Review of Chemical-Mechanical Planarization Modeling for Integrated Circuit Fabrication: From Particle Scale to Die and Wafer Scales

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Abstract— Modeling and simulation are critical to transfer CMP from an engineering 'art' to an engineering 'science'. Research efforts in CMP modeling have been attempted in the last decade. There is an urgent need to review the current models including their limitations and future research directions systematically. In this paper, chemical mechanical planarization modeling is reviewed systematically, from particle scale to die and wafer scales.

Keywords: CMP modeling, IC fabrication, particle scale, die scale, wafer scale.

1. Introduction

Although chemical mechanical planarization (CMP) is widely applied in integrated circuit fabrication, it is still a process of trial and error. Understanding the basic mechanism of this process has initiated the research efforts from both industry and academia in the last decade. This report gives a review of the previous CMP modeling efforts.

There are issues at three scales of CMP to be modeled, namely, the particle scale, die scale and wafer scale. The models at the particle scale are needed to address the roles and interactions of slurry particles, slurry chemicals, polishing pad and wafer materials. The material removal process in CMP can be considered as a sliding of the slurry particles over a chemically influenced thin layer over the wafer surface. The mechanical action, including the slurry abrasive indentation into the wafer surface under the down force and its sliding due to the relative movement of the wafer and polishing pad, and the chemical action, including the passivation of the wafer materials, the etching of the wafer materials, the hardening/softening of the slurry particles and polishing pad by the slurry chemicals, work together to remove the wafer surface material. Finding out what parameters and how they contribute to the mechanical-chemical actions is critical for understanding the issues related to the material removal mechanisms, e.g. the material removal rate (MRR) and the surface qualities (the roughness and scratching).

The models at the feature and die scales are needed to address the topography evolution of integrated circuit (IC) chips as a function of pattern density, line width, pitch width and polishing time. In the earlier stage, CMP is used in the planarization of inter-layer or inter-metal dielectrics (ILD/IMD) in the multi-layer IC fabrication to satisfy the depth of focus (DOF) requirements of the lithography process. With the copper and low-k

dielectrics taking place of aluminum and silicon oxide as the preliminary interconnection and inter-layer/metal dielectric materials, CMP is becoming an indispensable process for the patterning of copper in the IC fabrication. As predicted by the Semiconductor Industry Association (SIA)'s Technology Roadmap [1], the electric properties such as the time delay of the chips will depend on the resistivity and coupling capacitances of interconnection lines in the sub-micron era, which are functions of the geometry/topography of the interconnection metal lines and dielectrics [49]. A better understanding of the formation mechanism of the topography issues such as the pattern density effects, dishing, and erosion, can help to optimize the IC design, for instance, the design of the pattern layout or the dummy filling in the lower density area from the beginning of the design stage, and the process parameters, for instance, the selectivity of material removal rates of the metal to the dielectrics /barriers at the fabrication stage. The final goal of modeling efforts at this scale is to facilitate the development of electronics design automation (EDA) or electronics computer aided design (ECAD) software tools in terms of design for manufacturability.

The wafer-scale model is intended to address the issues related to the material removal non-uniformity over the wafer surface. To satisfy the manufacturability requirement in the sub-micron IC fabrication, the margin of the profile non-uniformity is usually limited in the range of several hundred nanometers. The material removal non-uniformity across the wafer is rooted in the non-uniform distributions of pressure and velocity over the wafer surface, which in a large degree are determined by the configurations of CMP machines. A model at this scale, therefore, needs to address the machine configurations properly.

In last decade, various kinds of models have been proposed by researchers, concentrating on different aspects of CMP. All of them can be put in one of the above three categories and success in a certain aspect. They will be reviewed in this report, one by one, from the particle scale to the die and wafer scales. A framework of an integrated model to consider the interactions among the models at the three scales will be proposed at the end of this report to address the issues including material removal rate, scratching, dishing and erosion, with-in die non-uniformity and with-in wafer non-uniformity, in a comprehensive way.

2. Particle Scale Models

The two most important issues at the particle scale are the material removal rate (MRR) and the surface qualities (the surface roughness and scratching). With the low-k dielectrics, usually soft polymer materials with pores, taking place of the oxide dielectrics as the preliminary dielectric materials in the next generation of IC chips, the de-lamination of the dielectrics and interconnection metals during polishing is becoming a critical surface quality issue as well. A full understanding of these problems requires proper answers to the following three questions:

What are the most important consumable and wafer parameters in the CMP material removal process?

What roles are these parameters playing once they are identified as critical parameters? How do these parameters interact to affect the material removal?

The four most important elements in the CMP material removal process are the slurry abrasive particles, slurry chemicals, polishing pad and wafer materials. There are six interactions among these four elements, namely, wafer-abrasive interaction, wafer-pad interaction, wafer-chemical interaction, abrasive-pad interaction, abrasive-chemical interaction and pad-chemical interaction. The first step to answer the above three questions depends on the understanding of these interactions independently. In the following sections, we review the previous particle-scale modeling efforts, which are mostly concentrated on one to two of the interactions. Integrated modeling efforts and a framework considering all the above interactions will be discussed at the end of this section.

2.1. Models considering the interaction between slurry particles and wafer surface

The most famous material removal equation is the experimental Preston's Equation [2], which is initially introduced for glass polishing,

$$MRR= K_e PV \tag{1}$$

where MRR is the material removal rate, K_e an all-purpose coefficient, P, the down pressure and V the relative velocity between the wafer and the pad. It demonstrates a linear dependency of material removal rate on the down pressure and velocity. An equivalent equation is the Archard's equation [3] in the area of *wear*. Not all experimental MRR data in CMP, specially, in metal CMP, supports the linear down pressure times velocity dependency. Revised Preston's equations were therefore proposed by different researchers. For example, considering that the material removal rate does not extrapolate to zero, Maury et. al. [4] introduces a fitting parameter MRR_0 into Preston's equation:

$$MRR= K_e PV + MRR_0 \tag{2}$$

Later, a nonlinear experimental equation,

$$MRR= K_e P^\alpha V^\beta, \tag{3}$$

where α, β are two fitting parameters, was proposed by Wrschka et. al [5] to get a better fit of the experimental data.

The major problem with Preston's equation and its revision is that consumable and wafer parameters are not included explicitly. Therefore, process window in terms of

consumable effects cannot be obtained. By extending Brown's model [6] of the metal polishing to the silicon polishing, Cook [7] developed a physical model to address this limitation. The interactions between the abrasive particles and the wafer surface is proposed as a Hertzian elastic penetration [8] of a spherical particle under uniform pressure P into the wafer surface, sliding along the surface with a velocity V and removing glass volume proportional to the penetration, Figure 1. A MRR formulation was proposed as:

$$MRR = (2E)^{-1}PV \tag{4}$$

where E is the Young's modulus of the wafer materials. This model can be taken as a theoretical verification of the Preston equation since it supports the linear dependency of MRR on pressure and velocity. The relationship between the wafer surface roughness R_s, the down pressure P, and abrasive size can also be obtained based on this model:

$$R_s = 3/4x(P/2kE)^{2/3} \tag{5}$$

where k is the particle concentration and unity for a fully filled close hexagonal packing [7] and x the diameter of the slurry particles. A similar model was developed by Liu et. al. [9], based on the statistical method and Herzian elastic penetration. Besides the wafer material parameter including wafer hardness H_w and wafer Young's modulus E_w , this model includes pad hardness H_p and abrasive Young's modulus E_s:

$$MRR = C\left(\frac{H_w}{H_w + H_p}\right)\left(\frac{E_s + E_w}{E_s E_w}\right)PV \tag{6}$$

where C is a coefficient to account for the effects of slurry chemicals and other consumable parameters. This model, similar to Cook's model, suggests that the material removal is proportional to the applied pressure and relative speed.

