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Interfacial Failure Characterization of Electronic Packaging Component Using a Multiscale Modelling Approach

Zhen Cui[1,2,3], Yingying Zhang[1,2], Qun Yang[1,2], Guoqi Zhang[3], and Xianping Chen[1,2,3*]

[1]College of Optoelectronic Engineering, Chongqing University, Chongqing 400044, China.

[2]Key Laboratory of Optoelectronic Technology & Systems, Education Ministry of China, Chongqing University, Chongqing 400044, China

[3]Department of Microelectronics, Delft University of Technology, Delft, Netherlands.

[*]Corresponding authors: Xianping Chen (email: xianpingchen@cqu.edu.cn)

Abstract

Interfacial properties of Cu/SiO_2 in semiconductor devices has continued to be the subject of challenging study for many years because of its difficulties in experimentally quantifying the critical strength of interface. In this paper, a multi-scale modeling approach is built to characterize the interfacial properties between Cu and SiO_2. In this system, the Cu and SiO_2 are bonded together by three types of chemical bonds, Cu-OO, Cu-O, and Cu-Si, which cause three atomistic interfacial structures. For Cu-O and Cu-Si bonded interfaces, the fracture occurs exactly at the interface, however, the fracture for Cu-OO bonded interface occurs at copper layer near the interface, which indicate two different fracture criterions coexist in Cu/SiO_2 system. And, the calculated interfacial strength at macroscale is in agreement with available experimental results.

Introduction

In electronic packaging system, copper in particular, a common metal with high bulk thermal and electrical conductivities, and apparently low electromigration rate [1], is an excellent material for interconnects in integrated circuitry on silicon dioxide substrates. The interface strength and reliability between Cu and SiO_2 has been driving more and more attentions due to the brittle fracture often takes place at the Cu/SiO_2 interface [2] which is one of most easily damage part in electronics products. As we know, the interface is a complicate domain, where two separate materials are bonded together by chemical bonds with various bonding characteristics and adhesion strength. In the meantime, it is tremendous challenging for us to understand and predict the interfacial failure conditions due to the difficulties in experimentally quantifying the fracture energy of interfacial adhesion. And, the inner relationship between interfacial failure mechanisms at nano-level and interfacial strength at macro-level is still not clear for us, which seriously blocks the improvement of reliability for electronic devices.

In this paper, a multi-scale modeling approach was established to characterize the interface properties and simulate the Cu/SiO_2 interface failure under normal and shear loading.

Methodology

The proposed computational procedure of the multi-scale simulation is based on the following ansatz: (1) The micro-scale structure of interface at molecular level is obtained by first principles calculation with density functional theory. This method allows us to elucidate the effect of local chemistry on the binding nature between copper and silicon dioxide substrate. (2) The obtained interfacial microstructures at first step are used to run MD simulation, the simulation results can indicate many important interfacial mechanical properties, including the traction-separation constitutive relation. (3) The simulation results from the previous step was then applied into the macroscopic scale via the cohesive zone model in Finite Element Method (FEM), the interfacial damage at Cu/SiO_2 interface was then simulated when subjected to shear and normal loading.

On the top surface of SiO_2 substrate, the different oxygen density causes different substrate terminations, which results in three types of SiO_2 surfaces: OO-terminated, O-terminated, and Si-terminated surfaces, as shown in Fig.1. Thus, in first-principles calculations, the oxygen density at the top of SiO_2 slab is changed to mimic different substrate terminations, the SiO_2 slab consists of eight layers in the [001] direction with a 2×2 surface unit cell, and the Cu slab consists of four [001] layers $2\sqrt{2}\times2\sqrt{2}$ surface unit cell. The first principles calculations are carried out within the local density approximation (LDA) as implemented in the

plane-wave code Vienna ab initio Simulation Program (VASP), the ultrasoft pseudopotential is used for treatment of Cu and Si [3], and projector augmented wave potential is applied for O [4].

