Stochastic models for pad structure and pad conditioning used in chemical-mechanical polishing

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Abstract. Stochastic models are presented for the structure and conditioning of pads used in chemical-mechanical polishing of wafers. First the one-dimensional distribution function of surface depth in the case of a conditioned solid pad is described. Then, for characterizing the structure of a foamed pad, the theory of random closed sets is applied. An important distributional characteristic of a random closed set, the linear contact distribution function, yields the contribution to surface depth resulting from pores. As a special example the Boolean model is considered. This leads to a formula that describes the variability of the surface of a conditioned foamed pad after a certain time. Simulations and experimental data show a good agreement between theory and reality.

Key words: chemical-mechanical polishing, conditioning, pad, stochastic models, surface roughness

1. Introduction

The problem of polishing surfaces is a standard problem in various industries. There exists an extensive literature about rough surfaces and their polishing written by engineers, *e.g.* [1, Chapter 8–10], [2, Chapter 7–9] or [3, Chapter 4]. It is particularly important for the semiconductor industry because wafers must be very smooth. Namely, in the production process of integrated circuits lithography [4] is used to mark a pattern on the wafer surface, and this pattern cannot be exactly reproduced on the wafer surface if the wafer has excessive topography variations.

Today, chemical-mechanical polishing (CMP) has been widely accepted as a planarization process in the semiconductor industry. In that procedure a wafer is pressed against a rotating polishing pad, while a chemically-reactive slurry is sprayed onto the pad ahead of the wafer. The combination of slurry, pad roughness, pad motion and wafer motion is understood to be responsible for the planarization of the wafer surface, see for example the models in [5–7].

Because of the importance of the pad in polishing processes, many papers deal with this theme. Yu *et al.* [8] present a statistical description of pad roughness, where they also describe the interaction between pad and wafer, whereas the pad developement during polishing process is not considered. In Bajaj [9] this problem is investigated experimentally, pads are examined under different polishing conditions as well as different pads under the same polishing conditions. It was found that "the initial removal rate increases linearly with applied stress; however, rates of drop in polishing rate [...] decline much more rapidly at conditions of high applied stress". Pads with higher pore volume show higher initial polishing rates; the decrease of polishing rate, with progress of polishing time, is related to a decreasing number of open pores [9]. Therefore closed pores have to be opend again to reduce the decrease of the

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polishing rate. So an additional process step was introduced in CMP: conditioning. There a conditioner (a rotating plate covered with cutting elements, *e.g.* diamonds) is held against the pad for maintaining its roughness; glazed areas on the pad surface, generated during polishing, are broken up and the open pore volume is increased. For reaching a uniform polishing performance, the amount of conditioning should be the same for all points of the pad, as emphasized by Hooper *et al.* [10].

Following these results some further questions remain open, especially what the "ideal" pad surface is and how it can be obtained; "ideal" means low surface roughness of polished wafer and constant high removal rate. Therefore a model describing pad and conditioning parameters and their influence on the resulting pad surface is needed as a basis for further optimization of polishing processes. Borucki *et al.* [11] presented an excellent mathematical model for conditioning and wear of solid pads and made first steps also for the case of foamed pads. Based on his model, the present paper considers the case of a foamed pad, which is the typical case in industry. A formula is derived which describes the variability of the surface of a conditioned foamed pad after a certain conditioning time, taking account both of pad and conditioner properties.

The paper repeats first the simplifying assumptions of [11]. Then, in Section 3, the onedimensional distribution function of surface depth in the case of a conditioned solid pad is re-derived. Models for the structure of foamed pads are described in Section 4, namely random-set models. Finally the results of Sections 3 and 4 are combined in Section 5 leading to a formula for the distribution function of surface depth in the case of a conditioned foamed pad. In Section 6 the stochastic-model assumptions are verified by experimental data.

