Low-k BEOL Mechanical Modeling[*]

Xiao Hu Liu[#], Michael W. Lane, Thomas M. Shaw, Eric G. Liniger, Robert R. Rosenberg, and Daniel C. Edelstein
IBM TJ Watson Research Center, Yorktown Heights, NY 10598
[*] Invited Paper [#]xhliu@us.ibm.com

ABSTRACT

Low dielectric constant (low-k) is achieved often at the cost of degraded mechanical properties, making it difficult to integrate the dielectric in the back end of line (BEOL) and to package low-k chips. Development of low-k technology becomes costly and time-consuming. Therefore, more frequently than before, people resort to modeling to understand mechanical issues and avoid failures. In this paper we present three multilevel patterned film models to examine channel cracking in low-k BEOL. The effects of copper features, caps and multilevel interconnects are investigated and their implications to BEOL fabrication are discussed.

INTRODUCTION

Low-k materials have been aggressively pursued for the insulator to further reduce RC delay and cross talk in BEOL after copper replaced aluminum as the conductor. However it is very challenging to integrate low-k materials because their mechanical properties are severely compromised. Compared to oxide they generally have lower modulus and hardness, higher coefficient of thermal expansion (CTE), lower cohesive strength, and weaker adhesion. The properties usually get worse when pores are introduced to lower the k further. As a consequence, various mechanical failures, such as film cracking and delamination, may occur during BEOL integration, low-k chip packaging and reliability testing.

The driving force to advance a crack is the energy release rate (ERR). If it is above the cohesive strength of the ILD, the crack will grow. The cohesive strength of low-k materials, which depends on the chemistry and the environment, can be measured by carefully controlled experiments. The reader is referred to a recent review [1] and the references therein for the cohesive strength. Instead, this paper focuses on the driving force only.

The energy release rate can be calculated analytically for simple geometries, but numerical methods such as finite element have to be used for complicated structures. Generally the driving force calculated depends on the crack length. In the case of channel cracking the energy release rate increases with the crack length and levels off eventually. If the plateau value (steady-state energy release rate) is less than the cohesive strength, a defect of *any* size introduced during BEOL processing will not propagate. Therefore, in the worst case scenario, one only needs to consider a semi-infinite crack to calculate the energy release rate [2]. For given mechanical properties of a low-k material and copper/low-k integration process, we present channel cracking models to explore the dependence of the energy release rate on the interconnect structure and geometry.

Channel Cracking in Patterned Low-k Film

Channel cracking has been studied extensively because it may occur during film deposition, in particular, for low-k materials. For a blanket film on a substrate the energy release rate G increases with the film stress σ and thickness h as

$$G = Z \frac{\sigma^2 h}{\bar{E}}.$$

Here $\bar{E}$ is the film plane strain modulus, and Z depends on the modulus ratio between the film and the substrate [3]. A stiff film on a soft substrate has larger Z than a soft film on a stiff substrate. When a metal pattern is introduced in the film, the driving force for a channel crack in the overlayer can be enhanced by an order of magnitude [4, 5].
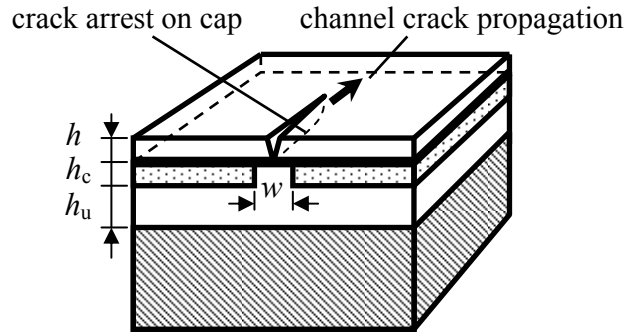

Figure 1. Structure of patterned copper and low-k underlayer below a blanket low-k film.

Figure 1 shows a patterned film structure of which the enhancement of the driving force for channel cracking was obtained by modeling and verified experimentally [5]. In a previous study we analyzed the effects of the gap spacing, as well as underlayer and overlayer thicknesses on the energy release rate [5]. In this paper we first explore how the cap and copper thickness affect the driving force, and then model two other structures for channel cracking.

