Pressure calculation using obstacle problem for CMP modeling

D Piliposyan\textsuperscript{1*}, R Ghulghazaryan\textsuperscript{1**}, M Poghosyan\textsuperscript{2,3}, and H Nersisyan\textsuperscript{2}

\textsuperscript{1}Mentor, a Siemens Business, Yerevan, Armenia
\textsuperscript{2}American University of Armenia, Yerevan, Armenia
\textsuperscript{3}Yerevan State University, Yerevan, Armenia

E-mail: \textsuperscript{*}davit.piliposyan@mentor.com, \textsuperscript{**}ruben.ghulghazaryan@mentor.com

Abstract. Chemical mechanical polishing/planarization (CMP) is one of the most important fabrication technologies in the semiconductor industry. CMP is used to achieve planar surfaces and remove excess deposited material from the wafer. During CMP, a chemical “slurry” containing abrasive particles and chemical reagents is deposited on the polishing pad. The polishing pad is then pressed against the rotating wafer. The combined action of the polishing pad and chemical slurry results in material removal and planarization of the wafer surface. Modeling of the CMP process allows detection of potential planarization defects in chips before manufacturing. Accurate computation of pressure distribution across the wafer surface is crucial for accurate modeling of the CMP process. The pressure distribution calculation is usually done using the Hertz contact theory and Chekina model, which involves computations of direct and inverse fast Fourier transforms (FFT and IFFT) and pad displacements updates. In this paper, we adopted an obstacle problem approach for calculating the pressure distribution across the wafer/die surface for CMP modeling. In an obstacle problem, the pad is assumed to be an elastic membrane with fixed boundaries that is displaced by the wafer surface. The goal is to find the equilibrium position for the pad and calculate the pressure distribution over the surface in contact. The main advantage of this approach is that computations of FFT and IFFT and recalculations of the pad displacements can be avoided. This can lead to a more accurate model that is independent of pad displacement update method. The approach is tested on several examples. The results show correct physical behaviour and are in agreement with expectations.

1. Introduction
Chemical mechanical polishing/planarization (CMP) is a process for removing excess conductive and dielectric materials from a silicon wafer to smooth and flatten the surface with the combination of chemical reactions and mechanical forces. It is one of the most important semiconductor manufacturing processes, and is critical for producing microprocessors, memory, MEMS and other integrated circuits (ICs). Fabrication of ICs can be divided into two main parts: the front end of line (FEOL) and back end of line (BEOL). The FEOL process is the first part of IC fabrication. It includes building architecture for the electrical isolation structures, transistors, capacitors, resistors, etc. The BEOL part connects all these integrated devices to create the necessary logic and memory circuits. CMP is used during both FEOL and BEOL sections to assure planarity of the layers. Usually a CMP tool consists of a polishing pad attached to the rotating table, a wafer attached to wafer carrier, a slurry dispenser and a dresser for
polishing/planarization conditioning. During the CMP process, a wafer is pressed face-down against the polishing pad while the wafer carrier and a polishing pad are rotating in the same direction. A slurry, containing chemicals and abrasive nanoparticles, is then injected through the slurry dispenser on top of the pad and transported to the pad-wafer interface through centrifugal forces. A three-body contact caused by the pad surface asperities (pores and grooves on the pad), slurry and the wafer surface lead to the removal of material from the wafer surface. The CMP results are very sensitive to the applied pressure, slurry chemistry, and the pattern printed on the wafer. An inappropriate combination of these parameters can lead to non-uniform material removal. This can lead to large values for the defects like dishing of metal lines and erosion of dielectrics causing hotspots like open, circuits shorting, timing delays and RC violations.

With the advent of high-k metal gates (HKMG) technology, additional CMP steps were added to FEOL loop. This leads to strong depth of focus (DOF) and wafer planarity requirements that increased the importance of CMP modeling and hotspots predictions prior to manufacturing [1–3]. CMP modeling is used to correctly predict materials removal and surface profile during polishing [2]. Typically, the material removal rate is described by Preston's law and is proportional to the pressure distribution over the chip area.

