CMP Modeling
Three-Dimensional Wafer Process Model for Nanotopography

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ABSTRACT

This paper proposes a three-dimensional wafer process model for nanotopography. This model allows us to predict the effect and behavior of nanotopography on the wafer processes especially for the wafer Mechanical/Chemical Lapping (MLP/CLP), wafer Single/Double Side Polishing (SSP/DSP) and device Chemical Mechanical Polishing (CMP).

INTRODUCTION

Nanotopography of the wafer front side is becoming very important for the Shallow Trench Isolation (STI) CMP process [1]. To realize the high performance and high yield of device, IC makers have to optimize their CMP by taking into account the characteristics of nanotopography induced by silicon wafer makers’ processes [2].

An ideal silicon wafer process for nanotopography is exemplified in Figure 1. This example clarifies the importance of generating a crystallographic flat surface before slicing the silicon crystal ingot. This surface is to be used as a reference plane in the following wafer process to improve the nanotopography. However, this quality-oriented process is too expensive for silicon wafer makers to invest under today’s excessive low-price-competition circumstances.

The conventional process is shown in Figure 2 with the features of the nanotopography and TTV (total thickness variation). Many silicon wafer makers have adopted the multi wire saw as their slicing technology on a cost-oriented policy. The wafer shape after slicing is modified by the following lapping process and then the etching process for the damage removal adds the roughness/waviness to it. Finally, the wafer shape is transmitted to various surface topographies according to the following polishing process such as SSP or DSP. The feature of the nanotopography after SSP heavily depends upon the mounting system such as a thin wax mount, thick wax mount or waxless (flexible) mount systems.

In this paper, we propose a three-dimensional wafer process model for nanotopography to elucidate the behavior and to help to optimize CMP process for efficient planarization.

Figure 1. An ideal silicon wafer process for nanotopography
MODEL FORMULATION

Wafer processes such as lapping and polishing, including CMP, use a common mechanism. As shown in Figure 3, higher parts of the wafer surface receive higher pressure by the elastic behavior of the pad or platen. Therefore, removal rates of the higher parts become higher than the other parts and evolve their planarity. Several CMP process models using this so-called contact wear model have been proposed so far, but the wafer was treated as a rigid material [3, 4, 5, 6, 7, 8]. In reality, the wafer will deform elastically by the pressure distributions of the front and back side during the wafer process. Because of the elastic deformation, nanotopography will be generated and the characteristics of the nanotopography reflect on the process parameters.

Figure 3 illustrates the wafer elastic deformation $U_{\text{wafer}}$ during the wafer process. In the case of SSP/CLP with wax mounting, the elastic deformation $U_{\text{wafer}}$ is generated by the mounting process and fixed during polishing/lapping. On the contrary, the deformation by MLP/DSP/CMP will change according to the balance of the pressure distributions on the front and back side.

In our three-dimensional model, we combine two-dimensional BEM and two-dimensional FEM to calculate pad deformation and wafer deformation. In this way, we can prevent time-consuming preparations such as element meshing for three-dimensional FEM.

Here, the polishing pad, lapping platen and insert/backing pad are assumed to be isotropic.
elastic bodies. The general form of the relationship between the pressure ($P$) and displacement ($W$) for them is expressed by Equation 1 with a $f$-function, which has a variable norm (r). We assume $f_1$ for single elastic plate as in Equation 2. The constants $E_i$, $v_i$ and $t_i$ denote Young’s modulus, the Poisson Ratio and the thickness of the plate, respectively. Curiously, this equation is the same form of the Yukawa potential and dissolves the infinity problem in Boussinesq’s solution [7, 9, 10, 11]. Equation 3 is the complete solution of the Hertz problem for plate bending on an elastic foundation and we can apply $f_1 + f_2$ for two-layer stacked polishing pads as in Figure 4 [12, 13].

$$W = P \cdot f(r)$$  \hspace{1cm} (1)

$$f_1(r) = \frac{(1-v^2)}{E_i} \cdot e^{- \frac{2[1-v^2]}{r}}$$  \hspace{1cm} (2)

$$f_2(r) = -\frac{j^2}{2\pi D} \cdot \text{keri}(\frac{r}{l})$$  \hspace{1cm} (3)

![Figure 4. $f$-functions for this model](image)