Channel cracking in a blanket film

The base line geometries for Figure 1, $h_c = h_u = w = 1 \mu m$ and $h = 0.5 \mu m$, are the same as in [5]. The mechanical properties of the materials are listed in Table I. Upon cooling from $400^\circ C$ to room temperature the structure undergoes mechanical stressing due to the thermal expansion mismatch between the BEOL materials. The strain energy stored in the structure releases partially, driving the channel crack to propagate. The energy release rate is evaluated by

$$G = \frac{1}{2h} \int_0^h \sigma(y)\delta(y)\mathrm{d}y.$$

The stress $\sigma(y)$ ahead of the channel crack and the crack opening $\delta(y)$ behind can be obtained using a commercial finite element code.

Because copper has a larger thermal expansion coefficient and is much stiffer than the low-k material, it is expected that the energy release rate strongly depends on the copper features. Figure 2 shows the energy release rate (ERR) as a function of the gap spacing between the copper pads for three different copper thicknesses. The ERR G as normalized by G_0 (the ERR

for a low-k film of the same thickness on silicon) shows the driving force enhancement due to the copper pads and the low-k underlayer. As reported before, the ERR peaks at some gap spacing [4, 5]. Therefore in the BEOL design a range of gap spacings between large metal pads should be ruled out to keep the driving force below the cohesive strength of low-k materials. On the other hand, the peak ERR is lowered with decreasing metal thickness. Shrinking the thickness dimension should help to avoid low-k film cracking.

Table I. Thermal mechanical properties of the BEOL materials

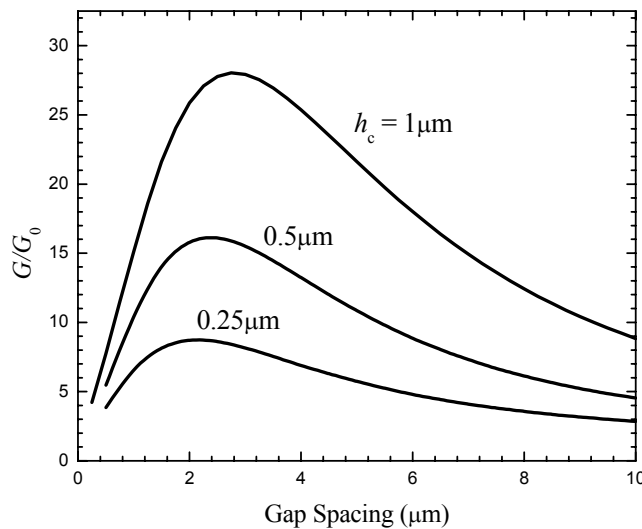| Material	Si	Cu	Nitride	Low-k Material
Modulus (GPa)	187.5	130	192	10
Poisson's ratio	0.28	0.34	0.3	0.3
CTE (ppm/^{o}C)	3	16.5	3	10

Figure 2. Energy release rate for the crack in Fig. 1 for various gap space and copper thickness.

In the model, a capping layer of 500A SiN is included between the metal and top low-k film. In Figure 1 the crack arrests at the cap and propagates only in the film plane. If the cap breaks, it will penetrate into the underlayer, relieving more strain energy stored there and adding more driving force for the in-plane crack propagation. To investigate the role of the cap we did parametric studies first by varying the thickness and then by changing the modulus. For each case the maximum ERR, G_{max}, was obtained by sweeping the gap spacing. The data points of G_{max}, when plotted against the cap stiffness (the modulus times the thickness) in Figure 2, falls on a "universal" curve for different caps. The normalized maximum ERR G_{max}/G decreases by about 40% when the cap stiffness increases from 2 kNm to 10 kNm. To reduce the driving force it is important to maintain stiffness by either adopting a high modulus cap or thickening the cap. Our modeling indicates that the intrinsic stress of the cap has little effect on the ERR. However, upon cooling from low-k film deposition temperature, a tensile stress is superimposed on the cap from the thermal mismatch between the metal and dielectric. Therefore a compressive cap with