Numerous deposition processes are used in modern semiconductor manufacturing for deposition of oxide, glass, metal and other layers. Even for advanced deposition technologies, the post-deposited profile is not uniform due to the underlying pattern variation and it might contain large variations. The non-uniformity post-deposition profile of a patterned wafer affects surface planarity after CMP. Thus, prediction of post-deposition profile is important for CMP modeling. Recently, a neural network-based full-chip deposition model for predicting the post-deposition profile surface was proposed [4–5]. Because the material removal rate is highly dependent on the local pressure, it makes the calculation of pressure distribution over the chip area crucial for accurate simulation of the surface profile dynamics for CMP modeling.

The pressure distribution calculation is usually based on the Hertz contact theory and Chekina model [6]. In this model, the pad is assumed to be a massive elastic body with a flat surface pressed against the wafer, which is assumed to be a rigid body. The calculations involve application of fast Fourier (FFT) and inverse fast Fourier (IFFT) transforms and pad displacements updates. Such an approach may generate numerical inaccuracies and instabilities of the algorithm.

In this paper, we applied an obstacle problem approach for accurate pressure distribution calculation across the wafer/die surface for CMP modeling [7]. In the obstacle problem, the pad is assumed to be an elastic membrane with fixed boundaries that is displaced by the wafer surface. The solution of the problem can be thought of as the equilibrium position of the pad, which lies above the wafer surface. In the region where the pad is above the obstacle, an elliptic partial differential equation (PDE) is solved, while in the other region, the pad coincides with the wafer. Using this approach, the computations of FFTs and IFFTs can be avoided. This method can lead to more accurate pressure calculation and automatic calculation of pad displacements.

2. Pressure calculation problem formulation

2.1. Obstacle problem

The obstacle problem is a classic model in the framework of variational inequalities and free boundary problems [4]. It usually describes the equilibrium state of an elastic membrane that is displaced by a physical obstacle, as shown in figure 1. Typically, these problems are modelled via a variational principle, using an inequality constraint that represents the physical obstacle.

Many important problems can be formulated by transformation to an obstacle problem: elastic-plastic torsion, phase transition, constrained heating, elasto-plasticity, optimal control and financial mathematics problems [7]. Because obstacle problems are highly nonlinear, finding accurate numerical solutions can be a challenge. Usually, Lagrange multiplier formulations are
used as numerical methods for the solution of obstacle problems [7].

The obstacle problem is defined as finding the minimum of the Dirichlet integral:

\[ D(u) = \int_{\Omega} |\nabla u(x)| dx, \]  \hspace{1cm} (1)

for all functions \( u(x) \) satisfying the condition \( u \geq \varphi, \varphi \in C^\infty \) in \( \Omega \subset \mathbb{R}^n \) domain. The Dirichlet boundary conditions are usually used for the problem with \( u = g \) at \( \partial \Omega \). The Euler-Lagrange equations of the minimization problem have the form:

\[ u(x) \geq \varphi(x) \quad \text{for} \quad x \in \Omega, \]  \hspace{1cm} (2)

\[ \Delta u(x) = 0 \quad \text{for} \quad u(x) > \varphi(x), \]  \hspace{1cm} (3)

\[ -\Delta u(x) \geq 0 \quad \text{for} \quad x \in \Omega. \]  \hspace{1cm} (4)

The equations (2)–(4) can be written as follows:

\[ \min \{ -\Delta u(x), u(x) - \varphi(x) \} = 0, \quad x \in \Omega \]  \hspace{1cm} (5)

2.2. Pressure calculation problem formulation

Suppose a rigid wafer is pressed against an elastic flat surface of a polishing pad with constant applied pressure \( P_0 \) (figure 2). Due to wafer surface asperities, the polishing pad deforms, leading to pad surface displacements and uneven distribution of applied pressure \( P_0 \) on the wafer surface. Our aim is to accurately calculate the pressure distribution throughout the wafer surface, which can later be used in a Preston equation to predict the material removal rate.

