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Fluid-Structure Interaction Modeling and Simulation of CMP Process for Semiconductor Manufacturing

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Abstract

Chemical mechanical planarization is one of the core processes in fabrication of semiconductors, which are increasingly used for information storage devices like solid state drives. For higher data capacity in storage devices, CMP process is required to show ultimate precision and accuracy. In this work, 2-dimensional finite element models were developed to investigate the effects of the slurry particle impact on microscratch generation and the phenomena generated at pad-particle-wafer contact interface. The results revealed that no plastic deformation and corresponding material removal could be generated by simple impact of slurry particles under real CMP conditions. From the results of finite element simulations, it could be concluded that the pad-particle mixture formed in CMP process would be one of major factors leading to microscratch generation.

Key Words : Chemical mechanical polishing, Contact stress, Finite element analysis, Fluid-structure interaction (FSI), Tribology

1. Introduction

Semiconductors are increasingly used for information storage devices, and the requirements of higher data capacity and more reliable systems have been making its fabrication processes more complicated and sophisticated. Chemical mechanical polishing or planarization (CMP), which is to planarize wafer surface using slurry with the combination of chemical and mechanical forces, is an essential process for semiconductor manufacturing[1,2]. As the size of semiconductors is required to be smaller, CMP becomes more important in the whole fabrication process, and accordingly more stringent control in the process parameters should be applied to achieve more accurate material removal.

Many research works have been reported for the mechanisms and the controlling factors to improve the CMP process and quality. However, there are still a lot of uncertainties and questions remained such as particle shape effect and predominance between chemical and mechanical actions. Especially, microscratch formation and within-wafer non-uniformity (WIWNU), which are must-kill factors in wafer, are one of the most important and critical issues in CMP[3-5]. However, no clear explanation or evidence in the mechanisms of their occurrences has been proposed.

Based on these backgrounds, in this study the effects of some process parameters in CMP were investigated using finite element (FE) simulations. The focus of FE simulations was on how microscratches can be generated during CMP process. The FE models in this study are very unique compared to other reported FE models including slurry fluid. In other words, fluid-structure interaction (FSI)[6] can be modeled and calculated, whose results thus can make it possible to get more accurate and practical analysis of CMP process.

2. Modeling and Simulation Details

Two-dimensional FE models are comprised of single nanoparticle, wafer, pad and slurry fluid, as shown in most of CMP systems. The wafer moves with constant speed and makes fluid flow in the slurry while the pad

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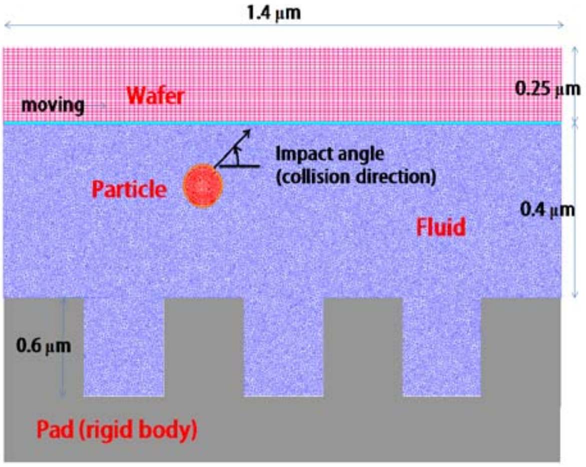
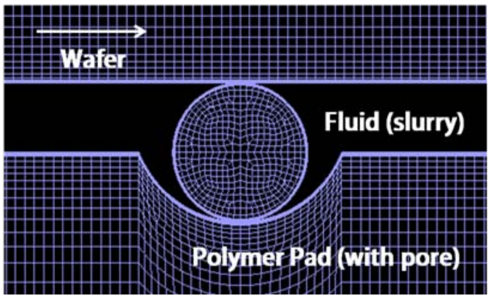


(a)



(b)

Fig. 1 2-D finite element model and configuration ; (a) a model for the observation of the effect of an abrasive particle impact on wafer surface, (b) a model for analyzing the situation of direct 3-body contact sliding

remains stationary. Unlike real CMP system, the FE model in this study considered single particle for simplification. As for the particle material, silica, ceria and alumina were selected, while Cu, Al, W, and Si_3N_4 were as applied for the wafer material. All of these materials were assumed to be isotropic and fully elastic-plastic materials in FE simulations.