sufficient cohesive strength should be selected to prevent the crack from propagating into the cap and lower layers.
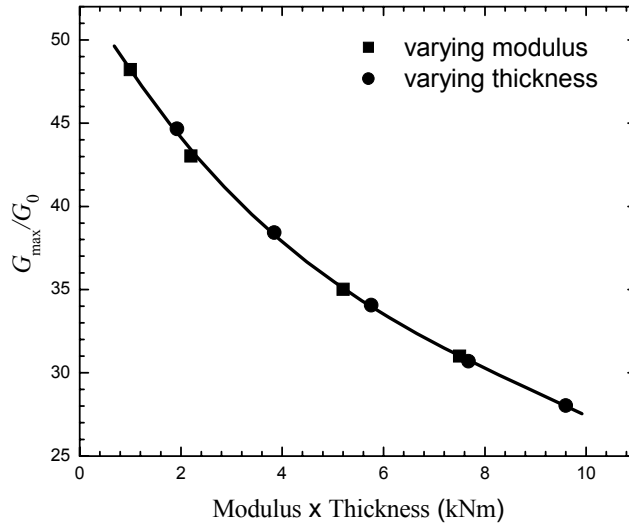

Figure 3. The maximum energy release rate decreases with the cap stiffness.

To explore further the low-k BEOL structural dependence of the driving force, we examine two variations of the model in Figure 1. The first one is to place the metal pads in the overlayer. The second considers multiple metal pads in the underlayers.
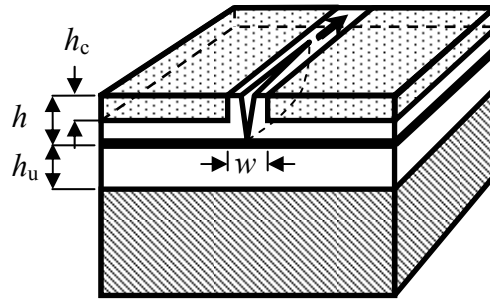
Channel cracking between two metal pads

Figure 4. Channel crack in a low-k patterned film with capped low-k under layer.

The structure in Figure 4 is used to investigate cracking propensity due to a copper pattern before the next blanket overlayer is deposited. A 500A nitride below limits the channel crack height to h. The base line dimensions are as before except that the layer thickness fixed at $h = 0.5 \mu m$ includes both the metal and the dielectric. The channel crack is again assumed to be at the center and the stress in the structure is applied by decreasing the temperature.

Figure 5 shows the energy release rate versus the gap spacing between the pads. In contrast to Figure 2 it has *no* peak at a given gap spacing. The driving force decreases monotonically when the gap spacing increases from zero. The limiting case of zero gap spacing corresponds to *one* blanket metal film on dielectric. The driving force is increased due to the elastic and CTE

mismatch between copper and the low-k dielectric [3]. In Figure 5 the ERR curves shift downward by as the metal thickness is reduced. Therefore, shrinking the metal thickness is beneficial to avoid cracking.
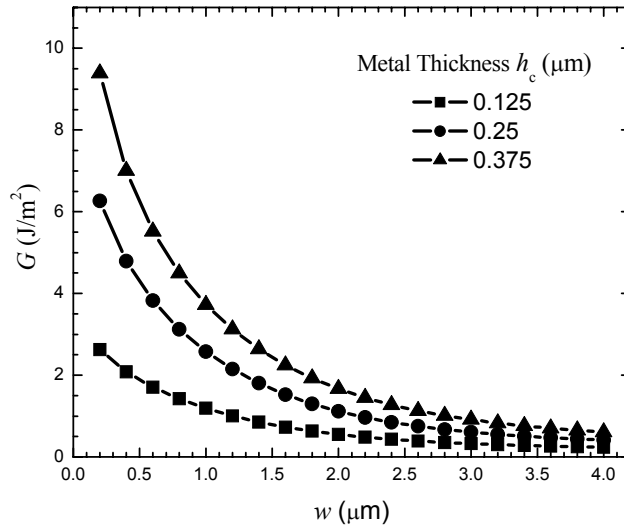

Figure 5. The driving energy for channel cracking as a function of spacing between metal pads at three different metal thicknesses.

