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Characterization of interfacial delamination in multi-layered integrated circuit packaging

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ABSTRACT

It is challenging to understand and predict interfacial delamination in multi-layered integrated circuit (IC) packaging due to the difficulties in experimentally quantifying the critical fracture energy of interfacial adhesion. This study takes a combined approach based on molecular dynamics (MD) simulation and finite element method (FEM) to characterize the interfacial fracture energy and predict delamination in the Cu/Ti/SiO_2/Si multilayer systems. MD simulation is first conducted on each interface of the multiple layers at the atomistic level to obtain the material parameters such as the critical interfacial fracture energy that are required for the interfacial cohesive constitutive relation. Then, FEM is used to model and predict the interfacial delamination of the multi-layered system under indentation loading at the macroscale with the cohesive zone being considered around the delamination or crack tips. Finally, the indentation damage test is performed to validate the modeling results. The proposed combined modeling approach will have the potential to provide guidance in design and applications of IC packaging for improved stability and reliability.

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1. Introduction

In the recent years, the mechanical robustness and reliability of three-dimensional (3D) integrated circuit (IC) packaging has become tremendously challenging due to its continuous reduction in size and increase in vertical integration [1]. Thermal problems such as cracking in the oxide layers and interfacial delamination are increasingly dominant due to the presence of high heat density in the small system size. Furthermore, the mismatch in the coefficients of thermal expansion between dissimilar materials induces thermomechanical stresses, leading to problems such as thermal warpage and eventually resulting in interfacial delamination failure.

Interfacial delamination is initiated by the nucleation of a crack at the interface or near the interface, which will then propagate when the stresses are sufficiently high and result in a catastrophic failure of the IC packaging [2]. The interfacial fracture energy, also known as the practical work of adhesion, is an essential property for the performance and reliability of the 3D ICs as it determines the amount of energy needed for delamination to occur. This property accounts for the thermodynamic work of adhesion between the interface and the energy dissipated by the materials probably due to plastic deformation and other inelastic contributions [3]. Thus, interfacial delamination failure is not only dependent on the mechanical properties of the layers, such as adhesion strength, reactivity and surface roughness but also the chemical and bonding characteristics at the interface and the stress distribution generated by external loading during the assembly and operating processes. There, an accurate failure prediction of interfaces cannot be made unless these material properties are well-considered [4].

The characterization of such interfacial fracture energies between the interlayers is an important but yet inadequately resolved problem. This problem is further exacerbated in the 3D ICs whereby the increase in vertical integration and reduction in size have resulted in the introduction of new material layers and high density interconnection. Many works have employed conventional numerical and experimental approaches such as, linear elastic fracture mechanics (LEFM), finite element modeling (FEM), four-point bend test, blister test, scratch test, indentation test and laser spallation technique, to analyze and characterize the interfacial delamination failure [5–11]. LEFM calculates the critical stress intensity factors and energy release rates at the crack tip as singular and infinite, which is physically unrealistic. Furthermore, as plastic deformation at the interface occurs before fracture, LEFM alone is inadequate to characterize delamination failure.

On the other hand, FEM based on the cohesive zone modeling (CZM) uses the critical interfacial energies of different interlayers as the governing criterion for failure and is commonly used to solve fracture mechanics problems at the macroscale [12]. During thermomechanical loading, the interface behaves like a nonlinear material, undergoing damage initiation and delamination propagation which can be

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described by a nonlinear traction-separation law based on CZM. The material parameters required to be input into the traction-separation law are usually experimentally derived.

Experimentally, the scratch test measures the force and displacement of the scratch tip to generate an interfacial crack and spalling, while the indentation test can be used to either induce spontaneous buckling of the film or create indentation blisters to drive delamination. In the event of a crack in the material, such as thin-film or substrate cracking, the corresponding load-displacement (*P*-*d*) curves would indicate a reduction in the stiffness. Subsequently, this will cause a change in the area under the *P*-*d* curve which corresponds to the work done for creak initiation. Such discontinuities are usually dependent on the failure mechanisms which may vary for different test systems. However, there is no evidence whether interfacial cracking will give rise to any discontinuities to the *P*-*d* curve [13,14].

Furthermore, when the system size approaches the nanoscale, it becomes more challenging to determine the interfacial properties accurately. A comprehensive and accurate description of the fracture at the interface cannot be provided based solely on the experimental or numerical approaches. The lack of knowledge in understanding of interfacial fracture has impeded 3D ICs design and technological advancement. Therefore, more viable methodologies are required to fully characterize the interfaces and predict interfacial delamination, so that the stability and reliability of the 3D multi-layered IC packaging can be improved.

One of such methodologies was developed by Namilae and Chandra [15] whereby a hierarchical multiscale model was used to study the mechanics of interfaces in carbon nanotube-based composites. This model used molecular dynamics (MD) simulation to derive the atomistic information of the interface and linked it to the macroscopic scale via the cohesive zone traction-displacement relations. Fan and Yuen [16] also used the same model to bridge the gap between the atomic and continuum levels. Similarly, the constitutive relations derived from MD simulation at the atomic level, in the form of traction-displacement curve, were incorporated into the CZM in FEM to investigate the interfacial fracture behavior at the continuum level. Subsequently, the corresponding failure force varying with the applied displacement was extracted from the simulated model and found to be in good agreement with the experimental data.

