Chemical mechanical planarization (CMP), also known as chemical mechanical polishing, is now widely recognized as the technology of choice for eliminating topographic variations and achieving near-perfect planarity of interconnection and metal layers in ultralarge scale integrated (ULSI) devices. During the CMP process, a rotating wafer is pressed face down against a rotating pad, while a slurry containing chemicals and abrasive particles is dragged into the pad–wafer interface. Polishing is then accomplished by the interaction of the pad and slurry with the wafer surface or by direct contact between the wafer and pad. To ensure stable and high performance of CMP, especially for wafers of larger diameters, it is important to optimize the slurry, pad, and other consumables. This has thus necessitated the use of grooved pads that help discharge debris and prevent subsequent particle loading effects.

Through theoretical modeling and numerical calculations, this paper aims to understand the effects of pad grooves on slurry flow at the pad–wafer interface, and to gain some insights into the optimization of pad groove designs thereby. In particular, a theoretical model previously used by Shan et al. is adapted to take into account the presence of grooves on the polishing pad. As a matter of fact, there have been a number of other theoretical models in the literature, each considering certain aspects of the CMP process. Specifically, among the works related to the calculation of slurry flow for grooved pads, Subramanian et al. computed the pressure flow and convective transport of a certain chemical substance in a single two-dimensional groove unit, using finite difference methods and periodic boundary conditions for the fluid pressure and velocity components. (Similar computations have also been carried out recently by Bakhtari et al. to analyze micrometer particle removal from deep trenches.) While such calculations are capable of capturing certain features of the transport phenomena in a single groove, the fluid dynamic interaction between neighboring grooves and the accommodation layer in the land area of the pad as porous cells (whose equivalent porosity and characteristic length were determined by an ingenious experimental apparatus; see also Muldowney and James). Of course, the approach of Muldowney and his co-workers is physically sound and presumably capable of revealing many detailed features of the slurry flow, but the necessity of resolving the slurry flow in each of the numerous grooves on the entire pad generally demands a very large amount of computational resources. It then appears to us that, to render the numerical computations less expensive, simpler simulation tools may still be desirable, and devising such a tool is one of the objectives of this paper.

As noted above, the theoretical model of Shan et al. was therefore adapted to take into account the presence of grooves on the polishing pad. Technically, when grooves are present on the pad, the geometry of the interface region apparently varies with time as the wafer slides over the pad surface; calculating the contact stress distribution and slurry flow at the pad–wafer interface is then more difficult than that for flat pads. To reduce the technical difficulties, we have chosen the simplest model that we are aware of (the model of Shan et al.) to be our point of departure. It is expected, however, that once the technical difficulties arising from the presence of pad grooves are resolved appropriately, similar approaches would also be applicable to other CMP models. Note also that previously Eaton et al. devised a hybrid Navier–Stokes/Lubrication theory approach to calculate the slurry flow for grooved pads. However, while the equivalent thickness of the slurry film is determined from the contact stress distribution in the model of Shan et al. (to be outlined below), it appears that a constant slurry film thickness has to be specified in the approach of Eaton et al. Therefore, in a certain sense, the present work integrates the groove modeling of Eaton et al. with the contact stress modeling of Shan et al.

Basically, to simplify matters, Shan et al. considered a two-dimensional (2D) model problem in which a rigid punch (modeling the wafer) slides over the surface of an elastic half-space (modeling the pad) at a constant relative velocity (see Fig. 1; but disregard the grooves for now). The resulting contact stress on the interface therefore has a one-dimensional (1D) variation along the direction of the relative sliding velocity, and, for a specified total load on the pad–wafer interface, can be calculated from an analytical expression of contact mechanics. Once the contact stress distribution is obtained, the equivalent slurry film thickness (i.e., the distance between the wafer surface and the mean asperity plane of the pad) is calculated by use of the Greenwood–Willkinson contact model for curved surfaces. Meanwhile, as the 2D slurry flow at the pad–wafer interface typically has a small Reynolds number, its dynamics can be described by the Reynolds equation of lubrication theory, which can also be supplemented with a “flow factor” (determined from an expression that was deduced by Fatir and Cheng) to take into account the reduction of slurry flow rate by surface roughness. Given the slurry film thickness, the Reynolds equation then can be integrated numerically, yielding the fluid (slurry) pressure distribution on the pad–wafer interface.
Here we emphasize that, according to the procedure described above, calculating the fluid pressure distribution requires first specifying the total load on the pad–wafer interface. However, with a prescribed back pressure on the wafer (as is usually the case in practice), the total load on the pad–wafer interface (and hence the contact stress between the wafer and pad) is affected by the fluid pressure distribution on the interface, and therefore is not known a priori. So, it inevitably takes a few iterations to obtain numerical results that observe force balance.

