# Development of Device-Level Chemical-Mechanical Polishing Simulation Module Using Cellular Automata Method

Hsiu-Ming Yeh and Kuo-Shen Chen

Department of Mechanical Engineering, National Cheng-Kung University, Tainan, Taiwan, 70101

### ABSTRACT

This work briefly presents the basic theory, the development, and a primary demonstration of a devicelevel chemical-Mechanical Polishing (CMP) CAD module. By integrating the phenomenological material removing relation such as Preston's equation, contact mechanics, finite element analysis, with a cellular automata environment, this CMP CAD aims to predict the rounding, dishing, and erosion effects commonly observed in modern copper CMP processes. Primary results indicate that this CAD can essentially catch the characteristics of polishing processes. Further modification of this CAD would enhance its accuracy for industrial applications.

*Keywords*: CMP, CAD, Contact Mechanics, Cellular Automata (CA).

### **1 INTRODUCTION**

Chemical mechanical polishing (CMP) process is a key fabrication route in states of the art IC fabrication processes. The predictions of both global and local uniformity and removing rate are critical for fabrication yield and device performance. In particular, the dishing and erosion for a copper process are particular important for the reliability of interconnections. Previously, Fu and Chandra proposed a model to predict the dishing of copper during a CMP process based on simple solid mechanics [1]. By that model, the extent of observed dishing and the model prediction were qualitatively correlated. However, this proposed model failed to count various practical effects such as structural aspect ratio, viscoelasticity, and geometrical imperfections, where those effects can only be obtained via numerical computation such as finite element (FE) method. However, since the topology of the device is constantly changing during the entire CMP process and FE simulations cannot emulate the material removal phenomenon during CMP without extensive re-meshing process, a cellular-automata (CA) based process emulator is therefore proposed to perform a more accurate evaluation for real interconnection parameter and process design.

#### 2 CELLULAR AUTOMATA (CA)

CA method bases on a defined transition rule to change the state of a specific cell [2]. By splitting the entire structure into numerous cells and using the contact stress level as the transition indicator, one can determine the existence or vanishing of a particular cell during CMP process. In this work, the curvature of a cell can be determined by the topology of itself and its neighborhood cells. The resulted curvature can further yield the contact stress and consequently, the material removing rate (*MRR*). The obtained MRR would effectively change the topology of the cell. This process would then start over again to simulate the entire polishing period. The entire procedure forms an auto-generation and auto-iteration process for modeling the polishing process.

#### **3 FRAMEWORK**

The device-level CMP simulation module would integrate with process parameters, polishing rule, material information and micromechanics. The schematic plot of the work is shown in Figure 1. The material removing rate (MRR) is determined by Preston's equation [3], i.e.,

$$MRR = KP_0 V \tag{1}$$

where  $P_0$  is the contact stress, V the sliding velocity, and K the Preston's constant, respectively. The determination of these parameters relies on simulations from mechanics and specific experimental data [4]. The average contact stress, q, can be determined by the applied loading and the local curvatures. I.e.,

$$q = \left(\frac{4E^*}{3\pi}\right)\frac{a}{R} \tag{2}$$

where  $E^*$  is the reduced modulus of the contact pair, *a* the effective contact radius, and *R* the local radius of curvature, which can be determined by the height of the specific cell and its neighborhood cells. As stated above, CA algorithm is then used to determine the state of the structure cells based on MRR. Figure 2a indicates the schematic plot of the typical microstructure of a copper interconnection just after electroplating. For simplicity, the periodic structure can be reduced to a single zone with periodic boundary condition. This serves as the basic simulation domain of this work. On the other hand, the stress information of that structure is obtained via a database, which has been built by extensive finite element analyses. The corresponding CA representation is shown in Figure 2b.



Figure 1: The framework of the device-level CMP CAD.



Figure 2: (a) schematic plot of the interconnect structure right after electroplating and (b) its CA representation.

### 4 DEVICE-LEVEL CONTACT STRESS

As mentioned in Section III, a contact stress database must be pre-built for executing the CA process. The polishing process, schematically shown in Figure 3, can be categorized into three stages, i.e., polishing of the upper feature copper only (stage I), polishing both of the upper and the lower features of copper (stage II), and polishing of the dielectric and copper (i.e., stage III). During the polishing, the squeezed polishing pad may contact the lower feature and cause the erosion of the desired pattern and this would cause dishing eventually. In order to obtain the stress and deformation information for subsequent analysis, Hertz contact analyses with extensive finite element simulations were performed to obtain a database for subsequent CA computation. A finite element model family was constructed and a typical deformed stress contour is shown in Figure 4. It can be seen that the stress distribution varies significantly along the contact surface with the maximum stress occurs around the corners. By varving the fillet radius and aspect ratio of the structure, the stress concentration factor also varies. Figure 5 shows a typical stress distribution for the upper copper feature. By regression analysis, the stress distribution along the upper surface with an applied pressure p can be expressed as

$$\frac{q(x)}{p} = c_1 \cdot \exp\left(\frac{c_2}{x + c_3}\right) \tag{3}$$

where  $c_1$ ,  $c_2$ ,  $c_3$  are fitted parameters related to the fillet radius *x*. Around the edge, the stress distribution is modeled by Hertz contact stress as

$$\frac{q(x)}{p} = p_{\max} \left[ 1 - \left(\frac{x}{A}\right)^2 \right]^{1/2}$$
(4)

where  $p_{\text{max}}$  is the maximum pressure on the feature, and *A* the contact area. By Eqs.(3) and (4), it is possible to update the stress information by using Eqs.(2), (3), and (4). The obtained stress then feed into Eq.(1) to determine MRR of each cell. For each step, after removing materials, the status of cells changes and the entire process would start over again.



