surface, when the approaching distance $Z_0$ is less than 3 nm, the van der Waals attraction between the particle and the surface is dominant. When the approaching distance is $Z_0$, the van der Waals attraction $F_0$ between a particle with the diameter of $D$ and a plane can be expressed as [3]

$$F_0 = \frac{AD}{12Z_0^2},$$  

where $A$ is the Hamaker constant of the adhesion system.

An expression of the molecular adhesion force $F_a$ between a particle and a plane is given by Bowling [13] as

$$F_a = \frac{AD}{12Z_0^2}\left(1 + \frac{2a^2}{DZ_0}\right),$$  

where $R$ is the diameter of the particle and $a$ is the contact radius between particle and plane, as shown in Figure 4.

The geometric relationship equation in Figure 4 is given as

$$a^2 = \left(\frac{D}{2}\right)^2 - \left(\frac{D}{2} - \delta_W\right)^2 = D\delta_W - \delta_W^2.$$  

Substituting (11) into (10) gives

$$F_a = \frac{AD}{12Z_0^2}\left(1 + \frac{2\delta_W}{Z_0}\right).$$  

Because the indentation depth of a particle into wafer surface $\delta_W$ is far less than the particle diameter $D$, (12) can be reduced as

$$F_a = \frac{AD}{12Z_0^2}\left(1 + \frac{2\delta_W}{Z_0}\right).$$  

Assuming the particle and the wafer surface are completely smooth, $Z_0$ can be taken as 0.4 nm [14]. $A$ is the Hamaker constant related to the material properties of the adhesion system of the particle/polishing slurry/wafer system, and the formula is shown as (14) to calculate the Hamaker constant of a three-component adhesion system [6]:

$$A = \left(\sqrt{A_{11} - A_{33}}\right)\left(\sqrt{A_{22} - A_{33}}\right),$$  

where $A_{11}$ is the Hamaker constant for a particle in a vacuum environment, $A_{22}$ is the Hamaker constant for wafer in a vacuum environment, and $A_{33}$ is the Hamaker constant for polishing slurry in a vacuum environment. As the abrasive particle and oxidant concentration in the slurry are not high, polishing slurry of CMP usually can be approximated as the water. The Hamaker constants of Cu-Water-Al$_2$O$_3$ system are listed in Table 1.

2.4. Comparison of $F_Z$ and $F_a$. To further study the relationship between the external forces on a single particle $F_Z$ by pad...
Table 2: Parameters calculating forces between wafer and abrasive.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young's modulus of wafer $E_W$ (MPa)</td>
<td>130000</td>
<td>[5]</td>
</tr>
<tr>
<td>Poisson’s ratio of wafer $\nu_w$</td>
<td>0.26</td>
<td>[5]</td>
</tr>
<tr>
<td>Wafer surface hardness $H_W$ (MPa)</td>
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<td>[7]</td>
</tr>
<tr>
<td>Young's modulus of particle $E_p$ (MPa)</td>
<td>310000</td>
<td>[4]</td>
</tr>
<tr>
<td>Poisson’s ratio of particle $\nu_p$</td>
<td>0.26</td>
<td>[4]</td>
</tr>
<tr>
<td>Particle density $\rho_p$ (kg/m$^3$)</td>
<td>3600</td>
<td>[4]</td>
</tr>
<tr>
<td>Young's modulus of pad $E_s$ (MPa)</td>
<td>10</td>
<td>[8]</td>
</tr>
<tr>
<td>Poisson’s ratio of pad $\nu_s$</td>
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<td>[8]</td>
</tr>
<tr>
<td>Mass concentration of particles $C_a$</td>
<td>0.034</td>
<td>[9]</td>
</tr>
<tr>
<td>Slurry density $\rho_f$ (kg/m$^3$)</td>
<td>1000</td>
<td>[9]</td>
</tr>
<tr>
<td>Particle diameter $D$ (nm)</td>
<td>200</td>
<td>[9]</td>
</tr>
</tbody>
</table>

and the molecular adhesion force between particle and wafer $F_a$, an example is used by theoretical calculation to compare $F_Z$ and $F_a$ that assumes an Al$_2$O$_3$ abrasive is pressed into the surface of Cu wafer. The Hamaker constant of Cu-Water-Al$_2$O$_3$ system is calculated as $9 \times 10^{-20}$ J by (13), the indentation depth $\delta_W$ is taken as 1 nm, and other parameters are listed in Table 2.