As one can clearly see from the above brief outline, despite being an oversimplification of the realistic CMP process, the model of Shan et al.7 still involves rather sophisticated calculations, reflecting the fact that CMP indeed is a complicated process where solid and fluid mechanics (and slurry chemistry, too) may interact in many interesting ways. Nevertheless, Shan et al.7 compared their numerical results with experimental data and obtained reasonable agreement. One of their major findings was that the average fluid pressure on the pad–wafer interface is typically subambient, and hence increases the total load and contact stress on the pad–wafer interface.

Now, as noted above, when grooves are placed periodically on the polishing pad, the geometry of the interface region clearly would change periodically with time as the wafer slides over the pad surface at a constant relative speed, resulting in periodic contact stress and fluid pressure variations. From a technical viewpoint, the task we propose to do in this work therefore is more complicated than that of Shan et al.7 But once appropriate approaches are devised to resolve the technical difficulties arising from the presence of pad grooves, similar techniques are expected to be applicable to other theoretical models of CMP as well.

In the remainder of this paper, we explain the details of the theoretical model of Shan et al.7 and our modifications for incorporating the presence of pad grooves into such a model. Numerical results are then discussed to understand the effects of pad grooves on slurry flow at the pad–wafer interface. Briefly, it turns out that the presence of pad grooves generally increases the slurry flow rate, which clearly facilitates debris discharge. Moreover, compared with a flat pad, the magnitude of the subambient fluid pressure on the pad–wafer interface also is increased by the presence of pad grooves, resulting in higher contact stress on the interface. The local material removal rate therefore is increased according to Preston’s equation.24 However, our numerical results suggest that, as a grooved pad has less contact area for the wafer to interact effectively with the polishing pad, the overall material removal rate is decreased by the presence of pad grooves. There is therefore a trade-off between slurry flow rate enhancement and material removal rate reduction in pad groove design.

**Modeling and Numerical Method**

Contact stress distribution on the pad–wafer interface.— Figure 1 shows the schematic of our 2D model problem for CMP. With respect to the 2D rigid punch of width 2a (hereafter referred to as the “wafer”), the grooved pad slides at a constant speed V. The coefficient of sliding friction between the pad and wafer surfaces is f, and the Poisson’s ratio of the pad is v. Suppose also that the total load on the wafer (per unit length in the direction normal to the plane shown in Fig. 1) is P, and ignore the presence of pad grooves for now. Then the contact stress distribution on the interface can be calculated from the following expressions20

\[
\sigma_{rd}(x) = \frac{P \cos \pi y}{\pi(a^2 - x^2)^{1/2}} \left(\frac{a + x}{a - x}\right)^\gamma
\]  

where

\[
\cot \pi y = \frac{2(1 - v)}{f(1 - 2v)}
\]

and the origin (x = 0) is located at the center of the wafer. Note that Eq. 1 was derived for a 2D rigid punch sliding on the surface of a half space,20 and the sliding speed V does not appear explicitly in Eq. 1. Furthermore, denoting the back pressure on the wafer by \(P_{\text{back}}\), and the spatial average of fluid pressure on the pad–wafer interface by \(P_{\text{AVG}}\) (see Fig. 1), we may express the total load P as

\[
P = 2a(P_{\text{back}} - P_{\text{AVG}})
\]

by invoking force balance. Equation 3 clearly indicates that a negative (i.e., subambient) average pressure would increase the total load on the pad–wafer interface. Note also that in practice the wafer typically is pressed against the pad by a fixture with a ball joint, and therefore cannot sustain a moment (see, for example, Borucki et al.25). In other words, the resultant moment with respect to the ball joint due to the contact stress, fluid pressure, and friction acting on the wafer surface has to be zero. This additional requirement amounts to taking into account the wafer surface tilting in the theoretical model. However, the tilting angle of the wafer surface usually is extremely small (on the order of a few microradians in the calculations of Jin et al.13), so for simplicity we shall not explicitly consider moment balance in the present theoretical model.

Now, when grooves are present, with a fraction \(\varphi (0 < \varphi < 1)\) of “land area” in each repeating groove unit of length \(a\) (see Fig. 1; hereafter \(\lambda\) is referred to as the “pitch” of the grooves), the total load on the pad is carried by the reduced land area, so that the contact stress on the land area is increased by a factor of 1/\(\varphi\). Moreover, the presence of pad grooves renders the geometry of the pad–wafer region varying periodically with time (with a period of \(T = \lambda/V\), and hence produces time-periodic contact stress and fluid pressure variations. To incorporate these considerations into our theoretical model, we find it convenient to use the “screening function” \(\zeta(x,t)\) to mark the position of pad grooves with respect to the wafer at a certain reference instant \(t = 0\); its value is assigned to be unity if the location \(x\) corresponds to a point in the land area of the pad and zero otherwise. [Note that \(\zeta(x)\) is periodic in \(x\) with period \(\lambda\).] Accordingly, because the pad is moving at constant speed \(V\) with respect to the wafer, the groove position at any instant \(t\) is given by \(\zeta(x - Vt)\), which for a fixed location \(x\) is time-periodic with period \(T = \lambda/V\). Meanwhile, as the geometry of the pad–wafer region changes continuously, the total load on the pad–wafer interface would also vary with time, i.e., \(P = P(t)\). Putting together these considerations, we then write the contact stress distribution on the pad–wafer interface as