The advantages of Cook and Liu's models over Preston's equation are that they provide insights into the roles and interactions of the consumable parameters. The contributions of the slurry abrasives and pad, for example, have been attributed to their size and
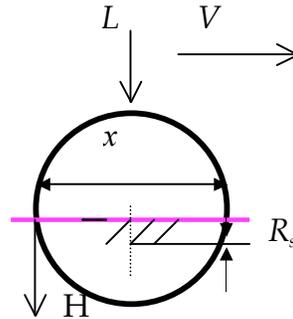

Figure 1. Mechanics of particle/glass contact (from Cook [7]).

hardness. An additional benefit is that not only material removal rate, but also surface quality issues such as roughness; see Equation 5, can be addressed using these models.

In Cook and Liu's models, the mechanical removal by abrasive particles is the dominant mechanism. Some researchers, instead, believe that the material removal is due to a mechanical-enhanced erosion. Runnel et. al. [10] are one of them, and developed an erosion-based model for CMP. They assumed that a fluid film exist between the wafer and pad interface, which affects the erosion/material removal rates at each single point through the fluid stress tensors over there:

$$MRR = C\sigma_t\sigma_n \tag{7}$$

where C is an all purpose coefficient, σ_t is the shear stress due to the slurry flow and σ_n the normal stress.

Runnel's model has been integrated into several particle-scale models by researchers including Tseng & Wang [11] and Zhang & Busnaina [12]. Tseng and Wang attributed the normal stress at the particle-wafer contact to the elastic indentation of the particle into the wafer surface, which is similar to that proposed by Cook [7], and calculated the normal stress over the wafer-particle interface as

$$\sigma_n = \frac{F}{\pi r_c^2} \tag{8}$$

where F is the force acting on the spherical particles, which is proportional to the down pressure P,

$$r_c = \left\{ \frac{3}{4}F(\frac{d}{2})\left[\frac{(1-\upsilon^2)}{E} + \frac{(1-\upsilon'^2)}{E'} \right] \right\}^{1/3} \tag{9}$$

the radius of wafer-particle contact, d the diameter of particles, υ and υ' the Poisson's ratios of wafer surface and the particle and E and E' the elastic modulus of the wafer and particles, respectively. The shear stress due to the slurry flow can be approximated as

$$\sigma_t = C\sqrt{\mu V P A} \tag{10}$$

where μ is the dynamic viscosity of the slurry and A the area of wafer surface. Substitution of equations (8) & (10) into (7) yields:

$$MRR = MP^{5/6}V^{1/2}, \tag{11}$$

where M is a parameter to account for material properties, slurry abrasive concentration and chemical processes. This model demonstrated a non-linear relationship between the material removal and the pressure times velocity. In comparison to the Cook and Liu's model, Tseng's model is attempting to connect the elastic indentation to the erosion rate instead of the mechanical abrasion. While the down pressure dependency (an exponent of 5/6) is still close to a linear dependency, the velocity dependency (an exponent of 1/2) is quite nonlinear. This is because the contribution of velocity has been attributed to the slurry flow instead of a sliding of abrasives.

Cook, Liu and Tseng& Wang's models attributed the penetration of the abrasive particles to Herzian elastic contact. Zhang and Busnaina [12] estimated the contact pressure between the particle and the contact surface and found that it is larger than the yielding stress of the polished materials. Therefore, they proposed that a plastic deformation is more likely deformation mechanism of polishing surfaces. The contact pressure over the abrasive particles-wafer interfaces is suggested to be equal to the hardness H_w of the wafer materials. Replacing the normal stress (Eq. 8) in Tseng and Wang's model with the hardness H_w yields the following material removal rate formulation:

$$MRR = M(PV)^{1/2} \qquad\qquad\qquad (12)$$

where M is a parameter to account for materials properties, slurry abrasive concentration and chemical processes. Both Tseng&Wang and Zhang& Busnaina's models suggest a nonlinear pressure times velocity dependency of material removal rate. However, Zhang and Busnaina attribute all the non-linearity to the fluid flow while part of the non-linearity in Tseng and Wang's model is from the elastic indentation of the abrasives. Moreover, it is noted that besides the external force applied on the particles from the pad, Zhang and Busnaina [12] also proposed that an adhesion force, either van der Waals force or electrostatic, depending on the separation distance between the particle and the wafer, contributes to the indentation. This has been integrated into another particle-scale model by Zhang et.al [13]. In a series of papers by Ahmadi and Xia [14] and Mazaheri and Ahmadi [15, 16], a thermodynamic work parameter W_a of adhesion is used to account for its effects on the indentation of abrasive particles. Lately, Mazaheri and Ahmadi [16] introduced double layer (dl) forces into the indentation force, whose magnitude is a function of the zeta potential of the abrasives and the wafer. Beside the abrasive wear, Ahmadi and Xia [14] also consider the adhesion wear of wafer in their model. Moreover, while most of the models treated the abrasives as spherical shape, Mazaheri and Ahmadi [15, 16] treated them as spheres with a number of hemispherical bumps around their surface. The penetrations of slurry abrasives are modeled as the penetrations of the bumps.

The above models imply that the abrasives are embedded into the pad and indented into the wafer surface. Beside these kinds of 'two-body' based models, it is noted that there are modeling efforts which assume that the abrasive particles float in the slurry and impact the wafer surface from time to time. It is these impacts that remove the materials. One model on this aspect has been proposed by Su [17], assuming a three-body abrasion of materials. Models similar to that by Tseng& Wang, attributing the material removal to

the erosion enhanced by the 'three-body' abrasive impact, instead of a 'two-body' indentation, may be developed.

2.2 Models considering the interactions between the polishing pad asperity and the wafer surface

The pad is assumed to be smooth in the earlier particle-wafer interaction models. It has been observed that the pad topography and pad material play an important role in material removal process. For example, the material removal rate increases with the pad surface roughness [18]. A softer pad yields larger material removal rate [18]. Without conditioning of the polishing pad surface, the material removal rate decreases exponentially with polishing time [19]. In consideration of this, Yu et. al. [20] developed a pad-based model. They approximated the peaks on the pad surface by hemispherical asperities with constant radius β, Figure 2. The asperity height is assumed to follow a Gaussian distribution $\Phi_Z(\mu_Z, \sigma_Z)$, where μ_Z is the mean and σ_Z the standard deviation of the asperity heights. Based on the model, the real contact area is smaller than the nominal contact area and proportional to the down pressure, see Figure 2. Steigerwald et. al [21] proposed that the material removal rate is proportional to the number of abrasive particles over the contact area. Combining this argument with Yu's model yields a linear dependency of the material removal rate on the down pressure. This agrees with Preston's Equation.

