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FAILURE ANALYSIS AND CHARACTERIZATION
FOR MICROELECTRONIC PACKAGING

PAMELA LIN

SCHOOL OF MECHANICAL AND AEROSPACE ENGINEERING

2016

**3D FAILURE ANALYSIS AND CHARACTERIZATION
FOR MICROELECTRONIC PACKAGING**

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Abstract

In the recent years, the mechanical robustness and reliability of three-dimensional (3D) integrated circuit (IC) packaging have become tremendously challenging due to its continuous reduction in size and increase in vertical integration. Thermal problems such as the silicon (Si) substrate cracking and interfacial delamination are increasingly dominant due to the presence of high heat density in the small multilayer IC packaging. Furthermore, as the manufacturing and processing steps of the 3D ICs are significantly different from that of the conventional ICs, new defect and failure mechanisms that are unique to 3D ICs are not well-investigated. The reduction in size has also increased the sensitivity of the 3D ICs to microdefects that had not previously threatened their reliability and integrity. The increased complexity and miniaturization of 3D IC packaging and its consequential problems demand for new failure analysis methods. Therefore, this PhD research is proposed to study the physical failure modes and mechanisms associated with 3D ICs via molecular dynamics (MD) simulation and finite element method (FEM), and to develop new failure analysis methods for packaging characterization, thereby improving the packaging techniques and processes.

Si is commonly used as a substrate material in the IC packaging but yet its fracture behavior theoretical framework is still not well-developed. Thus, studies are first carried out on Si to understand its fracture mechanism through MD simulation and experiment. As the mechanical properties of Si are strongly influenced by the crystallographic orientation, defects, grain boundary (GB) and temperature, their effects on the tensile properties and failure mechanisms of Si are investigated. The results show that when Si is subjected to tensile loading, it undergoes brittle fracture and its (111) plane is the most favorable cleavage plane due to its high atomic packing density, thus resulting in the highest stiffness and lowest

fracture strength. The presence of structural defects generally weakens the integrity of Si, particularly for the (100) oriented Si subjected to tensile loading in the [010] direction, its integrity is much more sensitive to these structural defects. The three-point bend test is also performed to investigate the crystallographic orientation and defects effects and the experimental results are found to be consistent with the MD results.

The investigation of $\Sigma 25(710)\langle 010 \rangle$ tilt and $\Sigma 25(001)\langle 001 \rangle$ twist GBs in bicrystal Si nanofilms show that their fracture strengths are lower than that of single-crystal Si, which is caused by the change in crystallographic orientation of the grains. It is observed that these nanofilms generally fail through sliding dislocation mechanism. The reduction in size results in the increase of surface effect, and thus less energy is required for dislocation sliding to occur at the surface. The strength is further weakened by the addition of notch at the free edge of the GB. The increase in temperature (up to 600 K) has insignificant influence on the failure mechanism but generally lowers the fracture strength as expected. These combined simulation and experimental findings are then used to substantiate and explain the fracture behavior of bulk Si subjected at the macroscale, thereby improving the accuracy of root cause analysis.

Furthermore, understanding and predicting interfacial delamination failure in the multilayered IC packaging are essential for their performance and reliability. The MD study is first performed to investigate the effect of voids and temperature on the interfacial fracture behavior in a-Si₃N₄/Si bilayer systems. When the bilayer system is subjected to tensile loading, its fracture behavior is found to be temperature-dependent. At 300 K, the interfacial strength of the bilayer system is ~22.5 GPa and it undergoes brittle fracture at the interface. However, failure occurs in the a-Si₃N₄ layer in a ductile mode when temperature is increased to 600K. With the existence of void in the Si layer in the a-Si₃N₄/Si system, crack initiates at the void and propagates towards the interface at 300 K. As the temperature increases to 600

K, the same bilayer system undergoes brittle fracture at the interface at a significantly lowered interfacial strength. With the inclusion of an interfacial void, the bilayer system fractures at the interface with a deteriorated strength regardless of the temperature. The simulation results also show that the presence of an interfacial void has a more adverse impact on the interfacial strength than having a void in the Si layer. Under the shear loading, the bilayer system deforms in three stages: elastic deformation, plastic flow in the a-Si₃N₄ layer and interfacial sliding. The presence of voids and the increase in temperature lower the stress required for interfacial sliding but they do not have significant effect on the shear deformation process.