\[
\sigma(x,t) = \sigma_{\text{rd}}(x,t)\zeta(x - Vt) = P(t)\cos \pi y \left(\frac{a + x}{a - x}\right)^\gamma \zeta(x - Vt)
\]

In Eq. 4, \(\sigma_{\text{rd}}(x,t) = \sigma_{\text{rd}}/\varphi\) incorporates the time dependence of the total load and the contact stress increase resulting from reduced contact area, while the screening function \(\zeta(x - Vt)\) renders the contact stress zero outside the land area (i.e., over the grooves) of the pad. Therefore, one may also think of \(\sigma_{\text{rd}}(x,t)\) as the contact stress distribution extrapolated outside the land area.
Note also that in Eq. 4 (and Eq. 1 for flat pads) the contact stress \( \sigma(x,t) \) tends to infinity at the two wafer edges \( x = \pm z \) due to stress concentration. To get around this singularity, following Shan et al., in numerical calculations we shall exclude a small length \( \Delta \) (to be specified later) from both edges of the wafer. The computational domain then has a total length of \( 2(a - \Delta a) \), and the spatial average of fluid pressure appearing in Eq. 3 can be calculated as

\[
P_{x,y}(t) = \frac{1}{2(a - \Delta a)} \int_{-a - \Delta a}^{a - \Delta a} p(x,t) dx
\]  

where \( p(x,t) \) is the fluid pressure distribution (the calculation of which is discussed later). We have checked that the numerical results are not significantly affected by small wafer edge exclusions. The minor inconsistency of using \( 2(a - \Delta a) \) for the total wafer length in Eq. 5 (and other spatial averages) therefore are ignored.

**Slurry film thickness calculation.**—With the contact stress distribution and its temporal variation determined, we then proceed to calculate the equivalent slurry film thickness, which is the distance between the wafer surface and the mean asperity plane of the pad. To that end, first the extrapolated contact stress distribution \( \sigma_0(x,t) \) is used to calculate the corresponding slurry film thickness variation across the wafer. Then, for points over the grooves, the groove depth (taking into account pad deformation) is added to the extrapolated film thickness to yield the total thickness of the slurry film there.

Specifically, assuming Hertzian contact between the pad and wafer, the Greenwood-Williamson contact model for curved surfaces relates the extrapolated contact stress distribution to the corresponding equivalent slurry film thickness \( h_0(x,t) \) by

\[
\sigma_0(x,t) = \frac{4E}{3(1 - \nu^2)} h_0 R^{1/2} \int_0^z (z - h_0)^{1/2} b(z) dz
\]  

where \( E \) is the elastic modulus of the pad, \( \eta \) and \( R \) are the density and average radius of the asperities, respectively, and \( b(z) \) is the distribution function of asperity height. Using an exponential asperity height distribution mentioned in Tichy et al., \( b(z) = e^{-z/\delta} \) (where \( \delta \) is the root-mean-squared average of the pad surface roughness), the integral in Eq. 6 can be readily evaluated, yielding

\[
h_0(x,t) = s \ln \frac{\sqrt{m} \pi E R^{1/2}}{(1 - \nu^2) \sigma_0(x,t)}
\]  

Now, to determine the total film thickness over the grooves, we use the Winkler or “mattress” model and view the land area in each groove unit in Fig. 1 as a column (a similar approach was also taken in Tichy et al.). When subjected to the compressive contact stress \( \sigma_0 \), the column height will be shortened by an amount of \( \sigma_0/K \), where the stiffness parameter \( K \) is related to the thickness \( l_{pad} \) and elastic modulus \( E \) of the pad. The bottom of a groove, however, is not subjected to significant stress and virtually retains its free (uncompressed) thickness. Therefore, the compressed groove depth under the wafer is calculated to be \( d_{groove} - \sigma_0/K \), where \( d_{groove} \) is the uncompressed groove depth. Adding then the compressed groove depth to the extrapolated film thickness \( h_0(x,t) \) for points over the grooves, we may write the film thickness distribution across the entire wafer as

\[
h(x,t) = h_0(x,t) + [1 - \xi(x - Vt)] \cdot [d_{groove} - \sigma_0(x,t)/K]
\]  