Zhao and Shi [22] also proposed a model based on wafer-asperity contact. Unlike Yu's model [20], the model does not consider the Gaussian distribution of the asperity heights. The contact area between an asperity and the wafer is given by $A_a \propto P^{2/3}$ based on Hertz elastic contact theory. By combining Steigerwald's argument, the material removal rate formulation can be obtained as

$$MRR = K(V)P^{2/3} \tag{13}$$

where $K(V)$ is a function of the relative velocity V and other CMP parameters. It is further considered by Zhao and Shi [22] that when the particles are rolling against the wafer surface, their contribution to material removal will be negligible. They argued that whether the particle is rolling or not is determined by the surface friction between the particles and the wafer, and only when the down pressure P is larger than a threshold down pressure P_{th}, the pure rolling can be avoided. This leads to the following material removal rate formulation:

$$MRR = K(V)(P^{2/3} - P_{th}^{2/3}) \qquad \text{for } P \geq P_{th}$$

and

$$MRR = 0 \qquad \text{for } P < P_{th} \tag{14}$$

The fundamental difference between the above pad-based models and the particle-based models by Cook and so on, is that pad-based models attribute the material removal rate to
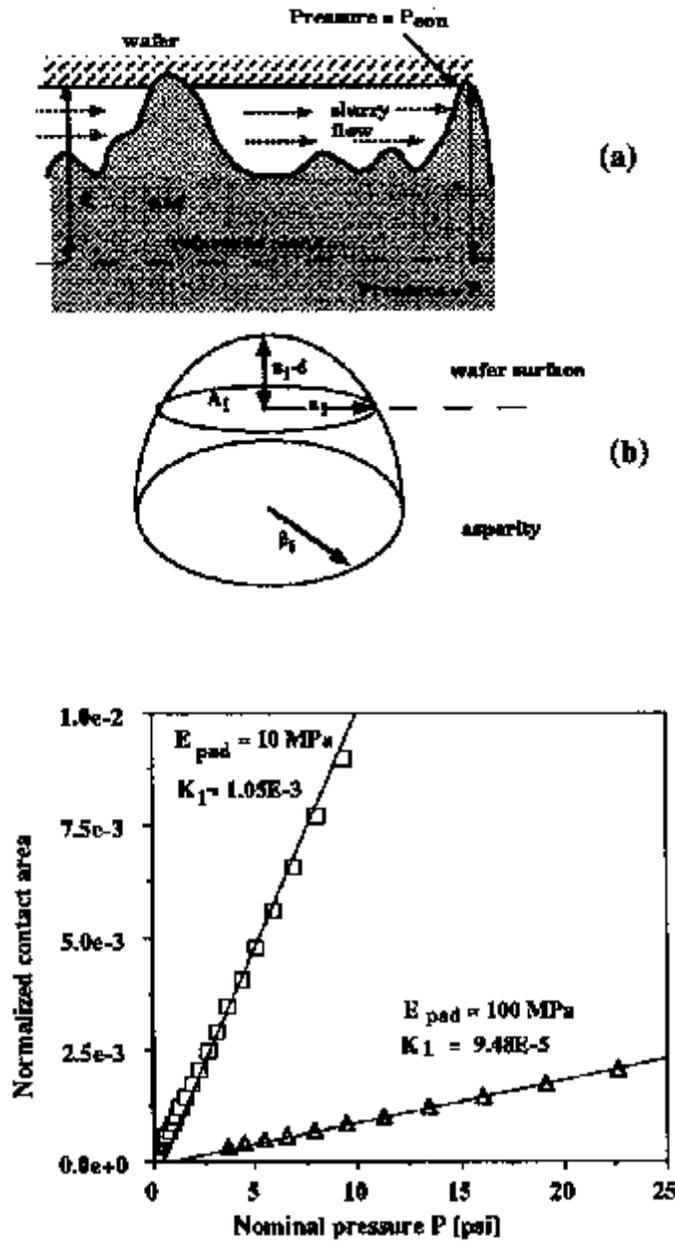

Figure 2. Wafer-pad contact model of Yu et. al [20].

the number of abrasive particle captured by the polishing pad while the later attributes the material removal rate to the interaction of a single abrasive and the wafer. Therefore, the down pressure dependency in Yu et. al [20] and Zhao & Shi's models [22] is due to the down pressure dependency of the contact area while in the particle-based models it is due to the down pressure dependency of the indentation of a single abrasive. Neither of them

may be sufficient. A complete model should consider that the material removal rate is equal to the number of abrasives times the material removed by a single abrasive. A particle-pad interaction model is critical for this purpose, considering that the function of the polishing pad is to hold the abrasive particles, transmit load forces to the particle-wafer surface, and conform to the article being polished.

It is also noted that, recently, numerical models based on finite element method have been used to investigate the wafer-pad contact [35, 60]. Fluid mechanics models considering a fluid film between the wafer and pad is to be discussed in the later sections.

2.3 Models considering the interactions between the slurry particles and polishing pad

Since the force supported by the 'cutting tools'-slurry abrasives is critical to determine the material removed by a single abrasive, and it is obtained from the polishing pad or slurry film, a successful particle-pad interaction model should first be able to evaluate the force. Several possible contact modes between the particles and pad exist. The first mode is that a slurry film is formed over the wafer-pad interface and therefore the particles are never embedded into the pad surface, but impact the pad only. In this case, the pad contributes to the force through the slurry film. A detailed fluid mechanics model considering the topography and deformation of the pad is needed to evaluate this force. Su's model [17] may be helpful in this aspect. The second possible mode is that the abrasives are embedded into the polishing pad. This is the case of the 'two-body' removal of materials. Cook's model [7] suggested a closely packing of spherical abrasives into the pad. It is assumed that the wafer and pad are separated completely by the abrasives and no pad-wafer direct contact exists. The force applied on a single abrasive under these assumptions is given by

$$F_p = \frac{2\sqrt{3}PR^2}{K} \tag{15}$$

where P the polishing pressure, R the abrasive size and K is the particle fill fraction on the pad. This particle-pad interaction model has been integrated into the material removal model of Cook [7]. It is also used by Ahmadi and Xia [14] to evaluate the force on a particle in the case of a hard-pad and larger concentration of abrasive particles. Later, Zhao and Shi [22] proposed that when the pad is soft enough, the abrasive particles will be embedded into the pad deeply and the force from the wafer is supported by the pad and abrasives together. This idea has been applied by Luo and Dornfeld [23, 24, 25] and Fu et. al [26] in their integrated material removal model. Luo and Dornfeld's model [23, 24, 25] suggested that this force is proportional to the contact pressure times the abrasive size by assuming that the abrasives are closely packed to each other and these closely packed abrasives are enwrapped by the pads so that the effective contact area between wafer and pad is equal to that without abrasives. Moreover, the size of the abrasives that may be captured by the pad is a function of abrasive size distribution and pad properties. Details on this abrasive-pad interaction model will be addressed in detail in Chapters 4

and 5 of [66]. Fu et. al [24] later assumed that the abrasives are dispersed evenly over the pad surface and use a beam model to evaluate the wafer-pad direct contact between each two single abrasives. The force supported by a single abrasive can be obtained from the beam model and is a function of abrasive size, down pressure and pad material properties [26].

Besides the force, the second purpose of an abrasive-pad interaction model is to evaluate the number of abrasives involved in the material removal process. Is this number simply proportional to the wafer-pad contact area, as that in the pad-wafer contact model by Yu et. al [20] and Zhao and Shi [22], or buried in more complicated scenarios? Fu et. al [26] simply took the number as an independent parameter in their model. This may be misleading considering that various parameters, say, the abrasive weight concentration and abrasive size, may have an influence on the number [23, 24, 25]. Luo and Dornfeld [23, 24, 25] considered a more complex scenario and suggested that only a portion of abrasives are involved in the material removal process. Similar to the size of the active abrasives, the portion is a function of the abrasive size distribution, pad topography, and material properties.