Assume that the wafer is given through its fixed contact surface:

\[ f(x, y): \Omega \to \mathbb{R}, \quad \Omega = [0, 1] \times [0, 1], \]  \hspace{1cm} (6)

where \( f(x, y) > 0 \) for any \( (x, y) \in \Omega \). We define a reference plane \( z = c \) with respect to which the pad and the wafer displacements will be calculated. This reference plane can be imagined as the top flat surface of the pad, where the actual pressure is applied. We define the displacement of the wafer \( w_{\text{wafer}}(x, y) \) as the distance between the top of the surface of the wafer and the reference plane \( z = c \), and displacement of the pad \( w_{\text{pad}}(x, y) \) as the distance between the pad surface and the reference plane \( z = c \) (figure 1b). The pad and wafer displacements can be written as follows:

\[ w_{\text{wafer}}(x, y) = f(x, y) - c, \quad (x, y) \in \Omega, \]  \hspace{1cm} (7)

\[ w_{\text{pad}}(x, y) = \ell(x, y) - c, \quad (x, y) \in \Omega, \]  \hspace{1cm} (8)
where \( l(x,y) \) is the pad’s profile at \((x,y)\). Our goal is to find the pressure \( P_w(x,y) > 0 \) on the pad/wafer surface at any point \((x,y) \in \Omega\), given the applied pressure \( P_0 > 0 \), wafer surface \( f(x,y) \), and polishing pad stiffness. We denote:

\[
p_{pt}(x,y) = P_w(x,y) - P_0, \quad (x,y) \in \Omega,
\]

and refer to \( p_{pt} \) as the perturbated pad pressure. The relation between the perturbated pad pressure \( p_{pt} \) and the perturbated pad surface displacement \( w_{pad} \) can be obtained from the formula [6]

\[
w_{pad}(x,y) = K \int \int_{\Omega} \frac{p_{pt}(\xi,\eta)}{\sqrt{(x-\xi)^2 + (y-\eta)^2}} d\xi d\eta, \quad (x,y) \in \Omega,
\]

Here \( K \) is the constant \( K = (1 - \nu^2)/(\pi E) \), with the Poisson ratio \( \nu \) and the Young modulus \( E \) of the pad. Note that in equation (5), both \( w_{pad} \) and \( p_{pt} \) are unknown. Additionally, because the total pressure on the pad must be \( P_0 \), the equilibrium condition will have the following form:

\[
\int \int_{\Omega} P_w(x,y) \, dx \, dy = P_0, \quad (x,y) \in \Omega,
\]

or

\[
\int \int_{\Omega} p_{pt}(x,y) \, dx \, dy = 0.
\]

So, if we calculate the value of \( p_{pt} \), we will find \( P_w \). The main idea behind the proposed solution is as follows: given a fixed value of \( c \), determine values of \( p_{pt} \) and \( w_{pad} \) from equation (10). If \( c \) is not correctly determined, the condition (11), (12) will not be satisfied.

We divide the wafer surface \( \Omega \) into two regions: \( \Omega_c \) is pad-wafer contact region and \( \Omega_{nc} \) is pad-wafer no contact region. For these regions, the following relations for displacements are true:

\[
\begin{cases}
  w_{pad}(x,y) = w_{wafer}(x,y), & (x,y) \in \Omega_c, \\
  w_{pad}(x,y) > w_{wafer}(x,y), & (x,y) \in \Omega_{nc}.
\end{cases}
\]

The pressure on the pad surface will be 0 at every point where there is no contact between the pad and wafer surfaces which mathematically can be written as:

\[
\begin{cases}
  P_w(x,y) \geq 0, & (x,y) \in \Omega_c, \\
  P_w(x,y) = 0, & (x,y) \in \Omega_{nc}.
\end{cases}
\]
In terms of perturbated pad pressure and displacements equations (13), (14) can be written as follows:

\[
\begin{aligned}
\begin{cases}
w_{\text{pad}}(x,y) = w_{\text{wafer}}(x,y), & \text{then } p_{\text{pt}}(x,y) \geq -P_0, \\
w_{\text{pad}}(x,y) > w_{\text{wafer}}(x,y), & \text{then } p_{\text{pt}}(x,y) = -P_0.
\end{cases}
\end{aligned}
\tag{15}
\]

2.3. Formulation of pressure calculation problem as an obstacle problem

Let us now formulate the solution of the pressure calculation integral equation problem (10)–(12) as an obstacle problem. We introduce the following notations for the sake of brevity:

\[
\begin{aligned}
z(x,y) &= w_{\text{pad}}(x,y), \\
g(x,y) &= w_{\text{wafer}}(x,y), \\
p(x,y) &= p_{\text{pt}}(x,y).
\end{aligned}
\tag{16}
\]