In MD simulations, a 4×4 supercell of the Cu/SiO_2 system is used to investigate the interfacial mechanical properties at molecular level, including the traction-separation constitutive relation. The top and bottom atoms of the system are fixed, then displacing the top fixed Cu layer along the z-direction at constant displacement of 0.1 Å until fracture occurs, as shown in Fig.2, further, the geometry optimization will be implemented after each step to get the minimized energy. The simulations are performed by using the commercial software Materials Studio®2017 [5]. All the simulations are calculated with the COMPASS forcefield, and 'Ewald' summation method is employed to calculate the electrostatic/van der Waals forces with a cutoff value of 9.5 Å.

In finite element simulation, first, a 3D Finite Element (FE) model in Abaqus was constructed to calculate the overall traction-separation constitutive relation of such multi-interactional interface, just as seen in Fig. 3. Since, we found that the Cu/SiO_2 interface actually is composed by three types of secondary interfaces, as it illustrated in Fig. 4, and approximate 15% and 16% area at the interface is bonded by Cu-O and Cu-Si bonds respectively [6]. Thus, the sample consists of four Cu-OO interface layer models, four Cu-O layer models, eight Cu-Si layer models and two rigid pads. Those interface layers are modeled by cohesive zone element [7]. After we obtain the overall interface traction-separation constitutive relation, the obtained results can be directly employed to simulate the interfacial delamination test of the Cu/SiO_2 system [8], as is illustrated in Fig.5. According to the geometric and loading configurations of this experiment test [7], the FE model is built, a columnar Cu dot of 50 nm height and 300 nm across on a SiO_2 substrate with a rigid-layer W of 50 nm, the material parameters are list in Table.1 and he 4-node axisymmetric elements, CAX4 and COHAX4, are used for the substructures and interfaces respectively.

Results and discussion

A. Atomistic interfacial structure

The atomistic structure of Cu-OO, Cu-O and Cu-Si bonded interfaces are shown in Fig.4. For Cu-OO bonded interface, the angle of O-Si-O is changed from 79° to110°, and the electrons carried by Cu atoms go from 0 to 0.03e, those large rearrangement would indicate bond formation between Cu and O atoms. The similar changes of atomistic structure and charges transition also can be found in Cu-O and Cu-Si bonded interface, but the magnitude of rearrangements at Cu-O and Cu-Si bonded interface are less than that at the Cu-OO bonded interface. Moreover, the relaxed bond length of Cu-O at Cu-OO and Cu-O bonded interfaces are ~1.962Å and ~1.963Å, respectively, and bond length of Si-Cu is ~2.269Å.

B. Fracture mechanisims

The MD simulation results show that there exist two different fracture mechanisms at Cu/SiO_2 system when subjected to tension loading. For the Cu-O and Cu-Si bonded interfaces, the fracture occurs exactly at interface, as shown in Fig.6 (b) (c), and their stress-displacement relations indicate that the fracture mechanism of Cu-O and Cu-Si bonded interfaces is the breaking of bonds between Cu and O/Si atoms at the interface. However, the fracture of Cu-OO bonded interface does not happen exactly at the interface but Cu layer near the interface, as illustrated in Fig. 6 (a), and the curve shows that the Cu layer goes through four stages: elastic deformation, yield stage, strengthening phase, and accelerated fracture stage. It is a typical stress-displacement curve for metallic materials, which indicates the fracture mechanism of Cu-OO bonded interface is the failure of copper material itself, because the bonding strength at the Cu-OO interface is stronger than that in copper material itself. Furthermore, the fracture energy of Cu-OO bonded interface is 1.32 J/m^2, which is much larger than the fracture energy of Cu-O and Cu-Si bonded interfaces, just seen in Table.2. Such differences indicate the interfacial oxygen density is very important factor influencing the strength of interfacial adhesion.

C. *Macroscopic interfacial strength*

The overall traction-separation constitutive relations are shown in Fig.7, and three important parameters of this relations are shown in Table.3, including the maximum traction N_{max}, the initial interface stiffness K_0 and fracture energy G. Then, the approximate parameters of stress-displacement relation are applied in the simulation of delamination test.