In summary, the pad-abrasive interaction is one of the most important interactions in the CMP process. One of the two material removal components, namely, the abrasive number, is a direct output of this interaction. The other, namely, the material removed by a single abrasive, is an output of the interaction through the wafer-abrasive interaction. An accurate model of this interaction will be critical for a successful particle-scale material removal model. There is not much modeling effort on this aspect before Luo and Dornfeld [24, 25], and more attention should be paid on it in the future.

2.4 Models considering the interactions between the slurry chemicals and wafer materials / surface kinetics models

The contribution of slurry chemicals to the material removal is either neglected in earlier models or represented by an all-purpose coefficient. Cook [7] suggested a complete but complicated scenario of the chemical effects. Besides the mechanical removal, he proposed that the surface removal during polishing should include the following five chemical processes: (1) the slurry chemical diffusion into the wafer surface; (2) the subsequent wafer material dissolution under the load imposed by the abrasive particles; (3) the adsorption of the dissolution product onto the surface of the polishing grain; (4) the re-deposition of the polishing materials back onto the wafer surface; and (5)……
These steps are not considered in most of the early models for two reasons: first, they are hard to be modeled quantitatively, and second, the contribution of these processes on the total material removal rate is believed to be minimal. From the knowledge of the authors, a recent model by Osseo-Asare [27] is the first to treat the adsorption rate of the dissolution product onto the surface of the polishing abrasives.

The major contribution of slurry chemicals on the material removal process has been attributed to the formation of a surface layer. This idea is well demonstrated by Kaufman

et. al in their Tungsten CMP model [28]. They used the following formulation to describe this tungsten passivation in the presence of ferricyanide, an oxidizer:

$$W+ 6Fe(CN_6)^3 + 4H2O \rightarrow WO42 + 6Fe(CN)64 + 8H+.$$
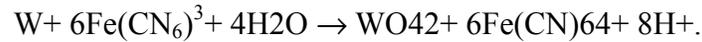
They proposed that this passivation layer is removed by slurry abrasives and the fresh tungsten surfaces are exposed, which is subsequently passivated and removed. This mechanism of passivation-removal-repassivation can be used to explain the copper, aluminum, and other metal CMP processes as well. Similar mechanism of surface modification-removal-remodification is supposed to work during silicon, silicon oxide and low-K material CMP. Paul [29] and Zhao et. al [30] have proposed detailed surface kinetics models to connect the slurry chemical concentrations and fresh metal surface sites available together to the formation rate of the surface layer. Their models can explain the material removal rate as a function of chemical and abrasive weight concentration. Lately, Borst et. al [31] proposed a five-step model for CMP of SiLK: (i). mass transport of reactant from the slurry to the slurry/wafer interface, (ii) adsorption of reactant to available surface site, (iii). reaction between adsorbed reactant and specific wafer surface to form an altered wafer surface layers, (iv), mechanical removal of the altered wafer surface layer, and (v) mass transport of removed material to the bulk slurry. This five-step mechanism is schematically shown in Figure 3. In their work, formulations to cover the steps (i), (ii) and (iii), which relate the mass transportation, slurry chemical concentration and reaction rate to the formation of the surface layer were presented. This detailed model is supposed to be able to be extended to the CMP of other materials.
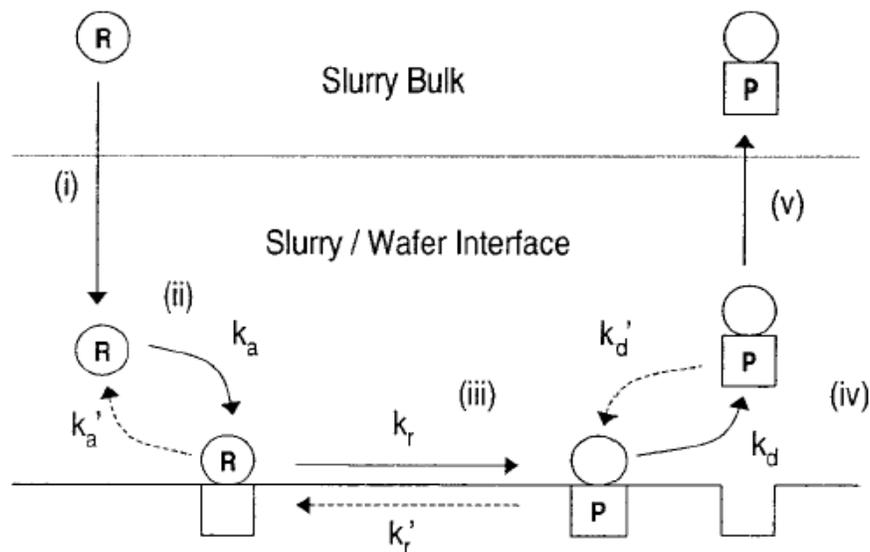

Figure 3. The five-step surface kinetics model [31].

The idea of the surface modification, removal and re-modification has been applied in Luo and Dornfeld's model [25] as well. They extended Kaufman's model by proposing that the surface layer is a bi-layer structure, one, softer hydrated layer and the other a

harder bottom layer. This is to be discussed in Chapter 4 of [66]. They did not cover the details on the formation rate of the surface layer as a function of slurry chemicals. However, they do connect the mechanical removal and chemical passivation rate together and propose MRR formulations as a coupling function of the surface generation rate, abrasive weight concentrations and wafer-pad contact area.

2.5 Models considering the interactions between the slurry chemicals and slurry abrasive particles and the interactions between the slurry chemicals and polishing pad

The slurry chemicals affect not only the wafer but also the slurry abrasives and polishing pad. Their contribution to material removal is therefore not only reflected through the surface kinetics, but also through the alteration of the abrasive and pad properties such as the abrasive shape, abrasive size, and the pad's Young's modulus. There are not too many modeling efforts on these two interactions yet. One of the efforts on the chemical-abrasive interaction is by Mazaheri and Ahmadi [16]. Mazaheri and Ahmadi proposed that the indentation of abrasives into the wafer surface is determined not only by the load from the pad but also the double layer (dl) forces F^{Ψ}, which are a function of abrasive size d and abrasive zeta potential Ψ. They proposed experimental equation of zeta potential Ψ as a function of slurry pH values for three different abrasive particle materials, namely, tantalum penoxide, alumina and silica. The zeta potential value can be substituted into the formulation of double layer forces to evaluate the material removed by a single abrasive using the indentation model. A recent model by Castillo-Mejia et. al [32] tried to explain the effect of wafer-pad interaction in CMP. The water is proposed to plasticize the polishing pad and reduce its elastic modulus. A formulation on the ratio of the Young's modulus of wet pad to the dry pad is suggested as a function of the water penetration depth. This is then used in a wafer-pad contact model to evaluate the material removal.