FE simulations were performed using various system parameters such as the shape of particle (trapezoidal, rectangular, spherical, and hexagonal), size of particle, system pressure, and wafer moving speed.

In this study, two different situations that can take place in real CMP process were simulated. First, impacts of the particle on the wafer surface were simulated under the slurry flowing into the micrometer-scale pad-surface gap in order to observe the feasibility of the microscratch generation by nanoparticle impact. To simulate this behavior, a slurry fluid in fluidic channel of a few micrometers between the wafer and pad asperities was modeled, and an abrasive particle was

Table 1 Material properties of slurry fluid and simulation conditions

Fluid	▪ Viscosity : 0.0015~0.0045 Pa·sec (at 20 °C) ▪ Slightly compressive flow in micro-fluidic channel ▪ Density : 1.5 g/cm^3
Particle	▪ Shape : Sphere, Trapezoid, Square, Hexagon ▪ Diameter : 30~200 nm
Simulation Conditions	▪ Pressure : 0.04~4 MPa ▪ Wafer moving speed : 1 ~5 m/s ▪ Initial speed of particle : 100 m/s ▪ Impact angle : 15~90 deg. ▪ Temperature : 20 °C

Table 2 Material properties of the particle, wafer and pad used in this simulation study

Material		Young's modulus (GPa)	Poisson's ratio	Density (g/cm^3)
Wafer surface	Cu	135	0.33	8.95
	Al	70	0.35	2.7
	W	411	0.28	19.2
	Si_3N_4	200	0.23	2.4
Particle	SiO_2	70	0.2	2.0
	CeO_2	181	0.311	7.65
	Al_2O_3	380	0.26	4.0
Pad	Poly-urethane	2.29 (MPa)	0.49	0.748

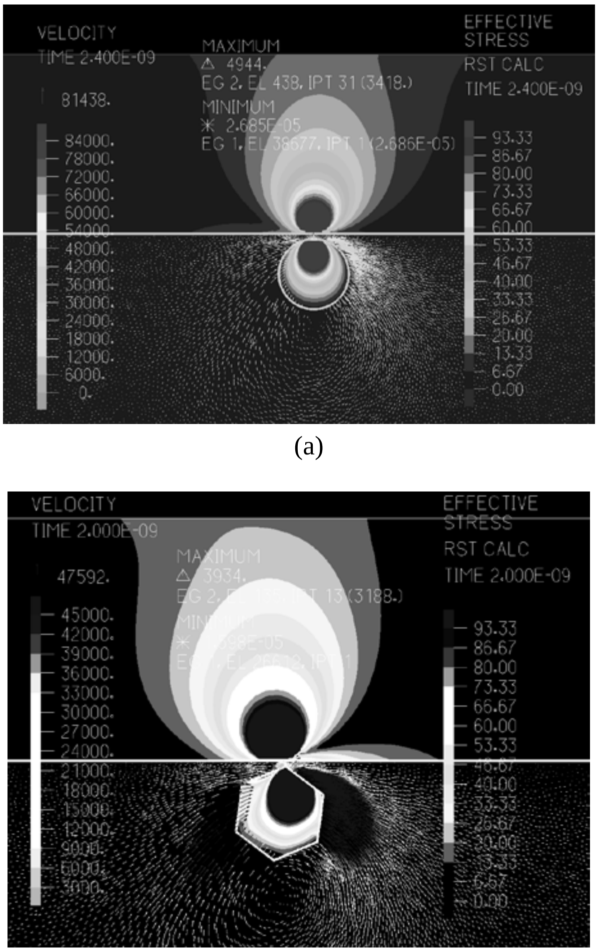
put in the slurry fluid (Fig.1a). Initial speed was given to the particle. The interfacial phenomena from the direct contact between the wafer/pad and particle or during their sliding contact was observed (Fig. 1b). Considering that commonly used polyurethane pad has many micro-pores on the surface, a particle is initially put inside a micro-pore of the pad in the FE model.