In FE simulation, it is observed that some of the cohesive elements have been removed at the lateral displacement of ~2.3 nm, which indicates that the onset of the interface damage, as shown in Fig. 8 (a). When the displacement increases to 3.2nm, the lateral loading deceases to zero, the Cu dot is totally separated from substrate. In this loading process, the maximum lateral force is ~30μN at lateral displacement of~2.8 nm, as shown in Fig. 8(b), which is in good consistent with the experimental result [8]. Furthermore, the FE model is used to calculate the normal interface strength of Cu/SiO_2 system, as shown in Fig. 9. The results show that the Cu dot is pulled out from the SiO_2 substrate under F=52μN. Thus, the interfacial strengths for Cu/SiO_2 are predicted as ~400Mpa and ~700Mpa in normal and shear directions, respectively.

Conclusion

A multiscale simulation approach is developed to characterize interface properties in Cu/SiO_2 component. The results show the interfacial oxygen density is very important factor influencing the strength of adhesion, the adhesion strength of oxygen-rich interface is larger than that of the low-oxygen density interface. Such interfacial properties cause two different fracture mechanisms in Cu/SiO_2 system. For Cu-O and Cu-Si bonded interface, the fracture happens exactly at the interface, however, the fracture for Cu-OO bonded interface occurs at copper layer near the interface, which, in turns, affects the overall structure of the Cu/SiO_2 system and, ultimately, its macroscopic property.

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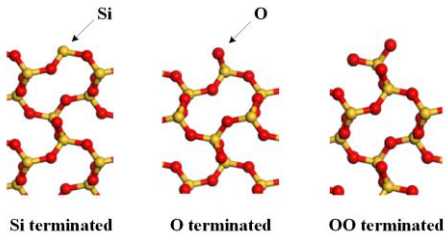

Fig. 1: Relaxed structures of the SiO_2 surfaces with different terminated atoms.

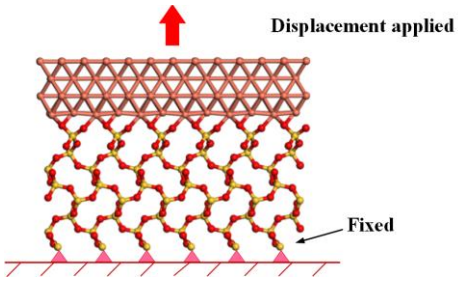

Fig. 2: Computational structure of the Cu-OO bonded

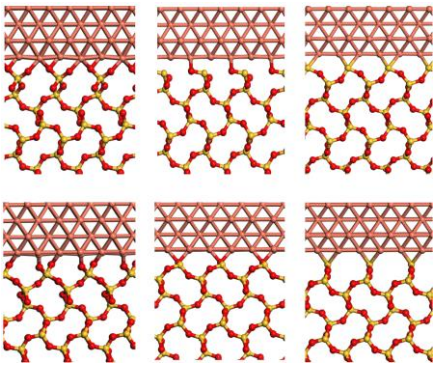

Fig. 4: The atomic structures of the Cu-OO, Cu-O, and Cu-Si bonded interface, respectively.

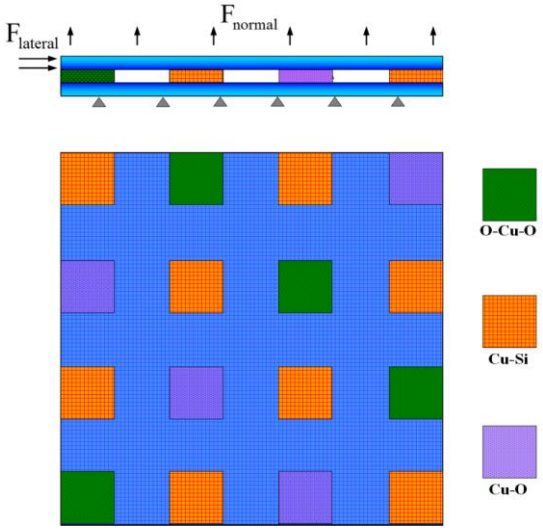

Fig. 3: The side and top view of multi-interactional interface structure, the lateral and normal loads are applied on the upper pad, respectively.