Note that the factor \( 1 - \xi(x - Vt) \) on the right side of Eq. 8 vanishes in the land area, and obtains the value of unity over the grooves. Furthermore, when the contact stress becomes too large so that at certain points \( \sigma_0 > d_{groove} \), this happens first at wafer edges \( x = \pm (a - \Delta a) \); see Eq. 4. Eq. 8 would give a smaller slurry film thickness for points over a groove than that for points over the land area. This is interpreted as groove failure, and simply indicates that our technical treatment is invalidated when the contact stress is too large. However, in practice the back pressure on the wafer should be properly set to prevent groove failure, so in our numerical computations the applied pressure and pad parameters are also chosen such that the grooves do not fail.

**Reynolds equation for calculating the fluid pressure distribution.**—Slurry flow at the pad–wafer interface typically has a small Reynolds number, so that as a good approximation its dynamics is governed by the Reynolds equation of lubrication theory

\[
\frac{\partial h}{\partial t} = - \frac{\partial q}{\partial x} - \frac{\partial}{\partial x} \left( \frac{Vh}{2} - \frac{1}{12 \mu} \psi(h) h^3 \frac{\partial p}{\partial x} \right)
\]  

where \( p(x,t) \) is the pressure in the fluid (slurry), \( \mu \) is the viscosity of the fluid. Also, assuming isotropic surface roughness, the volumetric slurry flow rate \( q(x,t) \) (per unit wafer breadth) is reduced by the “flow factor” \( \psi(h) = 1.0 - 0.9 \exp(-0.56h/s) \), which was determined in a numerical study by Patir and Cheng. Note that for flat pads, the slurry film thickness would not depend on time, \( \partial h/\partial t = 0 \), and Eq. 9 then reduces to the steady Reynolds equation used in Shan et al.

**Numerical method.**—To obtain the temporal variation of the fluid pressure distribution, one has to integrate Eq. 9 numerically, and here we discuss the technicalities. First, we discretize the \( \partial h/\partial t \) term of Eq. 9 in a two-step implicit manner, yielding

\[
\Delta t \left[ h^{n+1}(x) - h^n(x) \right] = - \frac{\partial}{\partial x} \left( \frac{V}{2} h^n(x) \right) - \frac{1}{12 \mu} \psi(h^n) h^n(x) \frac{\partial p^n(x)}{\partial x}
\]  

where \( \Delta t \) is the discrete time step (to be specified later), \( h^{n+1}(x) = h(x,(n+1)\Delta t) \), and \( p^{n+1}(x) = p(x,(n+1)\Delta t) \) are the slurry film thickness and pressure distributions at the discrete time instant \( t = (n+1)\Delta t \). Note that Eq. 10 is implicit in the sense that its right side involves slurry film thickness and pressure distributions that are unknown as yet. Furthermore, the spatial partial derivatives on the right side of Eq. 10 are discretized using standard central-difference schemes (the results are not elaborated here for brevity). For given slurry film thickness distributions \( h^n(x) \) and \( p^n(x) \), together with the boundary condition that the fluid pressure is equal to the atmospheric pressure at the wafer edges \( x = \pm (a - \Delta a) \), we have a well-posed matrix inversion problem for calculating the fluid pressure distribution \( p^{n+1}(x) \).

However, calculation of \( h^{n+1}(x) \) requires first calculating the extrapolated contact stress distributions \( \sigma_0[x,(n+1)\Delta t] \), which, in turn, depends on the total load \( P^{n+1} = P(n + 1)\Delta t \) at the corresponding instant (see Eq. 4, 7, and 8). But as pointed out earlier, the total load \( P^{n+1} \) depends on both the applied back pressure on the wafer (which can be prescribed) and the average fluid pressure (which remains to be calculated, however); a few iterations therefore are needed to obtain a converged solution of the fluid pressure distribution \( p^{n+1}(x) \). Specifically, at each discrete time instant \( t = (n+1)\Delta t \), an initial guess of the total load \( P^{n+1} \) is made to start the iterations. After going through the procedures described above to obtain the fluid pressure \( p^{n+1}(x) \), we can use Eq. 5 to calculate its spatial average, and use Eq. 3 to calculate the corresponding total load. The initial guess is then compared with the total load \( P^{n+1} \) just calculated, and corrected by Newton’s method. After a few iterations, a converged solution generally is obtained, and one can move on to the next discrete time instant.