Chemical mechanical polishing (CMP) is an indispensable processing step to fabricate damascene copper BEOL. Low-k materials, when integrated with copper, may have difficulty surviving CMP because they are so fragile. The industry has been developing low down-force CMP such as electro-CMP [6]. However, the down force is not the only concern. From our model here the stress in copper is also a possible source which may cause cracking.

Effects of metal stacks

Figure 6 shows another structure analyzed to study the effects of metal on the driving force for channel cracking. Compared to that in Figure 1, more metal pads (total number of N) have been inserted in the underlayer to simulate a multi-level BEOL structure. To simplify our analysis all the pads are assumed to have the same thickness ($h_c = 0.25 \mu m$) and the same inter-level spacing ($h_d = 0.25 \mu m$). The overlayer thickness is fixed at $h = 0.5 \mu m$. The metal pads are perfectly stacked and separated by the same gap spacing w.

First we compare the two structures in Figure 1 and 6 at the same total film thickness. Figure 7 shows one curve of energy release rate for $N = 3$ metal levels and the other one for the structure in Figure 1 calculated with $h_u = 1.25 \mu m$, $h_c = 0.5 \mu m$, and $h = 0.5 \mu m$. It is noted that they both attain a maximum at some gap spacing. However the maximum value is larger and occurs at larger gap spacing when there are stacks of copper pads. Adding two levels of metal pads raises the maximum ERR by about 60%.

Varying the total number of metal levels N one can examine the increase in driving energy imparted to the top low-k film. For a fixed N the maximum ERR was found with respect to gap spacing and then plotted against N in Figure 8. The maximum driving force increases significantly with the number of metal levels. Eventually it may overcome the cohesive strength

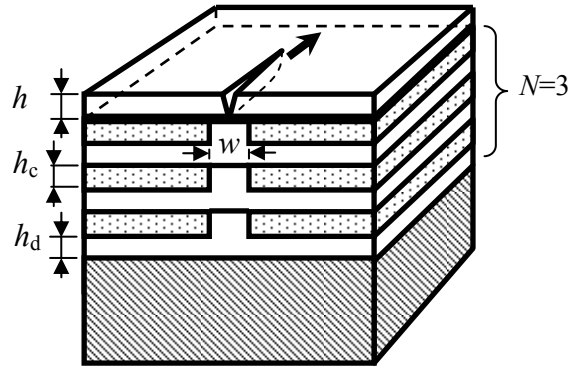of low-k dielectric, dictating a maximum number of BEOL levels on which a low-k film may be deposited.

Figure 6. Multiple level metal stack structure with a channel crack in low-k overlayer.
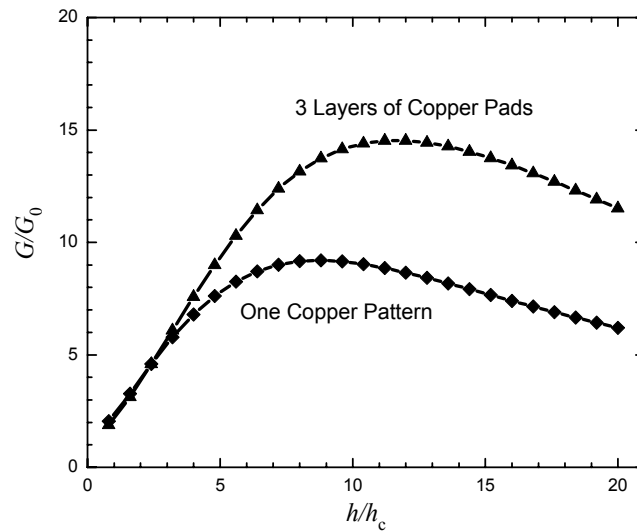

Figure 7. The driving energy for channel cracking for the structure in Figure 1 (lower curve) and Figure 6 (upper curve).