2.6 Integrated models considering the interactions among polishing pad, slurry particles, slurry chemicals and wafer surface

Most of the earlier models have been concentrated on one or two interactions of the CMP process. They are useful for identifying the input parameters. However, they may not be sufficient for understanding the whole material removal process. The effects of the same input parameters may be contrary to each other when acting in different interactions. For example, in the abrasive-particle interaction, larger abrasive sizes yield larger indentation depth and therefore benefit material removal rates, while in the abrasive-pad interaction, a larger abrasive size, however, may yield smaller number of abrasives and therefore smaller material removal rate. Relying on either the abrasive-wafer model or the abrasive-pad model to explain the effects of abrasive size may be misleading. A comprehensive model of CMP integrating the six interactions together is therefore

needed. In this section, several integrated modeling efforts at the particle-scale are discussed. Some of them have been mentioned earlier in above sections.

Xie and Bhushan [33] is one of the first to consider the comprehensive effects of mechanical elements including the abrasive particles and polishing pad topography in the polishing process. However, the slurry chemicals are not considered. The model cannot explain the effects of abrasive size distribution either. Chapters 2, 3 and 4 of [66], published in *IEEE Transactions on Semiconductor Manufacturing* [23, 24, 25], propose a model integrating the following four interactions, namely, the interactions of the wafer and pad, the interactions of the abrasive and wafer, the interactions of the abrasives and the polishing pad and interactions of the slurry chemicals and wafer surface, into one single material removal model.

The overall picture of the model can be described briefly here, Figure 4. The slurry is delivered into the wafer-pad interface, with slurry chemicals reacting with the wafer materials and forming a passive layer over the wafer surface. Since the pad surface is rough, only part of the pad asperities contact the wafer. This part of pad asperities captures the slurry abrasives and the abrasives captured will be deeply embedded into the pad and share the down force with the pad. These captured abrasives, called *active* abrasives, then remove the chemically influenced surface layer plastically. Among the four interactions, the wafer-abrasive interaction is modeled as a plastic indentation; the wafer-pad interaction is modeled as an elastic Hertz contact of sphere with a half space by assuming a uniform distribution of pad asperities; the abrasive-pad interaction is the
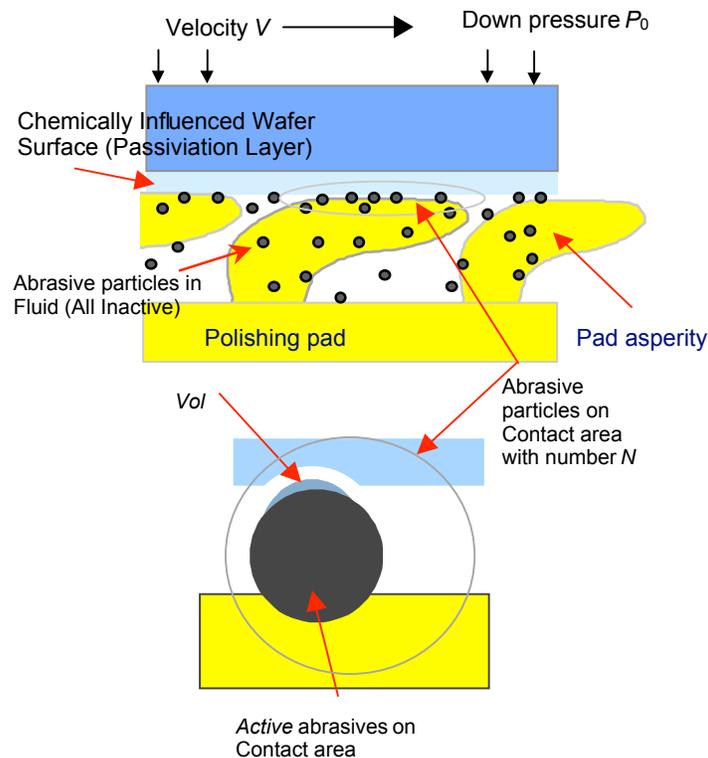

Figure 4. Interactions among wafer, abrasives and polishing pad [23].

key part of the model. The pad plays a role as a filter and only abrasives large enough can be captured; and the chemical-wafer interaction is modeled as a process of passivation, removal and repassivation.

One key idea of the model is that the material removal rate can be decomposed into two parts: one, the number *N* of the *active* abrasives, and the other, the material removed by a single abrasive per unit time. The advantage of separating the material removal into two parts is that the physical meanings of them are more apparent and therefore it is easier to identify and connect the input parameters to them. An additional benefit is that the connections between the four interactions can be easily obtained through their contribution to these two parameters. A framework of integrated particle-scale modeling connecting the four interactions has been proposed and shown schematically in Figure 5
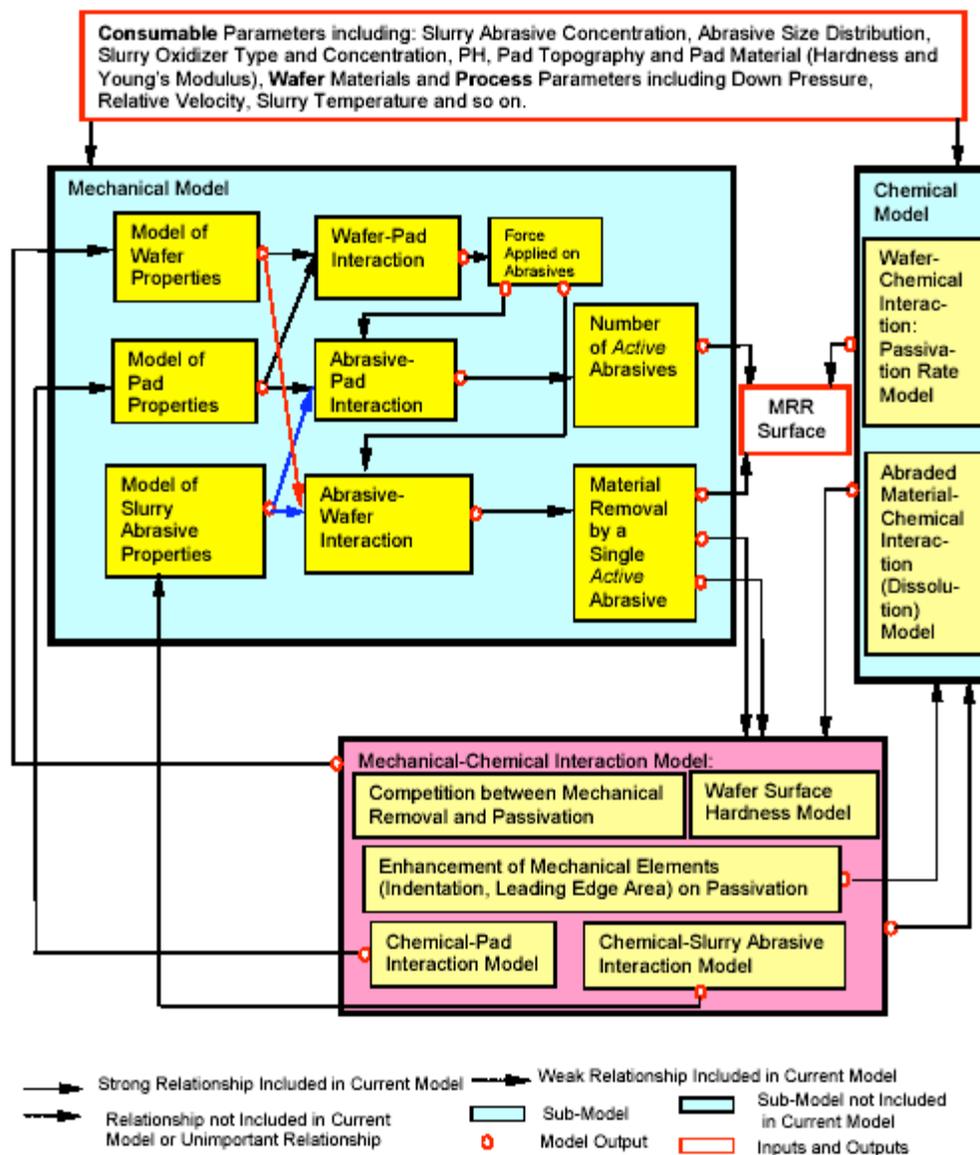

Figure 5. Detailed framework of the comprehensive material removal model.