Combining all the above observations, we obtain the following mathematical setting for the problem:

Find a constant \(c \in \mathbb{R}\) and functions \(z(x,y)\), \(p(x,y)\) such that the following conditions hold:

- the relation between the perturbated displacement and perturbated pressure satisfy the equation:
  \[
  z(x,y) = K \iint_{\Omega} \frac{p(\xi, \eta)}{\sqrt{(x-\xi)^2 + (y-\eta)^2}} \, d\xi \, d\eta 
  \text{ for any } (x,y) \in \Omega;
  \tag{17}
  \]

- equilibrium condition
  \[
  \iint_{\Omega} p(\xi, \eta) \, d\xi \, d\eta = 0,
  \tag{18}
  \]

- contact condition
  \[
  p(x,y) \geq -P_0 \quad \text{for } z(x,y) = g(x,y),
  \tag{19}
  \]

- no contact condition
  \[
  p(x,y) = -P_0 \quad \text{for } z(x,y) > g(x,y),
  \tag{20}
  \]

- non-negativity pressure condition
  \[
  p(x,y) \geq -P_0 \quad \text{for all } (x,y) \in \Omega,
  \tag{21}
  \]

- obstacle condition
  \[
  z(x,y) \geq g(x,y) \quad \text{for all } (x,y) \in \Omega.
  \tag{22}
  \]

Equations (19)–(22) can be reduced to equivalent complimentary problem:

\[
\min\{z(x,y) - g(x,y), p(x,y) + P_0\} = 0 \quad \text{for all } (x,y) \in \Omega.
\tag{23}
\]

It can be shown that conditions (19)–(22) imply equation (23). Conversely, if the equation (23) is satisfied, then the both arguments of min function in (23) will be non-negative. If \(z(x,y) < g(x,y)\), then the \(p(x,y) + P_0 = 0\). Finally, the problem is defined as follows:

Find a constant \(c \in \mathbb{R}\) and functions \(z(x,y)\), \(p(x,y)\) such that it satisfies the relation between the perturbated displacement and perturbated pressure below:

\[
z(x,y) = K \iint_{\Omega} \frac{p(\xi, \eta)}{\sqrt{(x-\xi)^2 + (y-\eta)^2}} \, d\xi \, d\eta 
\text{ for any } (x,y) \in \Omega
\tag{24}
\]

and satisfy the following conditions:

- complementary condition
  \[
  \min\{z(x,y) - g(x,y), p(x,y) + P_0\} = 0 \quad \text{for all } (x,y) \in \Omega,
  \tag{25}
  \]

- equilibrium condition
  \[
  \iint_{\Omega} p(\xi, \eta) \, d\xi \, d\eta = 0,
  \tag{26}
  \]

where the conditions (24)–(26) hold in the whole domain \(\Omega\).
3. Integral equation discretization and numerical solution

In this section, we propose a numerical algorithm for solving the nonlinear problem (24)–(26). For a number \( n \) (chosen in advance), a mesh in \( \Omega \) is constructed that goes through the points \( x_k = kh, y_j = jh, \) with \( k, j = 0, \ldots, n \), and has a size of \( h = 1/n \). We denote:

\[
\tilde{x}_k = x_k + \frac{h}{2}, \quad \tilde{y}_j = y_j + \frac{h}{2}, \quad k, j = 0, \ldots, n - 1.
\]  

(27)

Our aim is to calculate approximately the values of the pressure function \( p(x, y) \) at the points \((\tilde{x}_k, \tilde{y}_j)\). For the sake of brevity, the notations \( p_{kj} = p(\tilde{x}_k, \tilde{y}_j) \), \( z_{kj} = z(\tilde{x}_k, \tilde{y}_j) \) are used. The discretized version of the problem (24)–(26) at the points \((\tilde{x}_k, \tilde{y}_j)\) has the form:

\[
z_{kj} = K \int_\Omega \frac{p(\xi, \eta)}{\sqrt{(\tilde{x}_k - \eta)^2 + (\tilde{y}_j - \eta)^2}} \, d\xi \, d\eta, \quad k, j = 0, \ldots, n - 1,
\]  

