

Numerical simulation of Interfacial Failure between Copper and Porous Low-k Dielectrics

Shunsuke Miyagawa^a, Masaki Omiya^b

Department of Mechanical Engineering, Keio University, 3-14-1, Hiyoshi, Kohoku-ku, Yokohama,
Kanagawa, 223-8522, Japan

^ashunsuke-miyagawa@a8.keio.jp, ^boomiya@mech.keio.ac.jp

Keywords: interfacial failure, Young's modulus, shear modulus, dielectric constant, porosity

Abstract. Higher performance large scale integration (LSI) requires copper (Cu) instead of aluminum (Al) as a wiring metal because of its superior electrical conductivity. These LSI also requires lower dielectric constant to decrease line-to-line capacitance. Recently, porous low-k dielectrics are introduced for low-k dielectrics because of its ultra lower dielectric constant. However, their poor mechanical strength causes cohesive failure of low-k dielectrics or interfacial failure between Cu/low-k dielectrics during Chemical Mechanical Polishing (CMP) process. Especially, the damascene structure of the Cu interconnect can give rise to complex stress states and this causes a lot of issues during the fabrication process. Therefore, it is important to study interfacial adhesion for wide range of stress condition for Cu/low-k dielectrics. In this paper, we studied the mechanical strength and dielectric constant of porous low-k dielectrics and the interfacial strength between Cu and low-k dielectrics by finite element analyses. The effects of mechanical strength, porosity of porous low-k dielectrics on interfacial failure were discussed.

Introduction

Recently, wiring distances become narrow because of higher performance large scale integration (LSI). The narrow wiring distances induce a signal cross-talk and resistance-capacitance delay. Then, copper (Cu) wiring technology instead of aluminum (Al) wiring and low-k dielectrics are introduced. Especially, low-k dielectrics with a dielectric constant less than 2.1 are necessary for the 65nm technology nodes. Porous low-k dielectrics have lower dielectric constants. However, the mechanical strength becomes lower. Then, the cohesive failure of low-k dielectrics and the interfacial failure between Cu and porous low-k dielectrics can occur during Chemical Mechanical Polishing (CMP) or packaging processes. Especially, the damascene structure of the Cu interconnect can give rise to complex stress states and this causes a lot of issues during the fabrication process.

A lot of research institutions are studying about porous low-k dielectrics. The structure of porous low-k dielectrics can be measured by small-angle X-ray scattering [1]. The method to make pores in dielectrics was confirmed [2]. The influence of pore size and distribution to Young's modulus and dielectric constant is being investigated [3,4]. Shear stress distribution on the surface of the low-k dielectrics during CMP process was studied [5] and shear stresses concentrated at the boundary layer between hard mask and low-k dielectrics. However, it has not been clarified the interfacial failure between Cu/low-k dielectrics and the effect of porous structures on the interfacial failure. In this study, the interfacial failures between Cu/low-k dielectrics are simulated by finite element analyses with cohesive zone model. We also investigated the relationship between the mechanical strength and dielectric constant for the porous low-k dielectrics.

Numerical models

Elastic moduli and dielectric constant

We consider the dielectric material as silicon oxy carbide (SiOC) in this paper. The dielectrics are assumed to be isotropic and Young's modulus is 22.7GPa, Poisson ratio is 0.3, dielectric constant is 2.9 [6,7]. Figure 1 shows the numerical models for porous low-k dielectrics. We set the porosity of the models are 0~50%. The pore shapes were cylinder, sphere and 2D voronoi. At cylinder models and sphere models, the pore distributions shown in Fig. 1 were random, midmost, vertical that pores were lined lengthways and oblique that pores were lined asquint. The pore radii of the random structure were Weibull distribution. Weibull distribution function is

$$f(r) = \frac{m}{\eta} \left(\frac{r}{\eta}\right)^{m-1} \exp\left\{-\left(\frac{r}{\eta}\right)^m\right\} \quad (1)$$