The elastic body field such as pad/platen is expressed by $[F]$ matrix for BEM, which is generated by the integration and discretization of $f$-functions with boundary elements $A_j$ as in Equation 4. When the patterns of surface topography are periodic in the direction of $x$ and $y$ by the basic vector $c_x$ and $c_y$, their linear combination with the integer $k$ and $l$ appears here [8], Pressure $q$ and deformation $w$, which are difference forms against the reference pressure $Q_{\text{ref}}$ and reference plane $W_{\text{ref}}$, are expressed by Equation 5 and expanded as in Equation 6 and 7.

$$[F_{ij}] = \sum_{i=0}^{N} \sum_{j=0}^{N} \int f_1(r_j + (k \cdot c_x + l \cdot c_y)) \cdot dr_j \cdot dA_j$$  \hspace{1cm} (4)

$$[F]_{\text{before}} = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} w_{\text{known}} \\ w_{\text{unknown}} \end{bmatrix} = \begin{bmatrix} q_{\text{known}} \\ q_{\text{unknown}} \end{bmatrix}$$  \hspace{1cm} (5)

In Equation 6, wafer elastic deformation $U_{\text{wafer}}$ is added to the front side of the wafer surface $W_{\text{wafer, front}}$ and subtracted from the back side of the wafer surface $W_{\text{wafer, back}}$.

$$w_{\text{known}} = w_{\text{ref}} - w_{\text{wafer}}$$  \hspace{1cm} (6)

$$q_{\text{known}} = q_{\text{wafer}} - q_{\text{known}}$$  \hspace{1cm} (7)
The pressures that act on the surfaces of front and back side of the wafer are expressed by Equation 8.

\[ Q_{\text{front, } \text{back}} = Q_{\text{ref}} - q_{\text{unknown, } \text{front, back}} \]  

(8)

The elastic deformation of the wafer produced by the pressures acting on the surfaces of the front and back side can be expressed by Equation 9 using a stiffness matrix \([L]\) constructed by FEM [14].

\[ U_{\text{wafer}} = [L]^{\text{front, back}} \cdot \left( Q_{\text{front, } \text{back}} - Q_{\text{wafer, } \text{wafer}} \right) \]  

(9)

When the surfaces on both sides of the wafer contact everywhere on the polishing pad, insert (backing pad) or wax, the elastic deformation of the wafer by Equation 9 is transformed to Equation 10 explicitly in regard to \(U_{\text{wafer}}\). When the non-contact conditions exist, a loop procedure is required to gain the elastic deformation. In this case, Equation 11 ~ 12 are being employed with an initial value from Equation 10 until the value of recalculated deformation \(U_{\text{wafer}, n}\) is converged as in Equation 13. An appropriate coefficient \(\alpha\) should be chosen for a fast convergence in Equation 12.

\[ U_{\text{wafer}, 0} = \left( [L]_{\text{wafer}} + [F]_{\text{wafer}}^{-1} \right)^{-1} \left( Q_{\text{wafer, } \text{wafer}} + Q_{\text{wafer, } \text{wafer}} \right) \]  

(10)

\[ U_{\text{wafer}, n} = U_{\text{wafer}, n-1} + \alpha \left( U_{\text{wafer}, n} - U_{\text{wafer}, n-1} \right) \]  

(11)

\[ U_{\text{wafer}, n} = U_{\text{wafer}, n-1} \rightarrow 0 \]  

(12)

\[ U_{\text{wafer}, n} = U_{\text{wafer}, n-1} \rightarrow 0 \]  

(13)

The polishing rate can be calculated by substituting the gained pressure into the generalized Preston Equation as in Equation 14 [15, 16]. Using iterative procedures, we can get the processed wafer surfaces \(W_{\text{wafer}}\) of front and back side as in Equation 15 [6].

\[ \text{Rate} = R(Q, V, T) \]  

\[ = C_{1} \left( Q_{\text{front}} - C_{1} Q_{\text{wafer}} \right) + C_{2} \cdot e^{C_{2} t} \]  

(14)

\[ W_{\text{wafer}, \text{wafer}} = W_{\text{wafer}} + R_{\text{wafer}} \cdot dt \]  

(15)

Nanotopography is expressed by the deviations of \(W_{\text{wafer}}\) from the average as in Equation 16. Thickness variation (TV) is expressed by the addition of nanotopography of front and back side as in Equation 17. Therefore, TTV is expressed by the difference between the maximum and minimum of TV as in Equation 18. As we can see from these equations, when nanotopography of both sides is small, TTV is small. However, we have to notice that nanotopography is not necessarily small when TTV is small.