(will revise this figure to make the connections more clear). The abrasive-chemical and pad-chemical interactions are not included in the model yet. However, they are put in the framework for the purpose of completeness.

It is noted that following works of Luo and Dornfeld [23], similar integrated models have been proposed by Fu et. al. [26], Zhao and Chang [34] and Ahmadi and Xia [14]. Works by Mazaheri and Ahmadi [15, 16] are an extension to the modeling efforts of Ahmadi and Xia [14]. They are all based on the idea that the material removal can be separated into the number of abrasive size and material removed by a single abrasive. Besides the elastic Hertz contact of wafer and pad, they further consider the possibility of a plastic contact between the polishing pad and wafer. The adhesion force and dl forces are included in their models as well to calculate the material removal by a single abrasive. Following Luo and Dornfeld [23] and Fu et. al [26], Bastawros et. al [35] further proposed that three contact modes exist between the slurry particles and polishing pad: full contact mode, partial contact mode, and non-contact mode for a soft pad. However, unlike Luo and Dornfeld's model, all of them do not explore the effects of chemical surface passivation and abrasive size distribution (or pad-abrasive interaction) on the material removal process.

2.7. Summary of particle-scale models

Finally, in this section, as a summary, we list all the major physical models in Table 1, based on the interactions covered by them. Some integrated models are covering 3-4 interactions. It is noteworthy that most of the current particle-scale models are two-body based models. The effects of slurry are attributed to distribute slurry chemicals and particles to the wafer and pad interface. Due to its low selectivity of the material removal on high and low features, the existence of a slurry film that totally separates the wafer and pad may not be a favorite in terms of planarization capability. However, with the low-k materials applied as dielectrics, the existence of a slurry film may lead to a less aggressive wafer-pad contact and therefore reduce the de-lamination of metal and dielectrics during polishing. Therefore, models considering the slurry film and three body abrasions/removals as that in Su's work [17] may become more important in the low-k era. Most models on this aspect are at the wafer scale, and their discussion is postponed to the later sections.

3. Die-scale models

At the feature and die scales, the with-in die non-uniformity (WIDNU), which is referred as the non-uniform material removal on the areas with different pattern densities, is the major concern. With the application of damascene processes including the copper damascene and shallow trench isolation in the IC fabrication, the dishing and erosion are becoming concerns as well.

Table 1. List of particle-scale models.

Particle-Scale Model Category		Abrasive-Wafer Interaction	Pad-Wafer Interaction	Pad-Abrasive Interaction	Slurry Chemical-Wafer Interaction	Slurry Chemical-Abrasive Interaction	Slurry Chemical-Pad Interaction	Integrated Material Removal Model
References		[5][6][7][9][11][12][13][14][15][16][17][23][24][25][26][34][35][33]	[14][15][16][20][22][23][24][25][26][32][34][35][60][33]	[23][24][25][26][36]	[25][27][28][29][30][31]	[16]	[32]	[33][14][15][16][23][24][25][26][34]
Identified Input Parameters								
Abrasives	Abrasive Size	[6][7][9]		[23][24][25][26][36]		[16]		[33][14][15][16][23][24][25][26][34]
	Abrasive Size Distribution	[23][24][25]		[23][24][25]				[23][24][25]
	Abrasive Shape	[6][7][9][11][12][13][14][15][16][17][23][24][25][26][34][35]		[23][24][25][26][36]				[33][14][15][16][23][24][25][26][34]
	Abrasive Weight Concentration	[14][23][24][25][34][15][16]		[23][24][25]				[33][23][24][25][34]
	Dilution Ratio	[24][25][26]		[23][24][25]				[23][24][25]
	Abrasive Number			[26][36]				[26]
	Abrasive Young's Modulus	[9]						
	Zeta Potential*	[16]						[16]
	Abrasive Material Types					[16]		[16]
Pad	Pad Topography		[23][24][25][14][15][16][26][34][60]	[23][24][25][26][36]				[33][14][15][16][23][24][25][26][34]
	Pad Hardness		[23][24][25][14]	[23][24][25]				[14][15][16][23][24][25]
	Pad Young's Modulus		[14][15][16][23][24][25][26][34]	[23][24][25][26][36]			[32]	[33][14][15][16][23][24][25][26][34]
Wafer	Wafer Young's Modulus	[5][6][7][9][11]						
	Wafer Hardness	[9][12][14][15][16][23][24][25][26][34]						[33][14][15][16][23][24][25][26][34]
	Zeta Potential*	[16]						[16]
Chemicals	Oxidizer Concentration				[28][29][30][31]			[25]
	PH value					[16]		[16]
	Passivation Rate*				[25]*			[25]

3.1 Semi-empirical models

The MIT semi-empirical model is the most successful die-scale model. The framework of the model is first proposed by Stine et. al. [36]. They designed masks and associated measurement and analysis technology to characterize and model the polishing behaviors

of ILD as a function of pattern density, area, pitch and perimeter effects. The experimental data indicates that the *effective* pattern density $\tilde{\rho}(x,y)$, which is defined as the ratio of the raised area to the total area for a window of a given size, is the dominant factor for the WIDNU, while the structure area, pitch, and perimeter/area play only a minor role. Therefore, WIDNU is also referred as pattern density effects. The effects of pattern density on WIDNU can be attributed to the pressure non-uniformity. On the high-density area, where the oxide area contacted by the pad is larger, the *effective* pressure $P/\tilde{\rho}(x,y)$ is smaller and therefore the material removal is smaller. Analytical equations to address this are developed by Stine et. al. [37] based on Preston's equation of material removal rate [2]:

$$z = \begin{cases} z_0 - [K_i t \tilde{\rho}(x,y)] & t < (\tilde{\rho} z_1 / K_i) \\ z_0 - z_1 - K_i t + \tilde{\rho}(x,y) z_1 & t > (\tilde{\rho} z_1 / K_i) \end{cases} \tag{16}$$

where z is the height of the oxide pattern feature to the substrate, z_1 the as-deposited step height, $\tilde{\rho}(x,y)$ the *effective* pattern density, K_i the blanket wafer polishing rate and t the polishing time. Before $t = \tilde{\rho} z_1 / K_i$, the step is not totally removed. The reduction rate/removal rate is $K_i / \tilde{\rho}(x,y)$ based on Preston's equation. After that, t removal rate is equal to the blanket removal rate. Note here the usage of Preston's equation in the step height evolution model provides an interface to fit the previous particle-scale models in.