Table 1: Material parameters used in finite element simulation

	W	Cu	SiO_2
E	400Gpa	130Gpa	70Gpa
v	0.28	0.34	0.2

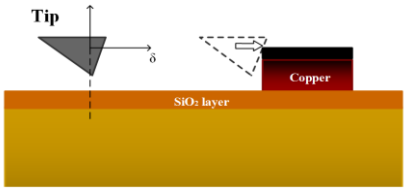

Fig. 5: Explanation of delamination test for Cu dot on SiO_2 substrate with lateral loading.

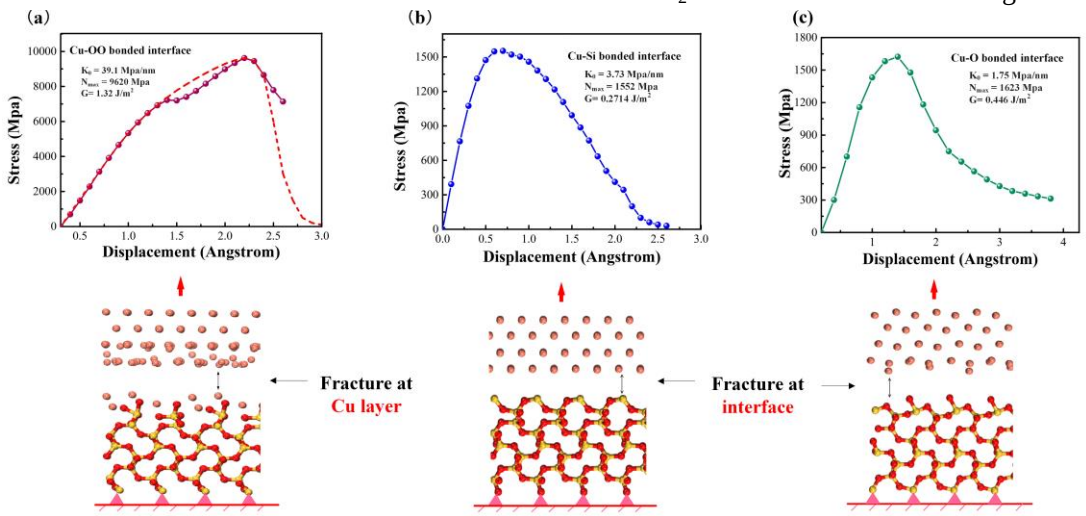

Fig. 6: The interface stress-displacement curves and atomic structure of interfaces under tension loading, (a) Cu-OO bonded interface, (b) Cu-Si bonded interface, (c) Cu-O bonded interface (the arrow represents the displacement applied on copper atoms).

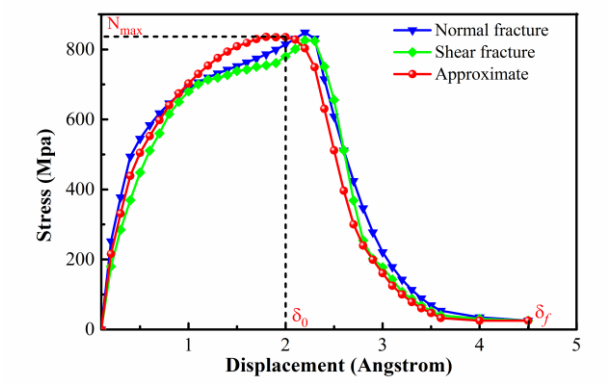

Fig. 7: The atomic structures of the Cu/SiO_2 interfaces, OO terminated, O-terminated, Si-terminated, respectively, with LDA simulations viewing along (a) [100] and (b) [001] directions.

Table 2: Calculated maximum traction (N_{max}), initial interface stiffness (K_0), and fracture energy (Gc)from MD simulation.

Type of interface	K_0 (10^3Mpa/nm)	N_{max} (Mpa)	G(J/m^2)
Cu/SiO_2:OO	39.1	9620	1.32
Cu/SiO_2:O	1.75	1623	0.446
Cu/SiO_2:Si	3.73	1552	0.271

Table 3: Calculated maximum traction (N_{max}), initial interface stiffness (K_0) and fracture energy (G_c) from FE simulation.