But there is one final loose end to tie up for the calculation procedures. Specifically, at the very beginning of the calculations (corresponding to \( n = 0 \), the slurry film thickness \( h^{0}(x) = h^{0}(x) = h(x,0) \), which also is essential for starting the calculations, is not known, because it depends on the total load \( P^{0} = P^{0} = P(0) \) that cannot be specified arbitrarily. (The groove position relative to the wafer can be specified arbitrarily for \( t = 0 \).)
but the corresponding fluid pressure distribution needs to be calculated.) To resolve this difficulty, recall that the geometry of the pad–wafer region varies periodically with period $T$. The total load $P(t)$ therefore should also be a periodic function of the same period, and it suffices to calculate the slurry flow for a complete period only. A tentative value of $P^{(0)} = P(0)$ therefore is specified, so that the initial slurry film thickness $h^{(0)}(x)$ can be obtained from Eq. 4, and 8 to start the calculations. After calculating for a complete period, the resulting total load $P(T)$ is compared with the tentative initial value $P(0)$; if the difference exceeds a preset tolerance, we then update $P(0)$ by $P(T)$ and carry out the calculations for one more period. Whether this iteration scheme does yield a solution for $P(0)$, and how to choose a solution when there are many, are discussed below for specific parameter values.

Results and Discussion

In all computations, the pad properties (listed in Table I) are taken to be the same as those used in Shan et al., 7 and the viscosity of water at room temperature $\mu = 0.001$ Pa $\cdot$ s is used for the slurry. The half-width of the wafer is taken to be $a = 50$ mm, the wafer–edge exclusion distance $\Delta a = 5$ mm, the applied back pressure on the wafer $P_{back} = 20$ kPa, and the relative sliding speed $V = 0.43$ m/s, as in Shan et al. 7 Furthermore, following Tichy et al., 9 the stiffness parameter for calculating the compressed groove depth is taken to be $K = 2.5$ MPa/mm (corresponding to a pad thickness on the order of a few millimeters). The friction coefficient between the pad and wafer surfaces is $f = 0.8$. The effects of the land-area fraction $\varphi$, number of grooves under the wafer $N$ [related to the pitch of the grooves by $\lambda = 2(a - \Delta a)/N$], and uncompressed groove depth $d_{groove}$ on slurry flow are investigated; their values are specified in the ensuing discussion.

As for the grid size and discrete time step used in the computations, we divide the computational domain into 18,000 equal divisions [the grid size therefore is $\Delta x = 2(a - \Delta a)/18,000 = 5$ $\mu$m] so that even the narrowest grooves encountered in the computations can be adequately resolved. Moreover, the discrete time step is chosen to be $\Delta t = \Delta x/V$, so that in each time step the pad moves a distance of $\Delta x$ exactly. It has also been checked that reducing the grid size (and the corresponding time step) does not alter the numerical results significantly.

Solution existence and stability issues.—First, let us check if our iteration scheme does produce solutions that make physical sense. As an example, suppose that there are 30 grooves under the wafer ($N = 30$), so that the pitch of the grooves $\lambda = 3$ mm and the period of the slurry flow $T = \lambda/V = 6.98$ ms. It was pointed out above that a tentative value of $P^{(0)} = P(0)$ (or, equivalently, a value of the spatially averaged fluid pressure $p_{avg}(0)$) for prescribed back pressure on the wafer; see Eq. 3) has to be specified to start the calculations, and an admissible periodic solution of slurry flow requires that the resulting total load $P(T) = P(0)$ [or $p_{avg}(T) = p_{avg}(0)$]. To see how $p_{avg}(T)$ varies with $p_{avg}(0)$, for a range of input values of $p_{avg}(0)$ we carry out the computations for one complete period, and plot the resulting values of the fluid pressure mismatch $p_{avg}(0) - p_{avg}(T)$ in Fig. 2. In particular, in Fig. 2a, the fluid pressure mismatch is plotted as a function of the input pressure $p_{avg}(0)$ for various values of the land-area fraction $\varphi$, taking the uncompressed groove depth $d_{groove} = 100$ $\mu$m, for prescribed values of $d_{groove}$, taking $\varphi = 0.5$. Other parameter values are detailed in the text.

Now, the results in Fig. 2a indicate that, for a prescribed uncompressed groove depth, no periodic solutions exist if the land-area fraction is too small ($\varphi < 0.483$ for $d_{groove} = 100$ $\mu$m). Meanwhile, Fig. 2b shows that, for a given land-area fraction, the groove depth has to be large enough ($d_{groove} > 61$ $\mu$m for $\varphi = 0.5$) for periodic solutions to exist. Recall that a smaller value of $\varphi$ implies less contact area and hence larger contact stress. Moreover, increased contact stress results in greater pad deformation that might cause groove failure for smaller groove depths. We therefore conjecture that the nonexistence of solutions when $\varphi$ or $d_{groove}$ is too small implies that in such cases the pad is not strong enough to support the wafer (in relative sliding motion) without groove failure.