Using (8), (13) to calculate the external forces on a single particle $F_Z$ by pad and the molecular adhesion force between particle and wafer $F_a$, the results are shown in Figure 5.

As shown in Figure 5, the critical value when the external force $F_Z$ is equal to the molecular adhesion force $F_a$ is 33 nm. When the particle diameter is less than the critical value, $F_Z$ is less than $F_a$. When the particle diameter is greater than the critical value, $F_Z$ is greater than $F_a$, and, along with increase of the particle diameter, the increasing extent of $F_Z$ is greater than that of $F_a$. The above analysis shows that when the particle diameter is small, the molecular adhesion force $F_a$ may be greater than or close to the external force applied on a single particle $F_Z$. Therefore, CMP models ignoring the molecular adhesion force between particle and wafer will bring about large errors. Only when the particle diameter is large enough and the external force $F_Z$ is much greater than the molecular adhesion force $F_a$, $F_a$ can be ignored. The critical values used to judge whether the molecular adhesion force in CMP can be neglected or not are related to Young's modulus of polishing pad, particle diameter, particle indentation depth, and particle volume concentration. In order to find the critical values, further study is needed.

3. Particle Indentation Depth considering the Molecular Adhesion Force

Substituting (1), (8), and (13) into (2) gives the specific force balance equation of the particle shown as

$$k_aE_pD + \frac{A}{12Z_0^2} \left(1 + \frac{2Z_0}{Z_0}ight) = H_W\pi\delta_W.$$  \(15\)

In (15), a dimensionless parameter $k_a$ is defined as

$$k_a = 0.19 \left(\frac{6C_aP_f}{\pi\rho_s}\right)^{-1/3}.$$  \(16\)

From (15), we have

$$\delta_W = \frac{(k_aE_p/H_W) + (A/12Z_0^2H_WD)}{\pi + (A/6Z_0^3H_W^2)}.$$  \(17\)

Two dimensionless parameters are defined as

$$\Pi_1 = \frac{A}{6Z_0^3H_W},$$  \(18\)

$$\Pi_2 = \frac{A}{12Z_0^2H_WD}.$$  \(19\)

If the $\Pi_1$, $\Pi_2$ items are ignored in (17), the particle indentation depth without considering the molecular adhesion force between particle and wafer surface can be expressed as

$$\delta_W = \frac{k_aE_p}{\pi H_W}.$$  \(19\)

The result of calculating by using (17), (19) is shown in Figure 6. Relative parameters are taken as follows: $E_p = 10$ MPa, $C_a = 0.01$, and the rest are listed in Table 2. In accordance with the analysis of Figure 6, when the particle diameter $D$ is equal to 25 nm or so, the relative particle indentation depths calculated by (17), (19) are equal; when $D$ is less than 25 nm, the relative particle indentation depth considering the molecular adhesion force is greater than that ignoring the molecular adhesion force, and with the decrease of the particle diameter, their deviation will increase; when $D$ is greater than 25 nm they are in small deviation and can be seen as equal. Therefore, in case of large particle diameter, the influence of the molecular adhesion force between particle and wafer on the indentation depth $\delta_W$ of particle into wafer is negligible. From the analysis of (17), the critical values used to judge whether the molecular adhesion force in CMP can be neglected or not still have relation with the Hamaker constant of CMP system, the approaching distance between particle and wafer surface, and wafer surface hardness.
4. Two Dimensionless Judicial Criteria