2. Basic assumptions

The pad surface is modeled as a (piece of a) homogeneous (stationary) and ergodic random field $\{Z_n(x)\}$, where x stands for a position on the pad surface. Often x is given in polar coordinates $x = (r, \theta)$ with $0 \le r \le r_{pad}$ and $0 \le \theta \le 2\pi$. $Z_n(x)$ is the surface depth of the pad at the point x at time n. The discretized time n depends on the rotation speed ω of the pad.

The coordinate system is chosen such that the starting value of the pad surface depth is $Z_0(x) \equiv 0$. The conditioning process increases the depth and therefore in the present paper $Z_n(x)$ is non-negative. Since we assume stationarity, the one-dimensional distribution function of the random field:

$$F_n(z) = P(Z_n(x) \le z)$$

is independent of the position x. In the following considerations we fix x and hence suppress it in the notation, *i.e.*, $Z_n = Z_n(x)$.

The approach in [11] for modeling the conditioning process is followed and the effect of a conditioner disk is approximated by the effect of a one-dimensional bar conditioner. The N cutting elements of the disk are assumed to be arranged on a line with mean spacing $l, l \leq r_{\text{pad}}$, (Figure 1). The point x encounters this simplified conditioner once per pad rotation. At each rotation the cutting elements displace independently from each other in their intervals of length l.

Under the simplifications described above it is sufficient to look at a fixed pad segment of length *l*. This segment lies on a ray of direction $\theta_0 \in [0, 2\pi]$ starting from the center of the pad. The segment center is taken as origin, denoted as $(0, \theta_0)$, and the segment is represented by the interval $(-a, \theta_0) \leq (r, \theta_0) \leq (a, \theta_0)$ with 2a = l. For simplification of notation the fixed θ_0



Figure 1. Schematic picture of the simplified conditioner with triangular cutting elements reacting on the pad surface.



Figure 2. The profile of a triangular cutting element is given by two parameters of the opening angle α , the depth h and the width l=2a. In a first step of conditioning (thick line) the cutting element center M_1 lies at 0. At the point r it generates the depth $V_1(r)$. In a second step (dashed line) the center may fall to the point M_2 . Then the depth at r is now $V_2(r)$, which is the maximum of the two depths $V_1(r)$ and $V_2(r)$. In the case drawn here it is $Z_2 = V_2(r)$.

is omitted. The interval $-a \le r \le a$ contains a cutting element at each rotation, and the center of the cutting element is uniformly distributed in [-a, +a].

For the calculations in this paper the conditioner stays at a fixed depth. For the case of a conditioner that moves in a deterministic manner into the pad the derivations in [11] can be applied.

3. Conditioning of a solid pad

As justified in Section 2, the considerations can be restricted to the interval $-a \le r \le a$. One cutting element encounters this interval once during a step (rotation). Borucki *et al.* [11] model the cutting elements, *e.g.* diamonds, by a saw-tooth function lying above the pad. (At the end of this section a generalization of the shape follows.)

The profile of one triangular cutting element (Figure 2) can be described by the following function, where the cutting tip lies at 0:

$$V(r) = h - \frac{h}{a} |r|, \quad -a \le r \le a, \tag{1}$$

with V(r) as the depth of the diamond in r. Here depth h and width a are the size parameters of the one-dimensional bar conditioner. Equation (1) is the same as (2.1) in [11] in other notation.

Since the center M_i of the diamond at time step *i* is uniformly distributed in [-a, a] (Figure 2), the depth of the cutting element V_i in *r* at time *i* is also uniformly distributed, due to the relation $V_i = V(r - M_i)$ and the assumption of periodic boundary. The corresponding distribution function is

$$F_1(z) = \frac{z}{h}, \quad 0 \le z \le h.$$

During *n* time steps *n* cuts happen at the fixed position *r*. The cutting depths V_1, V_2, \ldots, V_n are independent and uniformly distributed. By taking the maximum over V_1, V_2, \ldots, V_n the

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surface depth Z_n after *n* steps is obtained (Figure 2). Thus, the distribution function of the surface depth Z_n of a solid pad by interacting with a conditioner is:

$$F_n(z) = F_1(z)^n = \frac{z^n}{h^n}, \quad 0 \le z \le h.$$
 (2)