\[ \text{Nanotopography}_{\text{wafer}} = W_{\text{wafer}} - \overline{W}_{\text{wafer}} \]  

(16)

\[ TV_{\text{wafer}} = \text{Nanotopography}_{\text{wafer}, \text{front}} + \text{Nanotopography}_{\text{wafer, back}} \]  

(17)

\[ TTV_{\text{wafer}} = \max(TV_{\text{wafer}}) - \min(TV_{\text{wafer}}) \]  

(18)

\[ W_{\text{wafer}, \text{wafer}} = W_{\text{wafer}} + R_{\text{wafer}} \cdot dt \]  

(15)
The surface topography after CMP also produces nanotopography as in Equation 19. The accumulated nanotopography affects the performance of the following CMP process along with the wafer elastic deformation as in Equation 20 and Figure 5.

\[
\text{Nanotopography}_{\text{CMP+}} = \sum_{\text{CMP+}} \left( W_{\text{Wafer, CMP+}} - W_{\text{Wafer, CMP-}} \right)
\]

\[
w_{\text{known, \ front/ back}}_{\text{Wafer}} = W_{\text{Wafer}} - \left( W_{\text{Wafer, CMP+}} - W_{\text{Wafer, CMP-}} + \text{Nanotopography}_{\text{CMP+}} \right)
\]

Figure 5. Nanotopography during CMP process

RESULTS

We simulated the behavior of nanotopography for three cases, DSP, SSP with a thick wax mount and SSP with a thin wax mount. We assumed that the initial wafer has a completely flat surface on the front side and a sine curve topography with amplitude 200 (nm) and 10 (mm) pitch on the back side. For the polishing pad, we used the equivalence of SUBAIV. For the thick wax mount, strictly speaking, we should use the tacking behavior of Newtonian [17]. However, for simplicity, we used the mechanical properties of Politex SUPREME pad instead. For the thin wax mount, we assumed that the back side of the wafer contacts the surface of a mount block which has the mechanical properties of IC1000 pad. We used Equation 21 and 22 to get the wafer elastic deformation by a pneumatic stamp for wax mounting, and fixed the deformation during polishing.

\[
U_{\text{Wafer, 0}} = \left( [L_{\text{Wafer}} - F_{\text{Wax, back}}] \right)^{-1} \cdot \left( Q_{\text{Wax, back}}, U_{\text{Wafer, 0}} - Q_{\text{Pneumatic Stamp}} \right)
\]

\[
U_{\text{Wafer, t}} = [L_{\text{Wafer}}] \cdot \left( Q_{\text{Wax, back}}, U_{\text{Wafer}, t} - Q_{\text{Pneumatic Stamp}} \right)
\]

The results after polishing time 600 (sec) are shown in Figure 6. The surface topography of back side is transmitted to the front surface differently according to each system. Although, we can acknowledge better performance of DSP for both nanotopography and TV, the SSP with a thick wax mount shows the best performance for nanotopography. We should notice that thick wax mount technology will absorb the backside topography, prevent the wafer elastic deformation, and produce a crystallographic flat surface.
CONCLUSIONS

A three-dimensional wafer process model for nanotopography has been proposed. This model can give us a theoretical and practical basis to describe and predict the effect of nanotopography for both a silicon wafer process and device CMP process.

REFERENCES

Abstract: A previously presented model of CMP is extended to include the role of inhibitors. In CMP, a chemical reaction forms a surface film which is removed mechanically by abrasives. When inhibitor molecules bond to the surface film, the mechanical abrasion rate is reduced. The general model will be discussed, and then applied to W-CMP explaining differences in the reduction of polishing rates for different inhibitors.

Introduction: Chemical Mechanical Polishing is a complex, multi-scale process with an estimated 2 or 3 dozen input variables leading to output results. Linear dimensions can be used for an overview and can serve as a basis for modeling and understanding of separate facets of the overall process.

At the 100 mm scale, fluid dynamics can describe how polishing pressure and speed, combined with the mechanical properties of the fluid, pad and wafer, result in an applied pressure that forces the pad to envelop the abrasive and push it onto the wafer surface.

At the 10 μm scale, asperities on the pad surface deform under the applied pressure, increasing the contact area and leading to a constant effective pressure pushing the abrasive onto the wafer surface. Because the contact area is proportional to the applied pressure, and material removal is proportional to the contact area, it follows that the mechanical removal rate is proportional to pressure.