It is also seen in Fig. 2a that for a range of $\varphi$ values (e.g., $\varphi = 0.5$ or 0.6), there may exist two periodic solutions for the slurry flow. Note, however, that at the two solutions the curve of pressure mismatch has slopes of opposite signs, so that the two solutions have different stability properties. Specifically, for the solution hav-
ing a smaller magnitude of \( |p_{AVG}(0)| \), the slope of the pressure mismatch curve is positive. This means that if the input pressure \( p_{AVG}(0) \) is slightly perturbed for some reason, the resulting averaged pressure \( p_{AVG}(T) \) will tend to be restored to the correct value of \( p_{AVG}(0) \) after one period. That solution is therefore stable from a physical point of view, while the other solution can be shown to be unstable by a similar argument. Moreover, from the standpoint of numerical computations, when there indeed exists a stable solution, our iteration scheme will always converge to that solution with a reasonable initial guess of \( p_{AVG}(0) \). Therefore, it is both physically and numerically sound that the ensuing discussion only concerns stable solutions for the slurry flow.

An additional observation in Fig. 2a is that, as the land-area fraction keeps on increasing (for fixed groove depth), the magnitude \( |p_{AVG}(0)| \) of both the stable and unstable solutions increase; the unstable solution may eventually cause groove failure and then “cease” to exist in Fig. 2a (as the computations were not carried out beyond groove failure). Finally, as shown in Fig. 2b, for a given land-area fraction, both the stable and unstable solutions of \( p_{AVG}(0) \) become relatively independent of groove depth when the groove depth exceeds a certain value (roughly when \( d_{groove} > 100 \mu m \) for \( \varphi = 0.5 \)).

Basic features of the slurry flow dynamics.— Having addressed the issues of solution existence and selection, here we proceed to describe the basic features of slurry flow dynamics. As a particular example, let us take \( N = 30 \) as before (so that \( \lambda = 3 \) mm and \( T = \lambda/\nu = 6.98 \) ms), and, in addition, \( \varphi = 0.9 \) and \( d_{groove} = 200 \mu m \); the groove width therefore is \( \lambda(1 - \varphi) = 0.3 \) mm. The above parameter values are typical for commercial pads.

Using the parameter values specified above, the temporal variation of the spatial average of fluid pressure \( p_{AVG}(t) \) is calculated, and the result is shown in Fig. 3. As was observed by Shan et al.,7 here the average pressure is negative, and hence produces a suction force that increases the contact stress on the pad–groove interface. Also, because the slurry flow is periodic with time, the reference instant \( t = 0 \) does not have an absolute meaning. It is simply assigned here to the very instant when a groove is about to go under the wafer at \( x = -a \) (recall, however, that the computational domain extends from \( x = -a + \Delta a \) to \( a - \Delta a \)), as can be seen in Fig. 4 where the equivalent slurry film thickness distributions at \( t = 0 \) and \( T/2 \) are shown. Note that in Fig. 4 the “spikes” of larger film thicknesses correspond to the groove locations. Also, the right and left halves of Fig. 4 are plotted using different scales for \( x \), so that both the wafer-wide and local film thickness variations can be clearly shown. (The envelope of the wafer-wide film thickness distribution is approximately symmetric with respect to the origin \( x = 0 \).)

Moreover, Fig. 3 indicates that the relatively small groove size here (compared with the wafer half-length \( a \)) only produces an average fluid pressure variation on the order of a few Pa’s (while the back pressure on the wafer is 20 kPa). As a result, the spatial distribution of fluid pressure \( p(x,t) \) would only have a relatively weak dependence on time, as is illustrated in Fig. 5. However, Eq. 9 indicates that the volumetric slurry flow rate \( q(x,t) \) has a cubic de-
dependence on \( h(x,t) \) and hence is much more sensitive to the film thickness variation than the fluid pressure, resulting in the significant flow rate variations shown in Fig. 6 for \( t = 0 \) and \( T/2 \). (Like Fig. 4, the right and left halves of Fig. 6 are plotted using different scales for \( x \); the envelope of the wafer-wide slurry flow rate distribution is approximately symmetric with respect to the origin \( x = 0 \).) Looking more closely at the first few groove cycles (Fig. 5b), one also observes that the pressure gradient \( \frac{\partial p}{\partial x} \) in a groove is smaller than that in the land area, because the slurry film thickness is larger (corresponding to a smaller flow resistance) in a groove.

We now have a pretty good understanding about the basic slurry flow dynamics, and may go on to examine the effects of various pad groove parameters such as the land-area fraction \( \varphi \), number of grooves under the wafer \( N \), and uncompressed groove depth \( d_{\text{groove}} \) on the slurry flow dynamics. In particular, we wish to see how and to what extent the average fluid pressure and slurry flow rate vary with the aforementioned groove parameters. Moreover, the simple model of the Preston’s equation\(^24\) is used to calculate the dependence of the material removal rate on the groove pattern design characterized by such parameters.