(28)

\[
\min\{z_{kj} - g_{kj}, p_{kj} + P_0\} = 0, \quad k, j = 0, \ldots, n - 1,
\]  

(29)

\[
\int_\Omega p(\xi, \eta) \, d\xi \, d\eta = 0.
\]  

(30)

To discretize the problem further, equations (28)–(30) must be approximated using quadrature rules. Assuming that the mesh size is small enough, and that \( p \) is not changing much within one cell, we approximate the integral of \( p(x, y) \) on one cell by the value of \( p(x, y) \) at the midpoint of that cell multiplied by the area of the cell as follows:

\[
\int_\Omega p(\xi, \eta) \, d\xi \, d\eta \approx h^2 \sum_{m, i=0}^{n-1} p_{mi}.
\]  

(31)

The same approximation to calculate \( z_{kj} \) in (28) has the form:

\[
z_{kj} \approx \sum_{m, i=0}^{n-1} p_{mi} \int_{[x_m, x_{m+1}] \times [y_i, y_{i+1}]} \frac{1}{\sqrt{(\tilde{x}_k - \xi)^2 + (\tilde{y}_j - \eta)^2}} \, d\xi \, d\eta.
\]  

(32)

Integrals in the last sum can be calculated explicitly. By denoting \( a_{kmji} \) as:

\[
a_{kmji} = K \int_{[x_m, x_{m+1}] \times [y_i, y_{i+1}]} \frac{1}{\sqrt{(\tilde{x}_k - \xi)^2 + (\tilde{y}_j - \eta)^2}} \, d\xi \, d\eta,
\]  

(33)

we obtain:

\[
z_{kj} \approx \sum_{m, i=0}^{n-1} p_{mi} a_{kmji}.
\]  

(34)

Now, by inserting approximations (32)–(34) into (28)–(30), the complete discretization scheme for the problem is obtained as follows:

\[
z_{kj} = \sum_{m, i=0}^{n-1} p_{mi} a_{kmji} \quad \text{for} \quad k, j = 0, \ldots, n - 1,
\]  

(35)

\[
p_{kj} = \max \left\{ - \sum_{m \neq k, i \neq j} \frac{a_{kmji}}{a_{kkjj}} p_{mi} + \frac{g_{kj}}{a_{kkjj}} - P_0 \right\} = 0 \quad \text{for} \quad k, j = 0, \ldots, n - 1,
\]  

(36)

\[
\sum_{m, i=0}^{n-1} p_{mi} = 0.
\]  

(37)
In equation (36), unknowns \( p_{mi} \) appear on both the left and right sides. This allows us to use an iterative technique for solving the problem. We take an initial approximation \( p_{0kj} \), \( k, j = 0, 1, \ldots, n \) and update \( p_{mkj} \) using the Gauss-Seidel algorithm [8]. Theoretically, we will have that \( p_{mkj} \rightarrow p_{kj} \) as \( m \rightarrow +\infty \) for any \( k, j \), where \( p_{kj} \) is the solution of (30). The value of \( g_{kj} \) depends on the displacement \( c \). We must iterate the values of \( c \) to ensure that (30) holds. To this end, at each iteration, we increase or decrease the value of \( c \) depending on the sign of the integral in (30). If the integral is negative, we are increasing \( c \), otherwise we are decreasing \( c \). The increment size is dynamic, and tends to 0 as \( m \rightarrow +\infty \).

4. Results and discussion

In this section, we discuss the results of numerical experiments. For all cases, the pressure \( P_0 = 10 \text{KPa} \) is taken. The algorithm was tested on several profile patterns (figures 3–5).

In figure 3, profiles with constant length single and multiple prismatic patterns are considered. Simulations were done for two different pads: stiff (with stiffness of 1000 1/kPa) and soft (with stiffness of 301/kPa). For the profile with a stiff pad and constant length single prismatic pattern (figure 3a), a total pressure calculation error of 0.08% is achieved. For the same pad, but with a profile of multiple constant length prismatic pattern (figure 3b), the total pressure calculation error is as small as 0.04%. For the soft pad and constant length single prismatic patterned profile (figure 3c), the total pressure calculation error is decreased to 0.03%. For the same soft pad, but with a constant length multiple prismatic patterned profile (figure 3d), a total pressure calculation error of 0.07% is achieved.