Table 1 gives the material properties of slurry fluid and simulation conditions used as the input values for FE analysis. The properties of the wafer, pad and particle materials were presented in Table 2. These properties could be obtained elsewhere [7,8]

3. Results and Discussion

3.1 Effect of the particle impact

Fig. 2 shows representative of the simulation results obtained using spherical and hexagonal shaped particles, respectively. In real CMP process, slurry nanoparticles show various and irregular shapes rather than perfect spherical shape. The direction and size of the arrows displayed in the slurry fluid indicate the direction and velocity magnitude of slurry flow, respectively. In Fig. 2, it was observed that the particle collision causes mechanical stresses on the wafer surface. The contact stresses generated by the collision with various shaped particles were summarized in Table 3. From Table 3, it could be found that the stresses are much larger than the yield strength of aluminum wafer surface (generally, 50~120 MPa ; if annealed, 30~40 MPa) and plastic deformation can be generated in all cases of the particles. However, it should be noted that such high contact stress could be achieved only if the particle had high initial speed like



(a)

(b)

Fig. 2 Representative simulation results. Snapshots from the simulation obtained using the particle with the shape of (a) sphere, and (b) hexagon (in the case of CeO_2 particle and Al wafer surface, 0.04 MPa pressure, wafer moving speed 1 m/s)

Table 3 Maximum normal and shear stresses on the wafer surface induced by the particle with various shapes (ceria particle, Al wafer surface)

Particle Shape	Contact Stress (GPa)	Shear Stress (GPa)
Trapezoid	7.7	4.1
Sphere	4.94	2.59
Hexagon	3.93	2.06
Square	1.7	0.95

hundred of m/s enabling high impact energy. Considering that the particle jet speed in abrasive jet machining reaches several km/s, the result is quite reasonable. In real CMP process, it is impossible for the particle to have such large initial speed since the flow of slurry fluid containing particles is induced by the moving wafer and pad. Therefore, it can be concluded that any surface damage or material removal during CMP process cannot occur by simple nanosized particle impact.

Furthermore, from the investigation of the effects of other process parameters, it could be found that the stress and corresponding material removal induced by the collision of particle may decrease under relatively high wafer moving speed due to the slurry flow resistance. In addition, the increase in slurry fluid viscosity causes the reduction of material removal rate, but it should be noted that the viscosity effect could vary with the shape of abrasive particle. The result of the simulation on the change in abrasive size revealed that the larger abrasive particle induced the larger contact stress due to force transferring through slurry fluid as the particle moved and pushed the fluid. This observation brought an important finding that the slurry fluid could make the workpiece surface soften in addition to its inherent chemical action, then it change the mechanical properties of the surface layer such as elastic modulus and yield strength.

3.2 First observation on pad-particle mixture and its effect

As the next step to find microscratch generation mechanisms, a direct pad-particle-wafer contact (3-body contact) was modeled as illustrated in Fig.1b.