**Dependence of the averaged fluid pressure on pad groove parameters.**—Recall that the spatial average of fluid pressure \( p_{\text{AVG}}(t) \) is a measure of the resultant force acting on the wafer by the slurry (see Eq. 5). The contact stress on the pad–wafer interface (and the material removal rate) therefore would be dependent upon the averaged fluid pressure. As shown in Fig. 3, however, the spatially averaged fluid pressure varies periodically with time. Therefore, to examine the dependence of the spatially averaged fluid pressure on various groove parameters, we find it useful to calculate the temporal mean of \( p_{\text{AVG}}(t) \)

\[
\langle p_{\text{AVG}} \rangle = \frac{1}{T} \int_{0}^{T} p_{\text{AVG}}(t) dt \quad [11]
\]

In Fig. 7, the calculated mean values of the spatially averaged fluid pressure are plotted for a number of uncompressed groove depths: \( d_{\text{groove}} = 70, 100, \) and \( 200 \) \( \mu \)m. In particular, in Fig. 7a, the groove number is kept constant (\( N = 30 \)), while the land-area ratio \( \varphi \) is being varied. Note that in such cases, larger values of \( \varphi \) correspond to narrower grooves, and the limiting case \( \varphi = 1 \) corresponds to a flat pad (without any grooves). Meanwhile, in Fig. 7b the groove width is fixed to be 0.3 mm. Increasing the groove number then corresponds to reducing the pitch of the grooves and reducing the land-area ratio \( \varphi \) accordingly, with the limiting case \( N \rightarrow 0 \) again corresponding to a flat pad. It is seen in both Fig. 7a and b that the mean value of the spatially averaged fluid pressure \( \langle p_{\text{AVG}} \rangle \) generally is negative, consistent with the experimental and numerical results for flat pads in Shan et al.\(^7\). Furthermore, the magnitude of \( \langle p_{\text{AVG}} \rangle \) increases as the land-area ratio \( \varphi \) decreases (and, equivalently, as the number of grooves \( N \) increases). This in fact can be understood on physical grounds: as \( \varphi \) decreases, the pad has to sustain higher contact stress, resulting in a smaller slurry film thickness and hence a larger flow resistance, so that the averaged fluid pressure is higher. An additional observation in Fig. 7 is the rather weak dependence of \( \langle p_{\text{AVG}} \rangle \) on the groove depth. Like the results shown in Fig. 3, this again points to the fact that the relatively small size of the grooves does not affect the fluid pressure significantly.

**Dependence of the mean slurry flow rate on pad groove parameters.**—Here we calculate the mean value of the volumetric slurry flow rate

\[
\langle q \rangle = \frac{1}{T} \int_{0}^{T} q(x,t) dt \quad [12]
\]

and discuss its dependence on various groove parameters. Note that, as can be readily deduced from Eq. 9 (which is a statement of mass conservation in essence), the mean value of the slurry flow rate \( \langle q \rangle \) does not depend on the spatial variable \( x \). It is expected that a larger flow rate would facilitate discharge debris, and hence is beneficial for the CMP process.

Now, for the same groove parameter combinations used to obtain the results shown in Fig. 7, the calculated mean slurry flow rates are plotted in Fig. 8. Despite that the mean value of the spatially averaged fluid pressure appears to be relatively independent of the groove depth in Fig. 7, here in Fig. 8 the mean flow rate increases...
dramatically with the groove depth. As pointed out earlier, this results from the fact that the volumetric slurry flow rate has a cubic dependence on the slurry film thickness (see Eq. 9). More importantly, both Fig. 8a and b indicate that the slurry flow rate generally increases with decreasing land-area ratio (and, equivalently, with increasing groove number N). In other words, increasing the number and/or width of the grooves generally increases the slurry flow rate. Note, however, that as seen in Fig. 8a, for smaller groove depths, the mean slurry flow rate may reach a local maximum at a particular small land-area fraction (e.g., $\varphi = 0.52$ for $d_{\text{groove}} = 70 \mu m$). This is related to the fact that the pad deformation increases as the land-area fraction decreases, resulting in smaller compressed groove depths that prevent further slurry flow rate increase.