Subsequently, a combined approach based on MD-FEM simulations is adopted to characterize and predict delamination in a-Si₃N₄/Si bilayer system. The material parameters that are required to be input into the cohesive constitutive relation in FEM are derived from MD simulation. The work of interfacial fracture obtained by the FEM simulation is about 0.11 J/m² which is in good agreement with the experimentally obtained value of about 0.085 J/m².

The above approach is also extended to characterize the interfacial energies and predict interfacial delamination in the Cu/Ti/SiO₂/Si multilayered system. The thermodynamic work of adhesion W derived from MD simulation is used as the failure criterion for the FEM simulation as it is independent of the system geometry and applied strain rate. The interfacial fracture energy of 8.23 and 9.79 J/m² obtained from the MD-FEM simulations and the indentation damage experiment respectively, are also in good agreement. Hence, the combined approach is accurate and effective in characterizing and predicting the interfacial delamination in the multilayered IC packaging.

This PhD dissertation has investigated the fracture behaviour of bulk Si, bilayer systems and multilayered systems to understand their failure mechanisms and help in the failure

analysis process. This study is able to provide useful information for 3D ICs design and applications and helpful in improving their stability and reliability.

List of Publications

- [1] **Lin P**, Babicheva R, Xue M, Zhang H S, Xu H, Liu B and Zhou K, Tensile response of bicrystalline Si nanofilms with twist and tilt grain boundaries. *Computational Materials Science*, 2014 **96** 295-299.
- [2] **Lin P**, Babicheva R I, Xue M, Zhang H S, Xu H, Liu B and Zhou K, Effects of temperature and voids on the interfacial fracture of Si/a-Si₃N₄ bilayer systems. *Physica Status Solidi B*, 2015 **252**(9) 2013-9.
- [3] **Lin P**, Chai C M, Xue M, Xu H and Zhou K, An approach for the prediction of interfacial delamination of a-Si₃N₄/Si bilayer system. *Journal of Physics D: Applied Physics* 2016 (in press).
- [4] **Lin P**, Shen F, Yeo A, Liu B, Xue M, Xu H and Zhou K, Characterization of interfacial delamination in multilayered integrated circuit packaging. *Surface and Coatings Technology* 2016 (to be submitted).

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Chapter 1. Introduction

In the recent years, there has been increasing interest in the development of three-dimensional (3D) integrated circuit (IC) packaging due to its high performance, functionality and small system size. However, the increase in vertical integration and reduction in size of these 3D ICs have resulted in the introduction of new material layers and high density interconnection. Subsequently, when the multilayered IC package is subjected to thermal loading, thermomechanical stresses are induced as a result of mismatch in the coefficients of thermal expansion (CTEs) between dissimilar materials, and problems such as substrate cracking and interfacial delamination will occur. In this chapter, the failure of 3D IC packaging is briefly introduced. Subsequently, the motivations and objectives of the failure analysis of 3D are illustrated. Lastly, the organization of the whole thesis is presented.

1.1 Background

ICs play a vital role in many electronic devices. It consists of many different electrical components such as transistors, resistors and capacitors that are connected together in many different ways, resulting in different functionalities. With technological and social change, productivity and economic growth over the last few decades, the design of ICs has been moving towards 3D and miniaturization, wherein multiple layers of planar devices are stacked and interconnected using through silicon vias (TSV). A typical 3D IC comprises of a stack of silicon (Si) substrate topped with thin film of oxide and other metallization layers followed by a dielectric layer, such as silicon nitride. Similar stacks are built on top of the next, creating a compact IC package as shown in Fig. 1.1.

Figure 1.1. Schematic diagram of a 3D IC package (Lu *et al.*, 2002).

The advantages of 3D ICs include the enhancement of circuit performance as the long interconnects used in the conventional ICs are replaced by the short vertical interconnection, and thus reduces the chip size and interconnect delay problems. The increased vertical integration also increases functionality and allow the combination of different technologies (Davis *et al.*, 2005; Jung *et al.*, 2012). Despite their distinct advantages, 3D technology still faces many technological challenges and serious reliability issues. For example, the high-density interconnection gives rise to an increase in heat density that may affect circuit performance if not properly addressed (Vandeveld *et al.*, 2008). Other problems include the mismatch of CTEs in the multilayered structure which induces thermomechanical stresses, and eventually results in cracking in the bulk materials, interfacial delamination and performance degradation (Jung *et al.*, 2011).

The failure of IC can be categorized into three failure stages: the early life, the useful life and the wear-out life. In the early life stage, failures usually arise from quality issues while in the useful stage, failures are due to operating conditions and random anomalies. In the wear-out stage, failures usually occur due to the fatigue of the components. Besides, the package design, fabrication and assembly processes introduce inhomogeneties, such as defects,

contaminants, and residual stresses, causing stress-related failure such as substrate cracking and interfacial delamination.