When using a stiff pad, the pressure is distributed only on profile bumps over the prismatic
patterns for both the structures containing single and multiple prisms (figures 3e and 3f). When using a soft pad, the pad arches, resulting in some pressure dissemination on the bottom of the profile figures 3g and 3h). However, as with the stiff pad, the pressure distribution’s maximum values are concentrated on the edges of the profile bumps over the prismatic patterns for both the structures containing single and multiple prisms (figures 3g and 3h). In both cases, the pressure distribution reaches its maximum values on the edges of these rectangular bumps.

Figure 4 demonstrates the results for structures with varying size prismatic patterns. Figure 4a shows that the maximum pressure distribution values are achieved on the corners of the short prisms, while figure 4b shows that the pressure on the edges of the prisms are higher than at the middle parts. Figure 4c presents a 2D plot of the pad pressure distribution.

Finally, we considered a profile with evenly distributed sinusoidal shapes (figure 5a). In figure 5b, the pressure distribution takes the maximum values on the peaks of the profile bumps, which is expected for the considered surface pattern, while figure 5c provides a 2D plot of the pressure distribution. The described behavior of the contact pressure profile is in agreement with expectations.

These results confirm that the proposed method predicts a correct pressure distribution and may be used for accurate CMP modeling.

Conclusion

Accurate CMP modeling is crucial for the detection of potential planarity defects in chips before manufacturing. Pad pressure distribution over chip area plays a critical role during polishing. Namely, pressure distribution is responsible for long-range pattern interactions or long-range effects in CMP. CMP long-range effects strongly affect erosion of dielectrics and dishing of wide metal lines after polishing. Contact mechanics methods are typically used to calculate the pressure distribution, which involve computations of FFT and IFFT of the kernel function with singularities. Due to technology innovation and the increase in the number of patterns printed on wafers, the size of wafers are increasing, requiring new, more accurate approaches for pressure distribution calculation for CMP modeling.

In this paper, we formulated the Chekina model problem as an obstacle problem, and solved it numerically using the Gauss-Seidel algorithm. Numerical testing done by the proposed method shows that the model demonstrates correct physical behavior. In the proposed method, computations of FFT and IFFTs and recalculations of the pad displacements are avoided. This results in a more accurate pressure model that is independent of the pad displacement updating method.

Acknowledgments

This work is done under the support of a joint collaboration project between Mentor, a Siemens business and the American University of Armenia. The authors would like to express their appreciation to Shelly Stalnaker for her editorial assistance in the preparation of this paper.
References

[1] Ghulghazaryan R, Wilson J, and Takeshita N 2017 CMP model building and hotspot detection by simulation In Proc. of 158th Meeting of Planarization CMP Committee (Japan) 55

[2] Ghulghazaryan R, Wilson J, and Takeshita N Building 2017 CMP models for cmp simulation and hotspot detection In Mentor, a Siemens Business

[3] Ghulghazaryan R, Wilson J, and Abouzeid A 2015 FEOL CMP modeling: progress and challenges In Int. Conf. on Planarization/CMP Technology (ICPT) (Chandler USA) pp. 1–4

[4] Ros-Oton X 2018 Obstacle problems and free boundaries: An overview SeMA J. 75 (3) 399–419

[5] Ghulghazaryan R, Hovhannisyan M, and Wilson J 2018 Full chip neural network-based deposition models for cmp modeling: Challenges and perspectives In Proc. Int. Conf. on Planarization/CMP Technology (ICPT) (Seoul Republic of Korea) pp. 15–17

[6] Ghulghazaryan R, Piliposyan D, and Wilson J 2019 Application of neural network-based oxide deposition models to cmp modeling ECS J. Solid State Sci. Technol. 8 (5) 3154–62

[7] Chekina O and Keer L 1998 Wear-contact problems and modeling of chemical mechanical polishing J. Electrochem. Soc. 145 (6) 2100–6

[8] Press W, Teukolsky S, Vetterling W, and Flanner P 2007 Numerical Recipes. 3rd Edition: The Art of Scientific Computing (Cambridge university press)