The corresponding probability-density function is

$$f_n(z) = n \frac{z^{n-1}}{h^n}, \quad 0 \le z \le h.$$
 (3)

The function $F_n(z)$ can be rewritten as

$$F_n(z) = \left(1 + \frac{1}{h}(z - h)\right)^n, \quad 0 \le z \le h.$$
(4)

Equation (4) is the same as Equation (3.3) in [11] in other notation. Note again that, when comparing this result with [11], the surface depth here is considered as a positive rather than a negative variable.

For small values of the term $\frac{z-h}{h}$ the distribution function (4) can be approximated by an exponential function, using the well-known approximation $(1+x)^n \approx \exp(nx)$:

$$F_n(z) = \exp(\lambda_1(z-h)), \quad \text{for } z \approx h, \quad \lambda_1 = \frac{h}{h}.$$
 (5)

Figure 3 shows the probability-density function (3) of surface depth of a solid pad after n=6 time steps with a cutting element depth of $h=5 \ \mu m$.

In the case of a general shape V(r) of cutting elements (instead of a triangle) the distribution function $F_1(z)$ of the random cutting depth V_i in the *i*th step is given by

$$F_1(z) = \frac{\nu(\{r : V(r) \le z\})}{2a}, \quad -a \le r \le +a,$$

where v is the Lebesgue measure and V(r) the depth of the cutting element in r.

In some industries, for example, brushes are used as conditioners. The brush conditioner can be imagined as a plate with bristles instead of diamonds. The edges of bristles are rounded (so the resulting cut is smoother). The shape of such a cutting element can be modeled as the following quadratic function

$$V(r) = -\frac{h}{a^2}r^2 + h, \quad -a \le r \le a.$$

Then the distribution function of surface depth becomes

$$F_n(z) = \left(1 - \sqrt{\frac{z+h}{h}}\right)^n \approx \exp\left(-n\sqrt{\frac{z+h}{h}}\right).$$

4. Random closed sets as models for foamed pads

Pads used in industry are typically not solid but porous. So one is confronted with a two-phase-medium with a solid and a void phase and it is natural to use models of stochastic geometry, where the solid phase is considered as a random closed set Ξ , which is assumed to be stationary [12, Chapter 6]. This means that Ξ is infinitely extended in the whole space, with the same random fluctuation everywhere. In the space a coordinate system is used with origin o, which choice is arbitrary.



Figure 3. Probability-density function of surface depth of a solid pad after n = 6 time steps, given by Equation (3). The depth of the cutting elements is $h = 5 \mu m$ as in [11].



Figure 4. The random closed set Ξ is shown in grey. If *o* does not belong to Ξ consider the vertical line *L* from *o* to the first contact with Ξ . The length of this line segment is a random variable with linear contact distribution function.

An important parameter of a stationary random closed set is its volume fraction p. It characterizes the mean volume occupied by Ξ in a region of unit volume. In the given case, 1-p corresponds to the porosity of the pad. Because of stationarity it is

$$p = P(o \in \Xi) = P(x \in \Xi) \quad \text{for all } x, \tag{6}$$

where $P(o \in \Xi)$ denotes the probability of o belonging to Ξ .

For the determination of p often stereological methods (see [12, Chapter 11]) are used, based on the formula

$$V_V = A_A = L_L = P_P = p, \tag{7}$$

with V_V as volume fraction ("volume per volume"), A_A as area fraction, L_L as line fraction, and P_P as point fraction. This means that for any arbitrary one- or two-dimensional cross-sections of the pad volume, the fraction of filled (or empty) space is always the same. Formula (7) is true in the case of stationarity. For example, p of a stationary three-dimensional set can be obtained from planar sections yielding A_A . Further explanations of stereological methods can be found in [13, Section 3.2] and in [14, Chapter 2].