A wafer is grown from a single-crystal Si, which is then cut into smaller dies. When the Si wafer is subjected to backgrinding and dicing, microcracks are induced on the surfaces and edges of the dies along with the residual stresses, which may later results in substrate cracking (Wu *et al.*, 2003). An example of the Si substrate cracking is shown in Fig. 1.2. Furthermore, the Si substrate is encapsulated in the mold compound for protection from external impact. During thermal loading, the mismatch of CTEs of the different materials causes the whole IC package to warp, inducing stresses within the package, and subsequently leads to delamination failure. Therefore, proper selection of materials and well-developed assembly processes are essential to minimize such stress-related failures.

Figure 1.2. Edge cracking in the Si substrate. Courtesy of Infineon Technologies Asia Pacific Pte Ltd.

As 3D ICs are used in critical applications such as, aviation and automotive industries whereby their failure may be consequential or even catastrophic, it is important to understand

the potential failure modes and mechanisms involved to ensure their quality and reliability. Failure analysis is the process of determining the physical root cause of the component failure, given the failure mode and characteristics. Firstly, non-destructive two-dimensional (2D) methods are used to locate the site of failure. Then, the characteristics of the failure are characterized and verified. Lastly, the root cause of failure and mitigation steps can be determined and carried out to improve the design, processes and reliability of 3D ICs (Soden and Anderson, 1993).

The current techniques for physical failure analysis include:

- Electrical measurement
- Optical microscopy (optical microscopy, infra-red microscopy)
- Physical (cross-sectioning, laser removal)
- Thermal imaging (infra-red thermography, fluorescent microthermography)
- Electron beam microscopy (secondary electron, backscattered electron)
- Light emission microscopy
- Ion beam (focused ion beam, secondary ion mass spectroscopy)
- Scanning probe microscopy (atomic force microscopy, scanning tunneling microscopy)

These techniques allow the failure analyst to inspect and navigate within and around the complex ICs, to locate and characterize failure. However, as ICs approaches 3D, these techniques which are catered for the planar ICs are inadequate to characterize the failure modes and mechanisms in 3D IC packaging, especially where materials such as Si and silica-interfaced with other materials are concerned.

In addition, as the system approaches the nanoscale, the preparation and handling of the samples for experimental analysis are becoming increasingly challenging. Also, the accuracy of the outcome is strongly influenced by the experience and skills of the analyst. As such, it is

necessary to validate the outcome with alternative data. The validation can be done via simulation tools such as finite element method (FEM) and molecular dynamics (MD) simulation.

In terms of fracture, FEM is able to simulate the operational and environment conditions and provide the stress distribution analysis at the macroscopic level by assigning the material parameters and boundary conditions. Hence, with the stress distribution map and material properties, FEM is able to predict the fracture properties and regions where failures are most likely to occur. Subsequently, the comparison can be made with the experimental findings to determine the root cause of failure. Therefore, the use of FEM in failure analysis has heavily increased over the last decade and is widely employed in the modelling of bulk materials to analyse and characterize the quantitative and qualitative approaches that are used to determine the root cause of a failure event.

FEM requires an understanding of the functionality of the component and the simulation is dependent on the material information and data input, and thus the quality of these factors is essential for the success of the simulation outcome. However, as some of the material parameters are based on the bulk values obtained by various experimental means, when the package size is reduced to the submicron length scales, the material parameters may defer due to the surface effect and the continuum description of the materials become questionable. Thus, in order to overcome this challenge, MD simulation is used to obtain the full atomistic information that is necessary to study the materials phenomena.

From the previous studies, MD simulation has proven to be a unique and powerful simulation tool to investigate the complex behaviour of dislocations, cracks and grain boundaries at very fundamental level. It is able to provide an understanding to the fracture mechanics of materials and give new insights to the fracture behavior of materials at the atomistic level. These are especially essential with the complexity and miniaturization of 3D

ICs and the experimental techniques can no longer determine the material properties accurately. MD simulation is based on Newton's laws and empirical interatomic potentials that define the interaction of atoms and consequently, the very complex phenomena can be simulated.

However, due to the costly computation time and calculation, the MD simulation only has the capability to model several thousand of atoms. It is impractical and almost impossible to use MD to build a full scale model. Therefore, by incorporating the benefits of MD into FEM, for instance, using the materials data derived from MD simulation for FEM, the limitations of both simulation tools can be overcome and more realistic and practical simulation at the macroscopic level can be achieved. Finally, a theoretical response of a particular failure problem can be deduced. Hereafter, the validation with the experimental findings can be carried out and finally the nature of the failure analysis problems can be characterized and better understood.