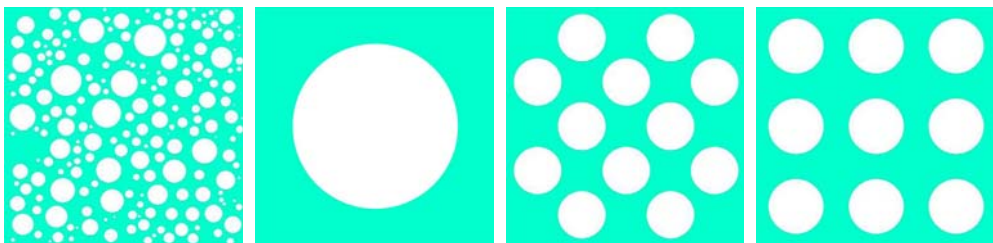
where r is the radius, m is the shape parameter and η is the scale parameter. The radii of the cylinder random structure models were Weibull distribution which was $m=2.47$ and $\eta=64.68$. The radii of the sphere random structure models were Weibull distribution which was $m=2.29$ and $\eta=60.52$ [8].

For boundary conditions, the top surface of the model was displaced to the vertical direction and the bottom surface of the model was fixed. Both side of the model was assumed as periodic boundaries. We got the normal stress on the top surface of the model after displacement and calculated Young's modulus. We also calculated the shear modulus of these models. For boundary conditions in this case, the top surface of the model was displaced to the horizontal direction and the bottom surface of the model was fixed. We got the shear stress on the top surface of the model after displacement and calculated shear modulus.

We also calculated the dielectric constants of those models. For boundary conditions, the top surface of the model was loaded 1V, and the bottom surface of the model was loaded -1V. The escape of the electric field to both side of the model was neglected because we assumed them as periodic boundaries. We got the electric charge on the top surface of the model after loading voltage and calculated dielectric constant. The dielectric constant is

$$\varepsilon = \frac{QS}{Vd} \quad (2)$$

where Q is the electric charge, V is the potential, S is the area of the model and d is the distance between the top surface and the bottom surface of the model.



(a) Random structure (b) Midmost structure (c) Vertical structure (d) Oblique structure

Fig. 1. The pore distributions of the porous low-k dielectrics models.

Interfacial failure

The models of the dielectrics for delamination analysis are shown in Fig.2. Figures 2 (a) and (b) show the models of the dielectrics for delamination analysis introducing porous structure in the left side of the low-k dielectrics and all of the low-k dielectrics, respectively. These pores are assumed to be cylindrical shape. These models are composed of Cu wiring, tantalum (Ta) barrier layer, silicon carbon nitride (SiCN) hard mask and SiOC low-k dielectrics. The target interface where the interfacial failure would occur is the interface between the hard mask and the low-k dielectrics. We introduce the interfacial cohesive zone models between these two layers. It is assumed that the energy release rate of this interface is 3.05 J/m^2 [9]. The Young's moduli and Poisson's ratios of the wiring and the dielectric materials are summarized in Table 1[5].

For the boundary conditions, the compression and shear forces are applied on the top surface of the model. The ratio of the pressure to the shear force was kept 0.1 or 0.2. The bottom surface of the model was perfectly fixed. The compression and shear forces increased gradually until the interfacial failure occur at the target interface.