For a blanket under layer (no metal pads in Figure 6) the driving force for a channel crack in the overlayer is proportional to the square root of the under layer thickness [7, 8]. Extended to the stacked pad structure in Figure 6 the maximum energy release rate as a function of total number of metal levels is expected to be

$$G_{max} / G_0 = \xi + \eta \sqrt{N} .$$

A fit to the data with $\xi = -4.6$ and $\eta = 10.8$ is given in Figure 8 by the shear lag model. It agrees well with the finite element model; even at a large number of levels it underestimates the driving force only by about 7%. The square root dependence is a good yardstick to extend the result of the maximum driving force from two levels to many levels of metal pads.
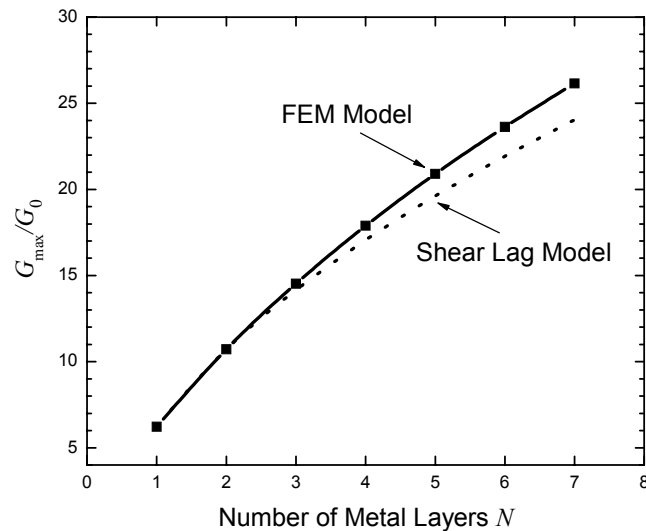
Figure 8. The maximum energy release rate for channel crack in overlayer increases as more levels of metal pads are built below.

CONCLUSIONS

Low-k dielectric films are susceptible to cracking because of poor mechanical properties. When integrated with copper it is more susceptible to cracking because of enhancement due to mechanical property mismatch. Models presented here have shown that the energy release rate is increased by an order of magnitude over that for a blanket low-k film on a silicon substrate. The data show a strong structural dependence of energy release rate on the copper features. An evaluation of a blanket low-k film on a silicon substrate is not enough; one has to examine its integration with copper to avoid cracking problems during BEOL fabrication from film deposition to CMP. Modeling is useful to highlight possible mechanical problems during copper/low-k BEOL integration.

REFERENCES

1. M. W. Lane, X. H. Liu and T.M. Shaw, *IEEE Trans. Dev. Mat. Reliability*, **4**, 142 (2004).
2. X. H. Liu, Z. Suo, Q. Ma and H. Fujimoto, *Eng. Fract. Mech.*, **66**, 387 (2000).
3. J. W. Hutchinson and Z. Suo, "Mixed Mode Cracking in Layered Materials" in *Advances in Applied Mechanics*, ed. J. W. Hutchinson and T. Y. Yu (Academic, 1991) pp. 63-191.
4. J. M. Ambrico, E. E. Jones, M. R. Begley, *Int. J. Solids Struct.* **39**, 1443 (2002).
5. X. H. Liu *et al*, *Proc. of Int. Interconnect Tech. Conf.*, pp. 93-95 (2004).
6. L. Economikos *et al*, *Proc. of Int. Interconnect Tech. Conf.*, pp. 233-235 (2004).
7. Z. C. Xia and J. W. Hutchinson, *J. Mech. Phys. Solids*, **48**, 1107 (2000)
8. Z. Suo, "Reliability of interconnect structures" in *Vol. 8: Interfacial and Nanoscale Failure* in *Comprehensive Structural Integrity* ed. W. Gerberich and W. Yang (Elsevier, 2003) pp. 265-324.