An important distributional characteristic of a closed random set is its *linear contact distribution function* $H_l(s)$. It can be explained as follows. Consider the origin o of R^3 . There are two cases: either o lies in Ξ or o does not belong to Ξ . If o does not belong to Ξ , we consider a vertical line L starting in o. The first contact of L with Ξ happens within some random distance (Figure 4). The length of the corresponding line segment is a random variable, the distribution function of which is denoted by H_l .

A popular model for a random closed set is the Boolean model; see [12, Chapter 3]. In the following this model is used both for the solid phase and its complement, the void phase.

A Boolean model is constructed as follows. There are two building elements: (1) $\Phi = x_1, x_2, \dots$ a stationary Poisson process in \mathbb{R}^d of intensity λ ,

- (1) $\Psi = x_1, x_2, \dots$ a stationary Poisson process in \mathbb{R} of intensity λ ,
- (2) Ξ_1, Ξ_2, \ldots a sequence of independent identically distributed random compact sets in \mathbb{R}^3 , which are independent of the Poisson process Φ .

Then the set

$$\Xi = \bigcup_{x_i \in \Phi} (\Xi_i + x_i) = (\Xi_1 + x_1) \cup (\Xi_2 + x_2) \cup \dots,$$



Figure 5. A Boolean model with elliptical grains.



Figure 6. In this schematic picture the pad has elliptic pores. The bold spiky line presents the surface depth Z_n assuming a conditioned solid pad. At point r_1 the cut passes in the solid phase and the surface depth $Z_n^*(r_1)$ is the same as $Z_n(r_1)$ in case of a solid pad. At point r_2 the cut hits a pore. Consequently, the surface depth $Z_n^*(r_2)$ is now the sum of the depth obtained by conditioning and the residual chord length in vertical direction in the pore.

is called a Boolean model (Figure 5). The points of the Poisson process are called "germs" and the sets Ξ_i "grains". The Boolean model is stationary and, in the case of isotropic distribution of the sets Ξ_i , isotropic.

The linear contact distribution function H_l in case of a Boolean model with convex grains is an exponential distribution of parameter λ_2 :

$$H_l(z) = 1 - \exp\left(-\lambda \frac{\overline{W}_1 b_{d-1}}{b_d} z\right) = 1 - \exp(-\lambda_2 z), \quad z \ge 0,$$

with λ as the intensity of the Poisson process, b_d as the volume of unit sphere in \mathbb{R}^d and \overline{W}_1 as the mean value of the first Minkowski functional of Ξ_0 .

To take a Boolean model for the solid phase of a foamed pad is perhaps not the best solution, since it would be considered as the union of many small objects. A more realistic alternative is perhaps the converse case, where the set of pores is considered as a Boolean model. Then the solid phase is the closed hull of the complement of a Boolean model.

Ramirez and Rider used just the latter model for describing the pad structure in [15]. They encountered the problem of needing to derive a formula for the corresponding linear contact distribution function, which is a notoriously difficult problem that cannot be solved in closed form. An exact analytical expression only exists for the case d=1 (see also [16, pp. 127 and 238]). In higher dimensions [16, p. 127] refers to a methodology that amounts to inverting a Laplace transform.

Fortunately, general statistical experience has shown that the linear contact distribution function is very often an exponential distribution or at least close to. This is equivalent to an exponential form of the covariance ([12, p. 205]). This empirical observation has led to coining the term 'set with exponential covariance' ([13, p. 145] and [12, p. 205]).

So it can be concluded for both applications of the Boolean model and for many other random closed sets that the linear contact distribution function is (approximately) exponential; see also Section 6.

Note that the statistical estimation of the model parameters p and λ_2 is straightforward. For the estimation of p stereological methods can be used and for the estimation of λ_2 methods of image analysis or the classical lineal method. There the random closed set is intersected with a line. The lengths l_i of the chords outside of the random closed set are measured. The mean chord length \overline{l} yields an estimate of λ_2 :

$$\hat{\lambda}_2 = 1/\bar{l}.$$

5. Conditioning of a foamed pad

After considering the conditioning of a solid pad (see Section 3) and the structure of a foamed pad (see Section 4), now the distribution of the random surface depth Z_n^* of a conditioned foamed pad after n steps can be determined.