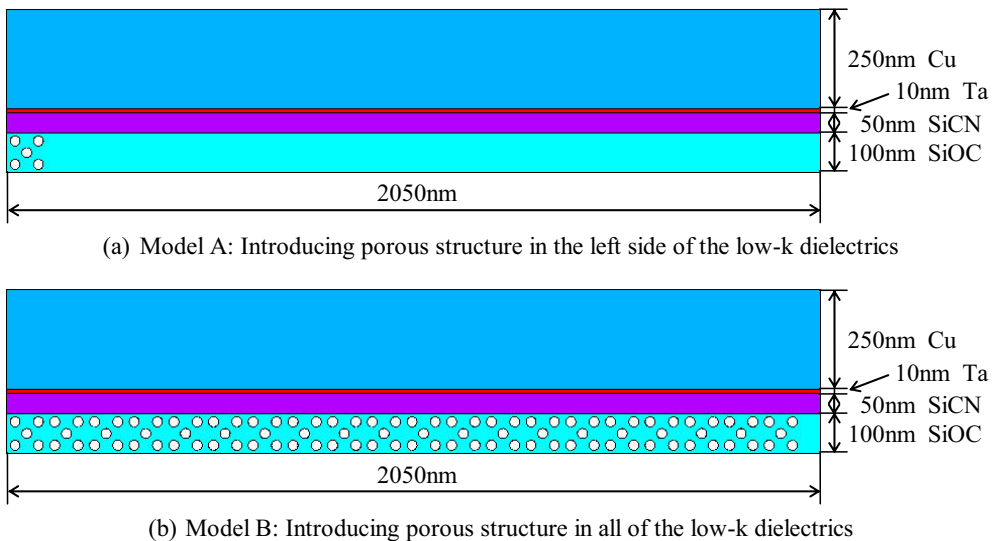


Fig. 2. The models of the dielectrics for delamination analysis.

Table 1. Elastic moduli of materials.

Layer	Material	Young's modulus [GPa]	Poisson's ratio
Wiring	Copper (Cu)	129.8	0.343
Barrier layer	Tantalum (Ta)	185.7	0.34
Hard Mask	Silicon carbon nitride (SiCN)	120	0.2
Low-k dielectrics	Silicon oxy carbide (SiOC)	22.7	0.3

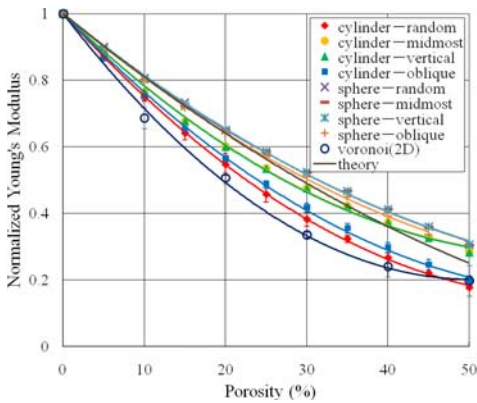


Fig. 3. Young's modulus of model as a function of porosity.

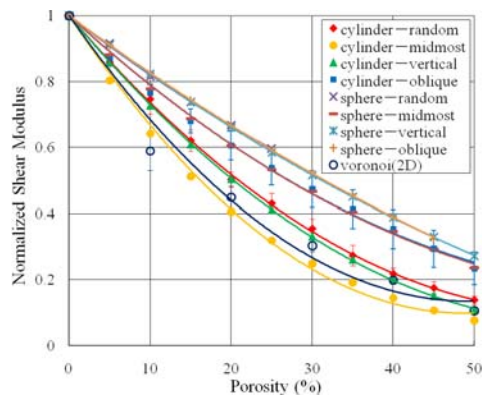


Fig. 4. Shear modulus of model as a function of porosity.

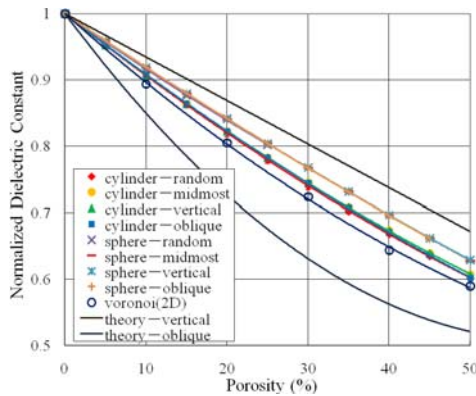


Fig. 5. Dielectric constant of model as a function of porosity.