1.2 Motivation and objectives

The increased complexity and miniaturization of 3D IC packaging and its consequential problems demand for new failure analysis methods. This demand is mainly driven by the following reasons.

Firstly, as the manufacturing and processing steps for 3D ICs are significantly different from the conventional ICs, new defect and failure mechanisms that are unique to 3D ICs are not well-investigated and known (Lee and Chakrabarty, 2009). The reduction in size has also increased the sensitivity of the 3D ICs to microdefects that had not previously threatened their reliability and integrity.

Consequentially, one of the failures that are commonly observed in 3D ICs is the cracking in Si substrate. During the assembly process, the Si substrate is subjected to mechanical loading, back-side grinding and wafer slicing. Inevitably, these processes introduce the stress concentrators such as the micronotches at the chip side and the groove lines at the backside of the substrate, which eventually lead to failure via crack propagation when subjected to high stresses. Failure can also occur as a result of intrinsic defects such as porosity and grain boundaries which weaken the integrity of Si. As Si is an anisotropic material, the intrinsic properties such as the crystallographic orientation also affect its strength.

While abundant knowledge and experience from handling metals in the conventional 2D packaging (van Silfhout *et al.*, 2004) are available, less is known about the fracture behavior of the nonmetals such as ceramic, silica or Si used in 3D IC packaging. This is because much of the necessary nonmetal fracture behavior theoretical framework is not yet fully developed (Anderson, 2005). Data on the fracture in the single nanocrystalline Si is limited due to the difficulties in performing precisely controlled experiments. There is also lack of the atomic scale simulation that allow quantitative comparison with the fracture experiments, such as the fracture strength of Si die that was investigated using the three-point bending test (Hauch *et al.*, 1999; Wu *et al.*, 2003; Chong *et al.*, 2004). The problem is further compounded in 3D IC packaging when there may be more than one die present.

Secondly, the increase in vertical integration and reduction in size of these 3D ICs have resulted in the introduction of new material layers and high-density interconnection. Thermal effects are therefore greatly exacerbated in 3D ICs as compared to planar ICs, and thus thermal integrity is a crucial challenge and can degrade the reliability and performance of these ICs. When the multilayered IC package is subjected to thermal loading, thermomechanical stresses are induced as a result of the mismatch in the CTEs between

dissimilar materials, and problems such as thermal warpage and interfacial delamination will occur.

Interfacial delamination is initiated by the nucleation of crack at the interface which eventually results in the failure of the IC packaging. It is important to predict interfacial delamination so that the stability and reliability of the multilayered IC packaging can be improved. However, it is challenging to experimentally quantify the critical energies of interfacial adhesion which is one of the most important properties that governs interfacial delamination. Furthermore, the delamination failure mechanisms are not only dependent on the mechanical properties of the layers but also the chemical and bonding characteristics at the interface and the stress distribution generated by external loading during assembly and operating processes.

The involvement of different layers also adds to the complexity of studying the physical failure mechanisms involved, making failure harder to predict with conventional 2D failure analysis techniques. It is therefore essential to develop new failure analysis methods to characterize and predict interfacial delamination. The lack of knowledge in the understanding of interfacial fracture has impeded 3D ICs design and 3D technological advancement (Snodgrass *et al.*, 2002; Vijayashankar *et al.*, 2011).

Therefore, new failure analysis approaches are required to study the physical failure modes and mechanisms for better understanding of the problems involved. Understanding of the crack behaviour in Si substrate and characterizing the material properties at the interface are helpful to lay foundation to the knowledge of fracture mechanisms involved in multilayered chip devices and essential for materials selection and process control.

The most fundamental way to understand the physical failure modes and mechanisms associated with 3D ICs, specifically for the case of cracking in Si and interfacial delamination between dissimilar materials, are via atomistic simulation. MD simulation is capable of

providing the most basic, or ab initio, description of the failure processes. With the advancement of computer science and technology, atomistic models have reached a level of accuracy that can often be compared with experimental findings. Therefore, this proposed research aims:

- To study the effects of crystallographic orientations, defects, grain boundaries and temperature on the tensile properties and the fracture behavior of bulk Si;
- To study the effects of defects and temperature on the interfacial properties and failure mechanisms of bilayer system;
- To develop new failure analysis approaches to characterize and predict failure in 3D IC packaging via MD and FEM simulations;
- To improve the current failure analysis techniques, the processes and the reliability of 3D packaging development, translating to increased yield in production of 3D ICs and lower costs.