Clearly, Z_n^* is obtained by superposition of the previous solutions; see Figure 6.

Firstly, the pad is treated as in the case of a solid pad. Let Z_n be the surface depth after *n* cuts. The corresponding probability-density function is approximately

$$f_n(z) = \begin{cases} \frac{n}{h} \exp\left(\frac{n}{h}(z-h)\right) & \text{if } 0 \le z \le h, \\ 0 & \text{if otherwise.} \end{cases}$$

Now consider any point $(r, Z_n(r))$, where $Z_n(r)$ is the value of the random field $\{Z_n(x)\}$ at the point x. (In the past this value was often simply denoted as Z_n .) Because of the stationarity assumption of the random closed set Ξ , this point can be treated like the origin of space. Consequently, the additional depth at r caused by a cut pore is either zero (with probability p) or positive, following the linear contact distribution function H_l . Consequently, Z_n^* is a sum of two random variables with density functions $f_n(z)$ and g(z), with

$$g(z) = \begin{cases} p\delta(z) + (1-p)h_l(z) & \text{if } z \ge h, \\ 0 & \text{if } z < 0, \end{cases}$$

$$h_l(z) = \lambda_2 \exp(-\lambda_2 z).$$

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The probability density function of Z_n^* is obtained by convolution (*) as

$$f(z) = f_n(z) * g(z)$$

$$f(z) = \begin{cases} \frac{n}{h}(1-p)\lambda_2}{n} (\exp(\lambda_2(h-z)) - \exp(-n-\lambda_2 z)) & \text{if } z > h, \\ p\frac{n}{h} \exp(\frac{n}{h}(z-h)) + \frac{n}{h}\frac{(1-p)\lambda_2}{n+\lambda_2} \left(\exp(\frac{n}{h}z-n) - \exp(-n-\lambda_2 z)\right) & \text{if } 0 \le z \le h, \\ 0 & \text{if } z < 0. \end{cases}$$
(8)

6. Verification of the stochastic model

This section aims to demonstrate that the basic assumption of the stochastic model of Section 4, the exponential form of the linear contact distribution, is realistic. Furthermore, it will be shown that the main result (8) is in agreement with empirical data.

We start with the linear contact distribution function. Figure 7 shows a thin section of a utilized Cake-pad ESM-013, obtained by SEM. It is clearly visible that the pores are spheres, which are considered as the grains in the random-set modelling. Their different grey tones are caused by different depths of the pores: dark pores have their centres deep in the slice. The spherical pores in Figure 7 seem to be disjoint, which is not a strong contradiction to the Boolean-model assumption, since for the sample porosity and intensity λ are small.

It is well known that the projection of a three-dimensional Boolean model onto a plane forms a planar Boolean model [12, pp. 81 and 82]. Consequently, a planar structure as that shown in Figure 7 should behave like a planar Boolean model if the spatial structure can be described by a spatial Boolean model. Measurement of the chord-length distribution function yielded the histogram represented in Figure 8. It can be well fitted by an exponential function (*p*-value 0.22 of χ^2 -goodness-of-fit-test). Exponentially distributed chord lengths are equivalent to an exponential linear contact distribution function ([12, Equation 6.2.5]). So it can be concluded that the linear contact distribution function of the projected random set follows an exponential distribution. Thus an important necessary condition of a Boolean model is satisfied.

Next we show in two ways that the result of stochastic modelling of conditioned foamed pads, formula (6), is in agreement with data obtained from direct measurement and from simulations.

In [9] the probability-density function of that part of the surface depth that results from pores was obtained by simulation. There a stochastic model of a porous pad was simulated and then the 'intrinsic probability-density function of the line-of-sight surface of foamed pad' was determined statistically. Figure 11 there is quite similar to our Figure 9; the function shown in [9] has the same exponential form. Also the function given in Figure 10, which represents the probability-density function f(z) for surface depth of a conditioned foamed pad, is quite similar to its counterpart in Figure 12b (solid curve) in [11].