From the results shown in Fig. 7 and 8, it can be concluded that, from the viewpoint of debris discharge, placing grooves on the pad is beneficial for the CMP process. Meanwhile, as the presence of pad grooves generally increases the contact stress on the pad–groove interface, the local material removal rate is expected to increase as well. However, placing grooves on the pad also reduces the land area of the pad for effective interaction with the wafer, and hence tends to decrease the overall material removal rate. It is therefore not clear at this moment whether the overall material removal rate is increased or decreased. This issue is addressed below using the simple model of the Preston’s equation.\footnote{ Dependence of the overall material removal rate on pad groove parameters.—Here we assume that the local material removal rate $R(x,t)$ is related to the contact pressure $p_{\text{back}} - p(x,t)$ and sliding speed $V$ between the wafer and pad by the Preston’s equation \footnote{ Note also that the estimated values of the Preston’s constant for the two cases are close to each other; so we shall simply take their arithmetic mean $C_0 = 4.0 \times 10^{-14} \text{ Pa}^{-1}$ in subsequent calculations.}

\begin{equation}
R(x,t) = C_0(p_{\text{back}} - p(x,t))V
\end{equation}

where $C_0$ is usually referred to as Preston’s constant. To have a reasonable estimate for the value of $C_0$, we have compared the experimental data of Thagella et al.\footnote{ Note that their data of material removal rate appear to be for flat pads. The geometry of the pad–wafer region therefore does not change with time; so it suffices to use the steady version of Eq. 9 and the numerical calculation is greatly simplified.} with the predictions of Preston’s equation.\footnote{ As shown in Fig. 9, the data of Thagella et al.\footnote{ For grooved pads, however, we shall make an additional assumption that only the land area of the pad in contact with the wafer polishes essentially, while polishing by the groove area practically is negligible. To calculate the overall material removal rate, therefore, one has to take into account the instantaneous groove position, and the spatial average of the removal rate is calculated to be} can be fitted with reasonable accuracy (minimized root-mean-squared error) by $C_0 = 4.35 \times 10^{-14} \text{ Pa}^{-1}$ for $p_{\text{back}} = 3 \text{ psi (20.68 kPa)}, 0.2 < V < 1.2 \text{ m/s}$; and by $C_0 = 3.67 \times 10^{-14} \text{ Pa}^{-1}$ for $V = 0.8 \text{ m/s}, 10 < p_{\text{back}} < 40 \text{ kPa}$. Here, the back pressure and sliding speed ranges cover the particular combination of $p_{\text{back}} = 20 \text{ kPa}$ and $V = 0.43 \text{ m/s}$ that has been used in our calculations.}

\begin{equation}
\dot{R}_{\text{AVG}}(t) = \frac{1}{2(a - \Delta a)} \int_{x = a + \Delta a}^{x = a - \Delta a} R(x,t)\zeta(x - Vt)dx
\end{equation}

Recall that $\zeta(x - Vt)$ is the screening function defined earlier to represent the instantaneous position of the grooves with respect to
The major advantage of placing grooves on the pad therefore seems to be the resulting greater slurry flow rate for debris discharge, at the expense of reducing the overall material removal rate. So, for practical groove pattern design, a careful decision must be made to achieve an optimized trade-off between the material removal rate reduction and sufficient slurry flow rate for debris discharge. Furthermore, although the average fluid pressure and overall material removal rate are relatively independent of the uncompressed groove depth, increasing the groove depth generally would increase the slurry flow rate significantly and reduce the possibility of groove failure. It is therefore advisable to use deeper grooves, as long as the land area of the pad does not buckle under the applied load.

Conclusion

Here, using two-dimensional lubrication theory supplemented with contact mechanics models, we have examined the effects of various pad groove parameters, such as the groove width, depth, and spacing, on the slurry flow dynamics and material removal rate. As oversimplified as our theoretical model may seem, we expect that the approach devised in this study to resolve the technical difficulties arising from the presence of pad grooves would also be applicable to other CMP models.

As it turns out, for uncompressed groove depths greater than about 100 \( \mu \text{m} \), the fluid pressure and contact stress on the pad–wafer interface are essentially independent on the groove depth. However, the presence of pad grooves generally increases the slurry flow rate significantly, and therefore is beneficial for debris discharge. It is also found that the magnitude of the subambient fluid pressure on the pad–wafer interface is increased by the presence of pad grooves. As the increased suction pressure implies higher contact stress between the pad and wafer, the local material removal rate therefore is increased as well. Nevertheless, our numerical results suggest that, because a grooved pad has less contact area with the wafer for effective polishing, the overall material removal rate is decreased by the presence of pad grooves. It is therefore concluded that the major advantage of placing grooves on the pad is the resulting greater slurry flow rate for debris discharge, while the overall material removal rate is reduced to some extent. Therefore, for groove pattern design in practice, one must seek an optimized trade-off between the material removal rate reduction and slurry flow rate increase. Moreover, as long as the land area of the pad does not buckle, it is advisable to use deeper grooves, as they would significantly increase the slurry flow rate and reduce the possibility of groove failure, without much sacrifice of the overall material removal rate.

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