At the 1 μm scale, abrasive particles can transfer from the slurry to the pad surface and back. Adherence of abrasive particles to the pad leads to a linear increase in the polishing rate with concentration at low concentrations, while saturation of the pad surface by abrasive particles leads to an asymptotic maximum polishing rate at high abrasive concentrations. This behavior has been observed experimentally and explained theoretically in previous work.

At the 100 nm scale, the pad envelops abrasive particles and pushes them onto the wafer surface.

At the 1 nm scale, chemical reactions between slurry components and the wafer form a surface film which is removed by abrasive action. The mechanism for this removal is not well characterized. It may involve plastic deformation caused by indentation of the abrasive into the surface. Or it may involve adhesion between the wafer surface film and the abrasive. The adhesion mechanism can be identified with chemical tooth1 and can be used to explain why different abrasive materials have different removal rates2.

The generally accepted mechanism3 for CMP involves alternating cycles of chemical formation and mechanical removal of a surface film on the wafer. The mechanism has been successfully modeled4,5 using methods of steady state chemical kinetics, and has been used to explain how the removal rate depends on the concentrations of oxidizer and abrasive and on polishing pressure and temperature for tungsten CMP. The model is described below. The current paper extends this model to include the effects of inhibitors in the slurry on the polishing rate.
The basic model: A simplified version of the model has two steps as shown in Table 1 below. In the first step, some chemical C reacts with the wafer W to form a surface complex WC*. The rate of this reaction is proportional to the concentration of chemical [C] and to the number of atoms on the wafer surface \( n_w \). In the second step, the complex is removed by mechanical action to reveal fresh W atoms on the wafer surface. The rate of this step is proportional to the number of surface atoms that are complexed, \( n_{WC} \). \( Y \) is detritus, removed from the surface.

### Table 1. Basic Reactions and Rate Equations in the CMP Model.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Rate Equation</th>
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<tbody>
<tr>
<td>( W + C \rightarrow WC^* )</td>
<td>( r_C = k_C [C] n_w )</td>
</tr>
<tr>
<td>( WC^* \rightarrow W + Y )</td>
<td>( r_M = k_M n_{WC} )</td>
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The mechanical rate constant \( k_M \) is proportional to the pressure \( P \) (because removal is proportional to the pad-wafer contact area, which is proportional to \( P \)), to the polishing speed \( v \) (because the area swept in time is proportional to \( v \)) and to the function \( f([A]) = [A] / (K_P + [A]) \) which depends on the particle concentration of abrasives \([A]\). Here \( K_P \) is the pad constant for abrasives adhering to and coming free from the pad surface. At low solid loading, the particle concentration \([A]\) is proportional to \( \%A \). Using \( k_{sodm} \) as a proportionality constant, \( k_M \) becomes

\[
k_M = k_{sodm} \frac{Pv[A]}{(K_P + [A])} \quad \text{Eq. 1}
\]

Letting \( n_{w0} \) be the total number of wafer atoms \( W \) on the surface of area \( A_0 \) in the complexed or uncomplexed forms, \( n_{w0} = n_w + n_{WC} = A_0 / d_w^2 \), with \( d_w \) as the distance between atoms. The material removal rate per area is \( R = \tau / A_0 = \tau k_M n_{WC} / A_0 \), where \( \tau \) is the removal depth. Using the relationship \( d(n_{WC})/dt = k_C[C] n_w - k_M n_{WC} \), an expression for \( n_{WC} \) can be derived, set equal to 0 at steady state, and solved using \( n_{w0} \) to give an expression for \( R \) which has the characteristic shape shown in Fig. 1, with \( X = P, v, Pv, [C], [A] \) or \( \%A \).

\[
R = \left( \frac{\tau}{d_w^2} \right) k_C[C] k_M / \left( k_C[C] + k_M \right) \quad \text{Eq. (2)}
\]

**Fig. 1** \( R = \tau X / (b + X) \) where \( X = P, v, Pv, [C], [A] \) or \( \%A \).

Each of these variables is limiting when their values are low, leading to initial linear increases in polishing rate as that variable increases. At high values, however, the system overloads with that variable and approaches an asymptotic maximum. In the case of large \([C]\) surface film formation is much faster than removal and mechanical factors become limiting. For large values of the mechanical variables \( P \) and \( v \), removal becomes much faster than formation.