Figure 3: Three stages of the device-level CMP process.



Figure 4: A typical contact stress contour of Cu/pad.



Figure 5: Contact stress distribution on upper-feature area.

## 5 CONSTRUCTION OF THE DEVICE-LEVEL CMP SIMULATION MODULE

Since the topology of the device is constantly changing during the entire CMP process, the pattern and pad have different contact interface. At a given step, the distribution of contact stress must be re-calculated. In this work, the device-level CMP simulation module is constructed by the database built from the above analysis of contact stress and Preston's equation. The definitions of the fundamental parameters are schematically shown in Figure 6, where *L* is the characteristic size, *w* the line width of copper,  $\lambda_w$  the line width of copper after electroplating,  $h_1$  the trench depth of copper, and  $h_2$  the trench depth of dielectric, respectively. The pattern density (*PD*) is defined as

$$PD = \frac{contact\ area}{total\ area} = \frac{\lambda_w}{L} \tag{5}$$

The device-level CMP process simulation module is programming by MATLAB. The overall flow chart of the simulation is shown in Figure 7. At first, the program judges whether the lower feature is contacted or not. If the deformation of polishing pad does not exceed the trench depth, the deformation can be categorized into stage I. On the contrary, if the deformation of polishing pad is over the trench depth, the polishing process would polish the upper and the lower feature of copper both. By the built-in database based on contact stress as well as other input parameters, the MRR of each location can be determined and the overall topology is therefore changed. This would alter the stress state, and therefore the distribution of MRR over the entire CMP processing period.

### 6 SIMULATION AND PARAMETRIC STUDIES

This section presents the essential demonstration and parametric studies using the emulator of constructed process. Figure 8 shows the distribution of contact stress with the loading=10KPa, *PD*=0.33, and trench depth=2nm.

In this study, the polishing pad contacts the lower feature area and the simulation results essentially agree with the FEM data.

Figure 9 indicates the influence of pattern density on the contact stress of the upper feature. In this study, trench depth is fixed as 2nm. It can be seen that essentially a larger PD yields a larger contact stress due to reduction in effective contact area. However, as PD is further increase, the contact of bottom feature actually take loads and the contact stress of upper feature gradually saturates. On the other hand, for the influence of trench depth, with a PD of 0.33, the simulation result is shown in Figure 10. It can be found that upper feature contact stress increases with trench depth since a large trench depth causes the polishing pad unable to contact with lower feature area. The tendency gradually becomes saturate, which indicates the contact occurs between pad and the lower feature.

A device-level CMP CAD demonstration is shown in Figure 11, which indicates a typical contact stress evolution (Figure 11a) during a 10 second polishing period and the corresponding topology variation (Figure 11b). It can be seen that the edges are gradually rounded off and the stress concentration become less significant during CMP. In the future, with more realistic process parameters included, the performance can be further improved and it should be very useful for engineering applications.



Figure 6: The definitions of necessary parameters.



Figure 7: The device-level CMP simulation flowchart.



Figure 8: Comparison between the FEM and simulation results for contact stress distribution.



Figure 9: The influence of pattern density on the upperfeature contact stress.



Figure 10: The influence of trench depth on the upperfeature contact stress.

### 7 CONCLUSION

The quality of CMP process is critical for modern IC fabrication and an efficient CAD system is highly demanded. This work briefly presents the basic theory, the development, and a primary demonstration of a device-level CMP CAD module. By integrating the

phenomenological material removing relation such as Preston's equation, contact stress analysis, finite element method, with a cellular automata environment, this CMP CAD aims to predict the rounding, dishing, and erosion effects commonly observed in modern copper CMP processes. Primary results indicate this CAD can essentially catch the characteristics of a typical polishing process. Further modification of this CAD would enhance its accuracy for industrial needs to improve the quality and reduce the cost.



Figure 11: A typical CA simulated CMP process. (a) contact stress evolution and (b) topology variation.

#### REFERENCES

- G. Fu and A. Chandra, "An Analytical Dishing and Step Height Reduction Model for Chemical Mechanical Planarization," *IEEE Trans. Semicond. Manuf.*, 16, 477, 2003.
- [2] T. J. Hubbard and E. K. Antonsson, "Cellular Automata in MEMS Design," *Sens. Mater. Conf.*, Tokyo, Japan, 7, 437, 1997.
- [3] F. W. Preston, "The Theory and Design of Plate Glass Polishing Machines," J. Soc. Glass Technol., 11, 214, 1927.
- [4] J-Y Lai, Mechanics, Mechanisms, and Modeling of The Chemical Mechanical Polishing Process, Ph.D. dissertation, Dept. Mech. Eng., MIT, USA, 2001.