The above closed-form analytical equation by Stine et. al. [37] concerns the topography evolution in the vertical direction. The complexity of the model is buried in the determination of the size of the pattern density window where an *effective* pattern density at location (x, y) is calculated. The *effective* pattern density and the corresponding pattern density window are needed because the pressure supported by a feature at location (x, y) is not only a function of the local layout density $d(x, y)$ (the location density is calculated in a window close to the feature size), but also a function of the features in the neighborhood. This is due to the macroscopic deformation of the pad. The polishing time t is usually larger than $\rho z_1 / K_i$ so that the as-deposit steps, by the second case of Equation 16, are totally removed. If the *effective* pattern density is calculated in the proper size of window, the slope of the oxide thickness as a function of the pattern density should be equal to the as-deposit step height z_1. This window size can, therefore, be extracted from experimental data using an iteration method until the condition of slope = z_1 is satisfied [37].

The size of the pattern density window is the key parameter to define/model the lateral topography across the whole chip. An implication in the *effective* pattern density calculation in Stine's model [36] is that all features in the pattern density window have the same contribution to the *effective* pattern density. Ouma et al. [38] realized that due to the smaller pad deformation, the features at the edge of the window may have less contributions. A weight density function $f(x, y)$ based on linear elasticity is applied to account for this. The *effective* density $\rho(x, y)$ in a pattern density window can be given by

the convolution of the layout density $d(x, y)$ and the weight density function: $\rho(x, y)= d(x, y) \otimes f(x, y)$. Following the same methods of Stine et al. [36], the size of the pattern density window can be extracted from the experimental data. The results are more accurate than those from Stine's model.

Under the framework of Stine's semi-empirical model, an accurate step height reduction model as Equation 6 is of the most interests. It provides not only the topography evolution information in the vertical direction but also extract the density window size in the lateral direction of the chip. The step height model by Stine et al. [37] (Equation 16) assumes no local compression of the polishing pad, so a step is completely removed before the pad touches the down areas. This may not be the case when the pad is soft and the step height is small. It is proposed by Tseng et al. [39] that for a soft pad the upper and bottom parts of the steps may be in contact with the pad simultaneously. The pressure difference over the upper and bottom parts of the steps is proportional to the step height times the pad stiffness. Based on this model the step height reduction is obtained as an exponential function of time. Combining Stine et al. [37] and Tseng et al. [39] models together, Smith et al. [40] proposed that the pad may touch the upper part of the step only at the beginning stage of the polishing, followed by a simultaneous touch of upper and bottom parts after the step height is reduced to a certain value (a function of pad materials, down pressure and feature geometry). Step height reduction formulations combining Tseng et al. and Stine et al.'s models were proposed. The size of the pattern density window extracted using these models will be different from that from the Stine et al. [36] and Ouma et al.'s [38] models.

By extending the exponential step height reduction model of Tseng et al. [39] from a single material over the upper and bottom parts of the steps to two different materials, Grillaert et al. [41] and Tseng et al. [42] developed a formulation to model the dishing and erosion in shallow trench isolation (STI). Tugbawa et al. [43] further developed a step height evolution model for the copper damascene process by combining the above models of Stine [36], Tseng [39], and Smith [40], which covers the bulky copper removal before the dielectrics are exposed, and the models of Grillaert [41] and Tseng [42], which covers the overpolishing stage after the dielectrics are exposed. Integrating this model into the framework of Stine and Ouma's models can extract the size of pattern density windows. With layout density information, the extracted window size can then be used to predict the topography evolution in both vertical and lateral direction including the copper dishing and oxide erosion in the copper damascene process.

It is noted, however, that while the model by Tugbawa [43] can predict the oxide erosion as a function of pattern density, it cannot capture the pattern density dependency of dishing in copper damascene process correctly. In Chapter 6 of [66], we propose a novel step height model for copper damascene process based on linear viscoelasticity, which can capture this feature and therefore may be more accurate for predicting the chip-level topography evolution in copper damascene and STI process. Moreover, it was realized by Maury et al. [4] that revised Preston's equations can capture the down pressure dependency of the material removal more accurately. In the development of the topography evolution model in Chapter 6 of [66], a revised Preston's equation is used in

the development of the topography evolution model. A final point worthy to mention is that all of the above models are based on the assumption of a direct solid-solid contact between wafer and pad.

3.2. Physical models

While the semi-empirical models of Stine et al. [36] and Ouma et al. [38] are the most successful models at die scale, other researchers are trying to developed physical models to explain the topography evolution. Ouyang et al. [44] assumed that a slurry film exist between and die and pad and developed pressure equations based on fluid mechanics to predict the pressure at the location (x, y, z). Preston's equation is then used to evaluate the topography evolution. Contact mechanics based model was developed by Chekina et al. [45] to evaluate the topography evolution as well. The disadvantage of these physical models is that they are computational intensity. Their accuracy is also still in question.

3.3. Electronics Computer Aided Design

One motivation for CMP modeling at the die-scale is to facilitate computer-aided design. In interconnect-dominant circuits, the topography, such as the ILD thickness variation, can lead to a more than 20% circuit performance variation, which is significant to cause concerns in design of high-performance microprocessors [46]. Since the underlying reason for the WIDNU is the pattern density, dummy patterns have been inserted in the low- density area to reduce the non-uniformity. The dummy filling should not hurt the original circuit function and design rule-correctness [47]. To satisfy this requirement, complicated filling algorithms have been developed by different researchers based on the *effective* pattern density models by Stine [36] and Ouma [38]. These include a series of recent works published in *IEEE Transactions on CAD* [47, 48, 49].

4. Wafer-scale models

The with-in wafer non-uniformity (WIWNU) of material removal rate is the major concern at the wafer scale. The preliminary reasons for the WIWNU are the non-uniform distributions of pressure and velocity across the wafer. To model these two distributions, it is needed to understand the configuration of the CMP equipments. There are two typical CMP configurations, namely, rotational type and linear type. For a rotational type of machine (Applied Materials Inc. and Novellus Inc.), the polishing head is rotated on a polishing platen, which is rotated around the center of itself. For a linear type of machine, the polishing head is rotated while a belt is moving under it linearly (LAM Research Inc.). The kinetics/velocity distributions associated with them were straightforward. Several researchers have investigated it for a rotational type of machine [50]. A conclusion of these analyzes is that the platen rotational speed times the offset of the head and platen centers is the major components of the relative velocity. When the platen speed is close to the head speed, the velocity distribution is more uniform. Similar

analysis can be done for a linear type of machine. They are given in Chapter 7 of [66]. The pressure distribution modeling is more complicated and can be put in two categories: models based on solid mechanics and models based on fluid mechanics.

4.1. Pressure distribution models based on solid-solid contact

The earliest wafer-scale CMP model for pressure distribution is that by Wang et al. [51] for the rotational type machines. They developed a finite element model to evaluate the pressure distribution based on the assumption of wafer-pad direct contact. The model results correlate with the material removal non-uniformity profile qualitatively well. The edge effects, e.g., the large material removal rate at the wafer edge can be well explained by the pressure singularity over there. This implies that solid-solid contact between wafer and pad dominates the pressure distribution. Several finite element models were developed after Wang et al. [51], for example, to investigate the improvement of the edge effects by a retaining ring. A model based on boundary element method, which is advantageous in thin structure analysis [63, 64, 65], is used in Chapter 7 of [66] to predict the pressure distribution with and without ring. Besides the numerical models, analytical models based on Hertz contact theory were proposed by Tseng et al. [52]. A unique property of their models is the effects of wafer curvature/film stress on the pressure distribution can be captured. More recently, Fu and Chandra [53, 54] have developed an analytical equation based on both linear elasticity and linear viscoelasticity. It is claimed that their linear viscoelastic model can explain the material removal degeneration with no pad conditioning.