According to (17), when assuming $\Pi_1 < 0.1 \pi$, $\Pi_2 < 0.1k_sE_p/H_W$; that is,

$$\frac{A}{Z_0^2 H_W} < 0.6\pi,$$

$$\frac{A \left(6C_a\rho_f/(\pi \rho_s)\right)^{1/3}}{E_p Z_0^2 D} < 0.231. \quad (20)$$

The $\Pi_1$, $\Pi_2$ items in (17) can be neglected; that is, the influence of the molecular adhesion force between particle and wafer on the indentation depth $\delta_W$ of particle into wafer is negligible.

Substituting the Hamaker constant $A = 9 \times 10^{-20}$ J, the approaching distance $Z_0 = 0.4$ nm, into (20) gives

$$H_w > 746 \text{ MPa}, \quad (21)$$

$$\frac{E_p D}{\left(6C_a\rho_f/(\pi \rho_s)\right)^{1/3}} > 2.435. \quad (22)$$

From the above analysis, when a CMP system is under the condition shown in (21), (22), the molecular adhesion force between particle and wafer can be ignored. Substituting the parameters in a typical CMP $E_p = 10$ MPa, $C_a = 0.034$, $D = 200$ nm, $\rho_s = 3600$ kg/m$^3$, and $\rho_f = 1000$ kg/m$^3$ into (22) gives

$$\frac{E_p D}{\left(6C_a\rho_f/(\pi \rho_s)\right)^{1/3}} = 7.626 > 2.435. \quad (23)$$

What is more, $H_w = 500$ MPa < 746 MPa. Hence, $\Pi_1$ item can be neglected while $\Pi_2$ item cannot be neglected during the course of this CMP. And then the relative indentation depth of the Cu-water-Al$_2$O$_3$ system can be simplified as

$$\frac{\delta_W}{D} = \frac{k_sE_p/H_W}{\pi + (A/6Z_0^2H_W)}. \quad (24)$$

From the above analysis, (20) are the two dimensionless judicial criteria that determine whether the influence of the molecular adhesion force between particle and wafer on the indentation depth $\delta_W$ of particle into wafer can be neglected or not. The two judicial criteria can apply to all CMP processes. It can be seen from these two criteria that the greater the wafer surface hardness $H_W$, the Young modulus of pad $E_p$, and the particle diameter $D$, the lower the particle concentration and the greater the possibility of neglecting the influence of the molecular adhesion force. It is by the inverse calculations indicated that, in typical metal CMP processes, if we take $E_p = 10$ MPa, $C_a = 0.034$, $\rho_s = 3600$ kg/m$^3$, and $\rho_f = 1000$ kg/m$^3$, average surface hardness of pure metal is generally less than 746 MPa, so $\Pi_1$ item cannot be ignored; when the particle diameter $D$ is greater than 64 nm, $\Pi_2$ item can be neglected. For a typical nonmetallic oxide CMP processes, under the same conditions, the nonmetallic oxide surface hardness is generally greater than 746 MPa, so $\Pi_1$ item can be neglected; when the particle diameter $D$ is greater than 64 nm, $\Pi_2$ item can be neglected.

5. Conclusions

By considering the influence of the molecular adhesion force between particle and wafer on the indentation depth $\delta_W$ of particle into wafer, the force equilibrium equation of a particle in wafer/particle/pad CMP system is established, and the external force on the particle conveyed by pad asperities and the molecular adhesion force between particle and wafer are compared and analyzed by quantitative calculation. The two dimensionless judicial criteria that determine whether the influence of the molecular adhesion force between particle and wafer on the CMP process can be neglected are educed through theoretical deduction. They can be applicable to every CMP system, which are important to construct mechanical model of CMP. According to the two criteria, the greater the wafer surface hardness $H_W$, the Young modulus of pad $E_p$, and the particle diameter $D$, the lower the particle concentration and the greater the possibility of neglecting the influence of the molecular adhesion force.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

References