This study adopts a similar approach to characterize the interfacial fracture energy and predict interfacial delamination in the Cu/Ti/SiO_2/Si multi-layered system via MD and CZM-FEM simulations. Such a system is chosen as it is a common multi-layered structure found in the 3D ICs whereby the Si substrate is first coated with a dielectric layer which is then coated by thin intermetallic layers. This simple and yet effective approach is capable of bridging the microscopic and macroscopic structures by deriving the necessary CZM parameters from the MD simulation, to model the interfacial behavior when subjected to indentation loading, and subsequently to quantify the interfacial fracture energy at the macroscale accurately. Lastly, the FEM model is validated with experimental findings from the indentation damage test which allows cracking to happen in a controllable manner and is capable of measuring very small and localized deformation in the nano to micron range [17–19].

From this approach, the atomic behavior at the interface can be transferred to the continuum model so that interfacial delamination in 3D ICs packaging under different operating conditions can be predicted. Henceforth, experiments that are usually time-consuming and challenging are no longer required. Ultimately, the crack behaviors and the interfacial properties can be better understood and characterized. This study will be helpful to lay foundation to the knowledge of fracture mechanisms involved in the multi-layered IC devices and essential for materials selection and process control so as to improve the reliability of 3D IC packaging.

2. Methodologies

MD simulation serves as an excellent tool for modeling the interfacial properties at the atomistic level [20–23], as it is able to account for the bonding characteristics at the interface and the stress distribution generated by an applied load. With recent technological advancement and increase in computational power, this tool has been widely employed to investigate the failure mechanisms such as fracture and dislocations for a vast variety of materials [24,25]. In this study, MD simulation is performed to extract the interfacial properties in the Cu/Ti/SiO_2/Si multi-layered system to provide the cohesive parameters needed for FEM simulation.

Fig. 1 shows the computation cell of the Cu/Ti bi-layer system which has a dimension of $120 \times 120 \times 200$ Å. The interface is assumed to be smooth with no surface roughness. A similar configuration is also adopted for the SiO_2/Si bi-layer system. Due to the lack of suitable interatomic potential to model the atomic interactions at the Ti/SiO_2 interface, MD simulation is not conducted for the Ti/SiO_2 bi-layer system and its interfacial properties is adopted from the literature [26]. The interactions among the Si-Si and Si-O atomic pairs are described by the Tersoff potential [27], and those among the Ti-Cu, Ti-Ti and Cu-Cu atomic pairs are described by the MEAM potentials [28,29]. Periodic boundary conditions are applied in the *x*- and *y*-directions, while free boundary condition is used along the *z*-direction to model a large-sized thin film. The simulation is conducted using the large-scale atomic/molecular massively parallel simulator (LAMMPS) [30].

Each material layer in the bi-layer system is initially relaxed to obtain the state with the minimum local potential energy. Afterwards, each layer is equilibrated at constant 300 K and zero external stress by using the constant pressure and temperature (NPT) ensemble via the Noose-Hoover thermostat for about 40 ps. Upon achieving equilibration, the system is then switched to the constant volume and temperature (NVT) ensemble. The structural information for each layer is then imported into a new simulation model to construct the bi-layer system as shown in Fig. 1.

In the new simulation model, the two layers are combined together with a separation distance of 10 Å. Such a large separation distance is chosen to allow ample time for the atoms at the periodic boundaries to rearrange themselves without the influence of the atoms from the other layer. Subsequently, the two layers are moved towards each other in steps of 0.05 Å followed by the relaxation of 0.5 ps until they are ~3 Å distance apart. At the short separation distance of ~3 Å, the bi-layer system will relax under the NVT ensemble for 10 ps to allow the interfacial bonds to form and to attain a globally stabilized structure. Subsequently, as high-stress sites at the interface may be present due to the formation of new interfacial bonds and the lattice mismatch between the two layers, energy minimization is then performed to ensure that local minimum energy state at the interface is obtained.

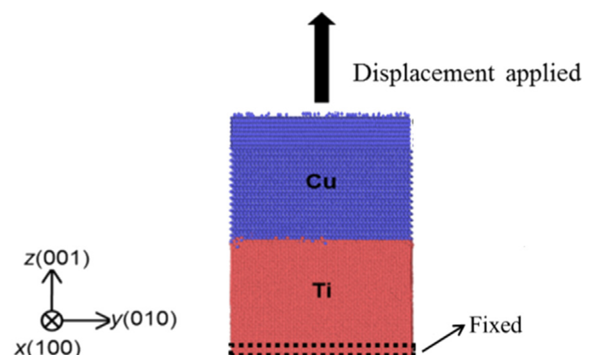

Fig. 1. Computational cells of the Cu/Ti system.

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