Development of Cu/insulation layer interface crack extension simulation with single crystal plasticity

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1. Introduction

Recently, LSI (Large Scale Integration circuit) is miniaturized to improve processing speed and performance. However, unexpected interfacial cracks extend in fabricating process and in use, because there are weak interfaces between Cu and SiN layers in LSI. However, local interfacial adhesion energy cannot be quantitatively evaluated because structures of LSI have sub-micron dimensions.

Micron-scale evaluation technique was developed where small blocks of the insulation layer material on Cu conductive layer were used as specimens, and crack extension was simulated by finite element method to evaluate Cu/SiN interfacial adhesion energy [1, 2]. Then, by using elastic-plastic finite element model, interface adhesion energy G not including plastic dissipation energy of Cu layer was evaluated, and the obtained values is almost constant which is independent of specimen size [3]. However, if specimen size become down to nano meter order, it is considered that local interfacial fracture toughness on micro Cu line is strongly affected by crystal anisotropy.

Then in this study, the impact of crystal plasticity on interfacial fracture toughness was investigated by simulating crack extension with three dimensional elastic-plastic finite element model.

2. Experimental procedure

In this study, interfacial fracture toughness was evaluated by using experimental results that have been obtained in a recent study [3]. Fig. 1(a) shows a photograph of experimental system which enables fracture test under in-situ observation with a sub-micron scale resolution. This testing machine as shown Fig. 1(b) is composed of a nano-indenter and a Focus Ion Beam (FIB) gun in Scanning Electron Microscope (SEM). In this testing machine, specimen preparation by FIB and testing by nano-indenter with 0.2 μ m tip radius can be carried out under in-situ observation.

The test structure is schematically shown in Fig. 2(a). The weakest interface in this structure is between the upper Cu line and the SiN cap layer. For evaluating local Cu/SiN interfacial strength, the specimen was fabricated by cutting a square section pillars out of the upper SiO₂ layer and removing the surrounding part of the layer. Fig. 2(b) shows a specimen whose size is $1 \times 1 \mu m$. With this specimen, crack propagates along the Cu/SiN interface and it enables to evaluate the adhesion strength of this interface.

3. Finite element model with crystal plasticity

In this paper, elastic-plastic analysis was conducted to evaluate interfacial fracture toughness G by using three dimensional finite element method. Figure 3 shows FEM model which was created by using commercial FEM code ABAQUS 6.10-2. The smallest mesh size of this model is 0.05µm. A user subroutine was used to incorporate Cu single crystal plasticity [4]. Material properties of the other material are shown in Table 1, whose values were obtained by indentation tests [5] and literatures [6].



Fig. 1 (a)The configuration of FIB-SEM and (b)testing system inside of SEM chamber.



Fig. 2 (a)The cross sectional view of with damascene Cu line and (b) Specimen fabricated by FIB.



Fig. 3 Three-dimensional FE model for crack extension simulation.

To simulate crack extension, bonding at the couple of nodes of the interfacial crack tip on the central axis of the model was removed in loading. Interface fracture toughness G was evaluated by using total energy method.

3. Crystal orientation and interface fracture toughness

Slip system of Cu crystal is shown in Figure 4. There are 12 slip systems of Cu crystal, because Cu crystal is Face Center Cubic (FCC) which has 4 slip plane and 3 slip direction in each slip plane. In this paper, energy release rate *G* was evaluate for three different Cu crystal orientations (100), (110), and (111) facing to the Cu/SiN interface, and angle between load direction and one of slip direction in interface, θ [degree], are 0 ° and 90 °, respectively.

Table 2 shows the obtained G values. For (100), crystal orientation of θ =0 ° and 90 ° were same because there are two slip directions in interface and these are orthogonal, Gvalue was 2.02 J/m². For (110), G values were 1.8 J/m² and 2.1 J/m². For (111), G values were 0.06 J/m² and 0.22 J/m². Comparing the G values of (111) surface to the G value of the other surfaces, G value of (111) surface is very smaller than the other surfaces. In the case of (111) surface, the slip of Cu crystal is likely to occur because the slip plane is parallel to the interface. Then, it is considered that G value becomes small because plastic dissipation energy becomes large due to Cu crystal slip. In Experiment, there were the cases that large plastic deformation of Cu interface occurred [7]. Then, this simulation can reproduce experimental result by considering the effect of Cu crystal orientation. For the (110) surface, G value of θ =90 ° is bigger than the value of $\theta = 0^{\circ}$

Figure 5 shows plastic zone near crack tip in the case of (111) surface. Comparing the plastic zone of Figure 5 (a) ($\theta = 0^{\circ}$) to Figure 5 (b) ($\theta = 90^{\circ}$), it is indicated that plastic zone of Cu layer near interface spreads easily in the slip direction. Then, in the same crystal orientation, it is considered that the interface fracture toughness depend on the angle θ .

4. Conclusions

Using a finite element model with crystal plasticity, the crystal orientation dependence of the interfacial strength was evaluated. For the finite element model, three different Cu crystal orientations such as (100), (110), and (111) facing to the interface were surveyed and also the effect of angle between load direction and slip direction θ was evaluated for the cases of 0 ° and 90 °. For the same crystal orientation, the energy release rate *G* obtained with $\theta = 90$ ° was higher than 0 ° because of the higher resistance against slip. However, *G* values for (111) were far smaller than the other cases. Consequently, it was considered that the *G* value depends mainly on how easily Cu crystal slips beneath the interface. It was demonstrated that the evaluated interface adhesion strength is dependent of the crystal orientation for the micro-scale Cu metallization systems in LSI.

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| Table 1 Material properties for finite element analysis. | | | | |
|--|--------------------------|------------------------|-----------------------|--|
| | Young's modulus (GPa) | Poisson's ratio (-) | Yield stress (GPa) | |
| Si ⁽⁶⁾ | 166 | 0.22 | - | |
| $SiO_2^{(5)}$ | 70 | 0.2 | 2.60 | |
| SiN ⁽⁶⁾ | 270 | 0.27 | - | |



Fig. 4 Set of slip system of Cu lattice.



Fig. 5 Plastic zone in the center cross section of FE model whose Cu crystal orientation of interface is (111). Radius between load direction and slip direction θ is 0 °(a) and 90 °(b).

| | 0 ° | 90 ° |
|-------|------------|-------------|
| (100) | 2.02 | — |
| (110) | 1.8 | 2.1 |
| (111) | 0.06 | 0.22 |