Numerical Results

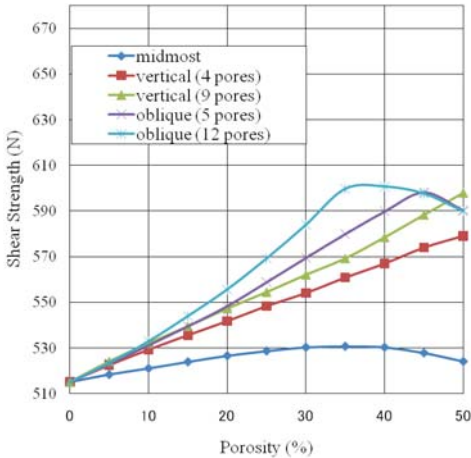
Elastic moduli and dielectric constant

Figure 3 shows the relationship between the porosity and Young's modulus of several porous structures. Young's modulus of spherical pore shape models is higher than the other models. At cylindrical pore shape models, Young's modulus of midmost structures and vertical structures is higher than that of random structures and oblique structures. At spherical pore shape models, Young's modulus of oblique structures is the lowest. Young's modulus of 2D voronoi models is smaller than the other models. It is concluded that the midmost structure and the vertical structure are strong against the loading to the vertical direction. The relationship between the porosity and shear modulus is shown in Fig.4. Shear modulus of spherical pore shape models is higher than the other models as the same as Young's modulus. At cylindrical pore shape models, shear modulus of oblique structures is the highest. At spherical pore shape models, there are no significant differences between them. Shear modulus of 2D voronoi models is smaller than the other models. It is concluded that the oblique structure is strong against the loading to the horizontal direction. The relationship between the porosity and dielectric constant is shown in Fig.5. The dielectric constant of cylindrical pore shape models is slightly larger

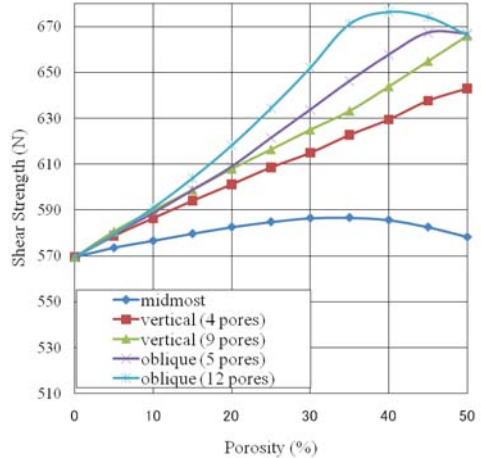
than the other models. It is concluded that pore distributions do not affect dielectric constants and the porosity is the important parameter for decreasing the dielectric constant.

Interfacial failure

Figure 6 represents the relationship between the porosity and the shear strength in model A. The shear strength is defined as the shear force at the initiation of the delamination between the hard mask and the low-k dielectrics. The shear strength of the oblique structures is the highest. Meanwhile, that of the midmost structures is the lowest. It is noted that the shear strength reaches the maximum value at 35%

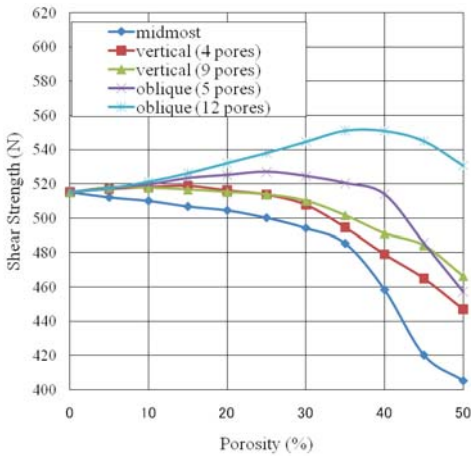


(a) the ratio of the compression force to the shear force is 0.1

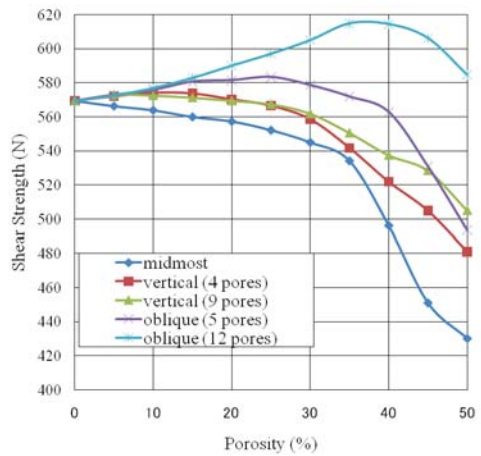


(b) the ratio of the compression force to the shear force is 0.2

Fig. 6. The relationship between the shear strength and the porosity in model A.