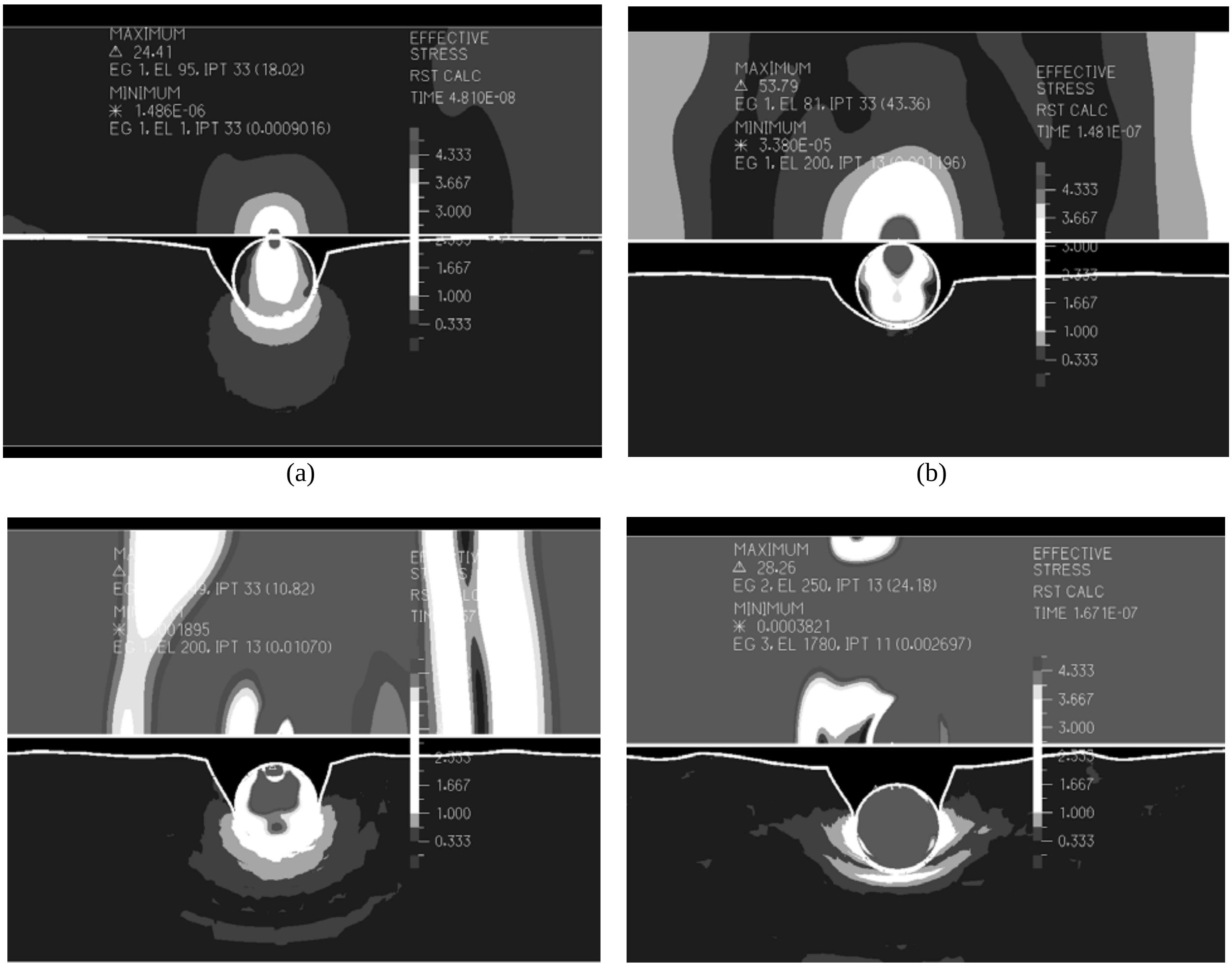


Fig. 3 Snapshots of the simulation results (silica particle, Si3N4 wafer, polyurethane pad) ; after (a) 481 time steps, (b) 1481 time steps, (c) 1571 time steps, and (d) 1671 time steps

Several snapshots of the particle-pad interaction according to time step evolution are presented in Fig. 3, which were obtained using silica particle, polyurethane (PU) pad, and Si3N4 wafer surface.

Examining the contact behavior in Fig. 3, it can be clearly seen that the abrasive particle interacts with both pad and wafer surfaces consequently moving up and down during CMP process. In the beginning, the particle on the pad pore starts to be pressed and moves toward the pad due to the pressure applied to the wafer. As the time step passes, the wafer becomes in contact with the pad and thereafter the particle rebounds from the pad and moves up due to the pad elasticity, as shown in Figs. 3a and 3b. Finally, the particle runs into and gets completely stuck in the pad as seen in Figs. 3c and 3d.

This is the first observation revealing that a pad-particle mixture could be newly formed during CMP process. In other words, the mechanical properties of the PU pad changes during CMP and the pad can be much harder than before. Therefore, this pad-particle mixture can be a major source to make microscratches on post-CMP surface. Moreover, as described above, the wafer surface can be soften by chemical action of the slurry. This may help the hard pad-particle mixture to induce microscratch on the wafer surface more easily. Recently a few experimental researches have suggested the feasibility of pad-particle mixture or particle-coated pad[9,10]. This simulation work is in good agreement with the experimental works. It is expected that if the simulations with multiple particles and another particle-pad material combinations are carried out as next step, the mechanism of microscratch generation will be revealed more clearly.

4. Conclusions

In order to investigate the mechanism of microscratch generation on the post-CMP wafer surface, finite element analysis considering fluid-structure interaction was carried out. 2-dimensional finite element models were developed to observe the effects of the slurry particle impact on microscratch generation and the phenomena generated at pad-particle-wafer contact interface. The results revealed that no plastic deformation and corresponding material removal could be generated by simple impact of slurry particle under real CMP situation. From the results of finite element simulations, it could be concluded that the pad-particle mixture formed in CMP process would be one of major factors leading to microscratch generation on post-CMP surface.

Acknowledgement

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