4.2 Pressure distribution models based on semi-solid-solid Contact and solid- fluid-solid contact

Some researchers believe that a slurry film may be formed over the wafer-pad interface under certain process conditions, say, when the down pressure is small and the relative velocity is large. Due to the small material removal selectivity over higher and lower regions, the existence of such a film may be unfavorable in terms of planarization ability. With the soft low-K materials replacing the hard silicon oxide as the dielectric materials in the sub-micron IC fabrication, a formation of slurry film, which makes the mechanical contact between wafer and pad less aggressive may be needed to avoid/reduce the de-laminations of metal and dielectrics. Several models have been developed to address the pressure distribution under the condition of a slurry film. Tichy et al. [55] assume that the thickness of the film is equal to the height of the pad asperities. Contact mechanics based on solid-solid contact is used to evaluate the deformation of the pad asperities. The asperity height after the deformation is equal to the slurry film thickness $h(x)$, which is then put in the Renold's equation to predict the fluid pressure. This model can be considered as a semi solid-solid contact model. One conclusion got is that the fluid pressure is negative under certain process conditions. Therefore the wafer is sucked to the pad. This implies that the solid-solid contact dominates the process in the process conditions. Besides the semi-solid-solid contact model, Thakurta et al. [56, 57, 58] and

Cho et al. [59] developed both two-dimensional and three-dimensional fluid models based on Renold's equation. Not only slurry flow in the lateral direction, but also slurry flow in the vertical direction, which is the case in Novellus CMP configuration, where slurry is fed from the bottom of the platen, is considered. The pad deformation due to the fluid flow is considered, as well and added into the film thickness. One boundary condition in the model is that the gimbals moment of the polishing head is zero under a zero friction force assumption. In Chapter 7 of [66], this model is extended to consider the friction force. The moment due to the friction force has to be balanced by an asymmetric distribution of normal pressure, leading to a change of the average normal pressure. One final point worthy to mention is that most of the previous 'two-body' based particle- scale models may not work any more in the case of fluid film.

5. Discussion and concluding remarks

From the viewpoint of industry, CMP modeling should satisfy the following requirements: i. reliability to be used as verification of process; ii. ability to give feedback for 'what-if' scenarios in lieu of time-consuming design of experiment (DOE) tests; iii. performance prediction for realistic, heterogeneous pattern effects; iv. prediction on not only wafer scale phenomena but also feature/chip scale interaction; v. integration of multi-scale (wafer-, die-, feature-level) interactions for global CMP modeling to be useful; vi. linkage of models to upstream (deposition, etc.) and downstream (lithography, etc.) process; vii. ability to address defectivity; and viii. ability to address new materials, consumables (pad, slurry, etc.) modeling and characterization [60].

Great progresses in CMP modeling have been made in last decade, which can help to address the above requirements from different aspects. The particle-scale models can give a feedback for 'what-if' scenarios to save up the DOE time. A more systematic design of experiment instead of trial and error can now be applied in the process development and optimization [61]. A successful particle-scale model to identify the critical input parameters of consumables, explain the roles and describe the interactions among them, will be particularly helpful for the consumable design. Optimal designs of pad topography and abrasive size distribution have been identified as two promising areas on this aspect. It is on-going research at UC Berkeley [61]. The defectivity issues, such as sratching and roughness, can also be addressed by the particle-scale models. The number of particles and their indentation depths into wafer are the two dominant factors on this aspect based on Luo and Dornfeld's model [23, 24, 25].

The die-scale model of MIT can now predict the performance of realistic pattern effects. Linkage of the copper models to upstream copper electrochemical plating process is underway at MIT [62]. Preston's equation and its revisions provide the interface for particle-scale, die-scale and wafer-scale model integrations. Combining the particle-scale material removal rate formulation with the pressure distribution prediction at die and wafer-scales can yield the with-in die and with-in wafer non-uniform material removal models. A framework of an integrated model connecting the models at the three scales together is shown schematically in Figure 6.
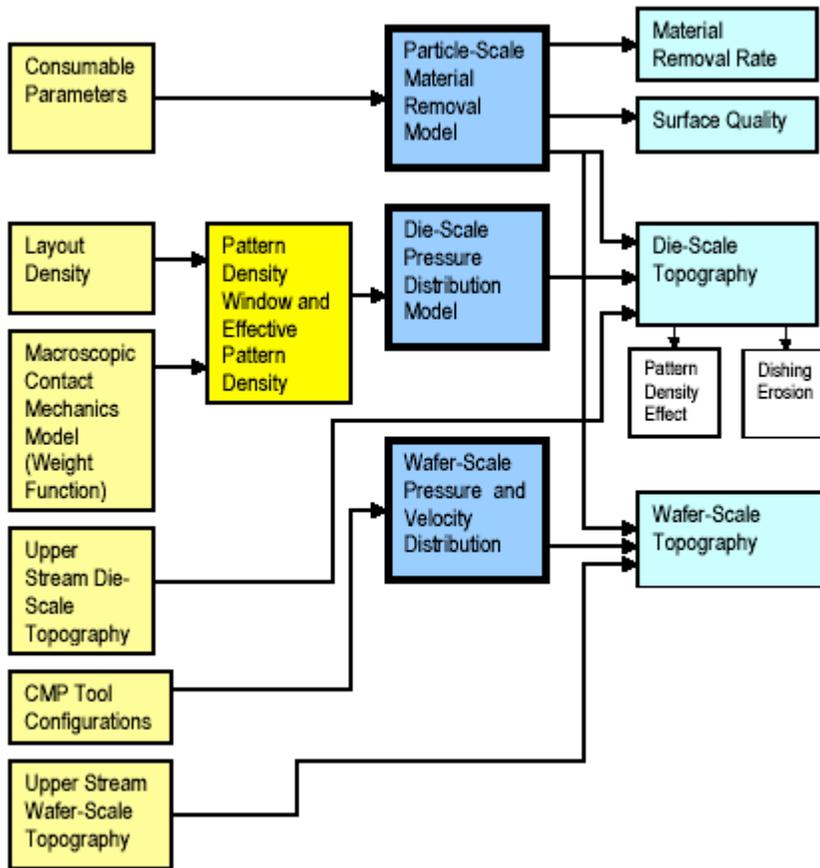
Figure 6. Framework of integrated CMP model.

There are still a number of problems to be solved. First, the particle-scale models, at the current stage, are only qualitative models. Calibration of the models under manufacturing environment has not yet been done. Obtaining many of the input parameters directly, say, the pad Young's modulus, abrasive size distribution, and so on, by experiment and their tabulation may be needed in the future. Currently, most particle-scale models are 'two-body' based. A 'three-body' removal model for CMP of low-k materials is needed. Second, the step height reduction model at the die-scale is based on solid mechanics. A viscoelastic model to calculate the weight function of effective pattern density may be needed for more accurate time-dependency prediction. With the application of low-k materials, a fluid mechanics-based model to understand the step height reduction is needed as well. Moreover, CMP of new materials for micro electromechanical system (MEMS) applications and its modeling are becoming interesting topics. These kinds of research will lead to a more predictable and reliable CMP process for the next generation of IC fabrication.

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