Finally, we performed our own measurements for a particular foamed pad. The surface of a utilized SUBA pad was analysed by means of a laser topograph. Figure 11 shows the histogram of the measured depths, which is based on 10000 values from a line of 1 cm length.



Figure 7. Cross-section of a utilized Cake-pad ESM-013, by SEM.



Figure 8. Histogram of chord lengths outside the pores measured in Figure 7.



Figure 9. Probability-density function $h_l(z) = \lambda_2 \exp(-\lambda_2 z)$ of the linear contact distribution multiplied by (1-p). The value for the volume fraction $V_V = p$ is taken from data by Letitia Malina, Motorola as p = 0.4. The value for the parameter $\lambda_2 = 0.4$ is estimated from Figure 11 in Borucki [11]: The value g(z)of the function in Figure 11 for z = 0 is about 0.24. The quotient of 0.24 and 1 - p = 0.6 yields λ_2 .



Figure 11. Histogram of the depths on the surface of a utilized SUBA 1250 pad.



Figure 10. Probability-density function f(z) for surface depth of a conditioned foamed pad obtained by Formula (8). The parameters are the same as in Figures 3 and 9 above $(n=6, h=5, p=0.4, \lambda_2=0.4)$.



Figure 12. Fitted probability density function to the data shown in Figure 11.

Comparison of the corresponding probability-density function estimate in Figure 12 with Figure 10 shows qualitative similarity. The peak at depth z=20 in Figure 12 corresponds to the peak at depth z=5 in Figure 10. In both figures a long tail to the right is clearly visible, a short one to the left. The cusp at depth z=40 on Figure 12 (visualized by the arrow) may correspond to that at z=5 on Figure 10.

7. Conclusions

In this paper we have developed a model for describing the surface of pads in their dependency on conditioner parameters and pad properties. For this purpose the theory of Borucki *et al.* [11] has been extended to the case of foamed pads. The structure of a foamed pad can be described by methods of the theory of random closed sets. Especially, the linear contact distribution function H_l yields the contribution to surface depth resulting from pores. In many cases H_l is (exactly or approximately) an exponential distribution. Superposition of the effects of conditioning (of a solid pad) and porosity then yields the probability-density function of surface depth of a conditioned foamed pad. The approximations are acceptable, as shown by comparison with computed results in [11] and own measurements for a utilized pad.

There are the following relationships between the conditioning process and surface depth distribution, which can be used to control the distribution of the pad surface depth.

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- The peak of the probability-density function of pad surface depth is at the point of cutting element depth h. Changing h causes a horizontal translation of the peak. Large hproduce much pad removal; much pad removal shortens pad lifetime. Therefore a small cutting depth h is intended in industry.
- The duration of conditioning expressed by time n is related to the shape of the left part of the probability-density function of pad surface depth. Longer conditioning yields steeper slopes. If in this left function part one or more local maxima can be seen, then some irregularities will exist on pad surface. For taking them off, conditioning has to be applied for longer times.
- The pad parameter λ_2 , which is related to the linear contact distribution function, contains important information about the pore distribution. If the pores are small with low variation, λ_2 is large and the right tail of the function is short and steep; large pores with a high degree of variability are correlated with a long right tail. The two extreme cases are not useful for polishing. In the first case the pad is too smooth, so the removal will be too small. In the second case the pad is too rough, which causes too large removal variation and consequently a rough wafer surface.
- The volume fraction p of pores is closely related to the height of the beginning of the right tail of the function at depth h (in Figure 10 at f(5)=0.18), for large p the tail begins at a higher point, for small p at a lower one. In the polishing process, too large and too small values of p are not useful.

Further investigations should concern the influence of different cutting elements (different to diamonds), different pad structures, different conditioning process parameters etc. Also the question of the ideal pad surface needs consideration.

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