Type of fracture	K_0 (10^3Mpa/nm)	N_{max} (Mpa)	G (J/m^2)
Normal	24.16	835	0.243
Shear	19.0	810	0.212
Approximate	21.5	820	0.228

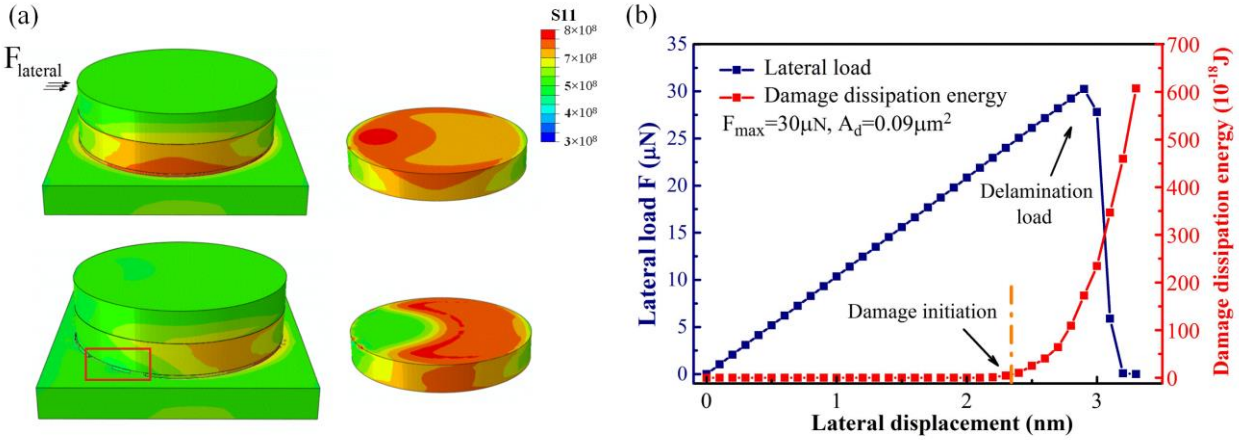

Fig. 8: (a) The stress contour of delamination test with lateral loading at the displacement of 1.5 nm/2.5nm, the right graph is the interface stress distribution of Cu dot; (b) the lateral load-displacement curve and the corresponding damage dissipation energy graph.

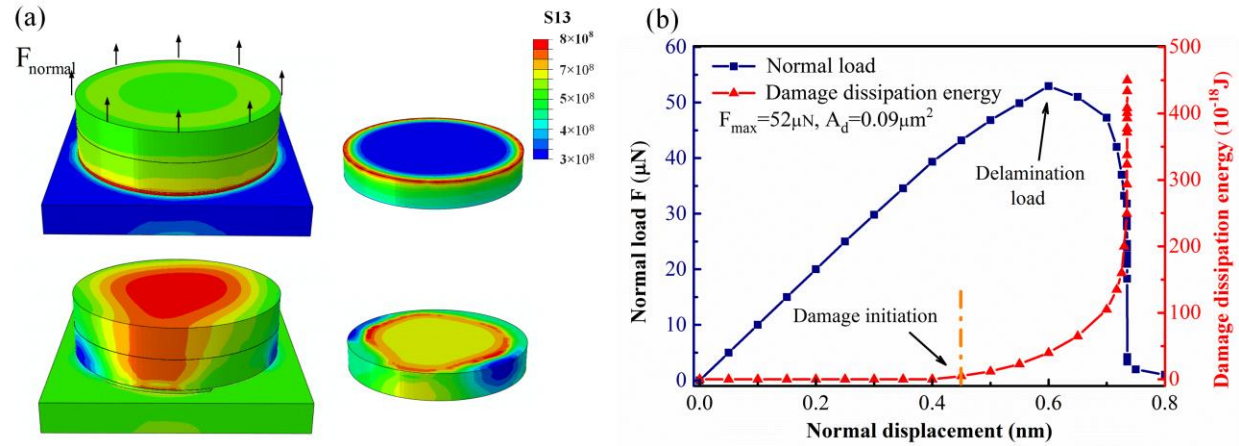

Fig. 9: (a) The stress contour of delamination test with normal loading at the displacement of 0.4 nm/ 0.7nm, the right graph is the interface stress distribution of Cu dot; (b) the normal load-displacement curve and the corresponding