(a) the ratio of the compression force to the shear force is 0.1



(b) the ratio of the compression force to the shear force is 0.2

Fig. 7. The relationship between the shear strength and the porosity in model B.

porosity in the oblique (12 pores) structures and then the shear strength decreases. This indicated that it is possible to make the structure which has the high strength and low dielectric constant to control the porosity.

Figure 7 shows the relationship between the porosity and the shear strength in model B. The trend is quite different from Fig.6. The shear strength tends to decrease as the porosity increase. However, it is noted that the shear strength of the oblique structures increases at the low porosities and the shear strength has the maximum value around 35% porosity in the oblique (12 pores) structures. It is also indicated that it is possible to make the structure which has the high strength and low dielectric constant to control the porosity.

Conclusions

The influences of pore arrangement on mechanical strength and dielectric constant of porous low- k dielectrics were investigated. The sphere models have the highest Young's modulus and shear modulus. The vertical structures have a high stiffness to tensile load and the oblique structures have a high stiffness to shear load. The pores distributions do not affect the dielectric constant and only the porosity is the important parameter to reduce the dielectric constant. The shear strength of the oblique structures is the highest in the porous structures. Thus, introducing the oblique structure in low- k dielectrics can increase the interfacial strength.

References

- [1] H. Hermann, A. Elsner, M. Hecker, D. Stoyan: *Computer simulated dense-random packing models as approach to the structure of porous low- k dielectrics*, Microelectronic Engineering Vol. 81 (2005), p. 535-543.
- [2] Ei Yano, Yoshihiro Nakata, Iwao Sugiura: *Low- k Interlayer Dielectrics for 65 nm-Node LSIs*, FUJITSU Vol. 56, No. 4 (2005), p. 272-278.
- [3] Hidenori MIYOSHI, Hisanori MATSUO, Yoshiaki OKU, Hirofumi TANAKA, Kazuhiro YAMADA, Noboru MIKAMI, Syozo TAKADA, Nobuhiro HATA and Takamaro KIKKAWA: *Theoretical Analysis of Elastic Modulus and Dielectric Constant for Low- k Two-Dimensional Periodic Porous Silica Films*, Japanese Journal of Applied Physics Vol. 43, No. 2 (2004), p. 498-503.
- [4] Xia Xiao, Reinhard Streiter, Gang Ruan, Renru Song, Thomas Otto, Thomas Gessner: *Modelling and simulation for dielectric constant of aerogel*, Microelectronic Engineering Vol. 54 (2000), p. 295-301.
- [5] Masako KODERA, Yoshihiro MOCHIZUKI, Akira FUKUDA, Hirokuni HIYAMA, and Manabu TSUJIMURA: *Shear Stress Analyses in Chemical Mechanical Planarization with Cu/Porous Low- k Structure*, Japanese Journal of Applied Physics Vol. 46, No. 4B (2007), p. 1974-1980.
- [6] Haruo TSUCHIKAWA, Yoriko MIZUSHIMA, Tomoji NAKAMURA, Takashi SUZUKI and Hirochika NAKAJIMA: *Simple Modeling and Characterization of Stress Migration Phenomena in Cu Interconnects*, Japanese Journal of Applied Physics Vol. 45, No. 2A (2006), p. 714-719.
- [7] Ken-ichiro HIJIOKA, Fuminori ITO, Masayoshi TAGAMI, Hiroto OHTAKE, Yoshimichi HARADA, Tsuneo TAKEUCHI, Shinobu SAITO and Yoshihiro HAYASHI: *Mechanical Property Control of Low- k Dielectrics for Diminishing Chemical Mechanical Polishing (CMP)-Related Defects in Cu-Damascene Interconnects*, Japanese Journal of Applied Physics Vol. 43, No. 4B (2004), p. 1807-1812.

- [8] H. Shen, S. M. Oppenheimer, D. C. Dunand, L. C. Brinson: *Numerical Modeling of Pore Size and Distribution in Foamed Titanium*, Mechanics of Materials Vol. 38 (2006), p. 933-944
- [9] S. Maitrejean, F. Fusalba, M. Patz, V. Jousseume, T. Mourier: *Adhesion studies of thin films on Ultra Low K*, Interconnect Technology Conference, 2002. Proceedings of the IEEE 2002 International (2002).