1.3 Dissertation outline

This thesis contains six chapters. Following this introductory chapter, a comprehensive review on the 3D IC packaging, its associated problems and the failure analysis methodologies employ in this work are provided in Chapter 2. The study of the fracture behaviors of bulk Si is presented in Chapter 3. Chapter 4 and 5 focus on the investigations of the interfacial delamination of bilayer and multilayer systems respectively. Chapter 6 concludes the thesis and proposes the future works.

Chapter 2. Literature Review

2.1 Integrated circuit packaging

3D integration technologies have become one of the fastest emerging IC design approaches that offer flexibility and cost effective integration and packaging solutions. The primary drivers for 3D integration are miniaturization, integration of different technologies in a small package and enhancement of system performance. It involves the stacking of chips, whereby each chip is built on a separate layer in the stack, which are then connected together via vertical inter-layer interconnects. Consequentially, the system size can be greatly reduced and more technologies and functionalities can be combined and integrated within a small package (see Fig 2.1) (Davis *et al.*, 2005). With vertical integration, the interconnection can be shortened to reduce the critical delay problems, and thus the circuit performance can be enhanced.

Figure 2.1. Vertical integration of ICs from 2D to 3D (Chanchani, 2009).

The 3D IC assembly can be separated into four different approaches, namely the monolithic, wafer-on-wafer, die-on-wafer and die-on-die. In the monolithic assembly, the electronic components and connections are built in layers onto the single Si wafer, which is then diced into individual 3D ICs. The advantage of this method is that the aligning, thinning, bonding or TSVs will not be necessary as only one substrate present. For the wafer-on-wafer,

the electronic components are built onto two or more Si wafers which are then aligned, thinned, bonded and diced into individual 3D ICs. Vertical connections are built onto the wafers before or after bonding. The TSVs are passed through the Si substrates between active layers and/or an external bond pad. As such, the yield is reduced for such assembly process as the failure of any one chip in the 3D ICs will lead to the failure of the entire 3D IC.

Similarly, for the die-on-wafer assembly, the electronic components are built on two Si wafers, whereby one is diced and then aligned and bonded onto the second wafer. For the die-on-die, the electronic components are built on multiple dies which are then aligned and bonded. Thinning and TSV may be carried out before or after bonding. One advantage of this method is that die testing can be carried out on each die in advance so that one bad die does not affect the integrity of the entire stack.

Figure 2.2. Schematic diagram of a 3D IC.

Figure 2.2 illustrates a simplified schematic diagram of the materials used in 3D ICs. Si is commonly used as substrate due to its excellent semiconductor properties. The Si wafer is first grown via Czochralski process. In this process, a cylindrical ingot of high purity single-crystal Si is melted at high temperature and dopant impurity atoms such as boron and

phosphorus are added to the molten Si to form p-type or n-type Si with different electronic properties. A precisely oriented rod-mounted seed crystal is dipped into the molten Si and slowly pulled upwards and rotated simultaneously. As a result, a large single-crystal Si ingot is formed. Subsequently, the ingot is then sliced into thin wafers and cleaned with acids to remove impurities and reduce defects induced by the sawing process.

The surface of the substrate is then oxidized to form a dielectric layer, which provides electrical stability. Etching is then carried out to remove unwanted regions of oxide. The process is then repeated each time with different layers of materials depending on the necessary functionality. Lastly, the entire wafer stack is coated with a layer of passivation such as, silicon nitride, to protect the wafer from contamination during the assembly process. The stack is then mounted on to lead frames and thin gold wires connect the chip to the frames to create an electrical path. Subsequently, a mold compound is pressed onto the stack to form an IC package.

As the current trend moves towards miniaturization, 3D vertical integration is able to offer higher connectivity and new design possibilities. The reduction in size and increased vertical integration results in high-density interconnection, and thus significantly shorten circuit delay and power consumption and thereby enhancing circuit performance. Furthermore, the stacking of multiple chips allow the layers with different processes to be built together, and thus more functionality is able to fit in a small space, leading to the generation of small yet powerful microelectronic devices.

Despite their distinct advantages, the complexity of size reduction and vertical integration in 3D technologies has resulted in many technological challenges and serious reliability issues that are not present in the planar ICs. Firstly, the high-density interconnection has led to high heat density that must be carefully managed, and if not properly addressed, it may induce thermomechanical stresses within the IC package and

threaten its reliability. Secondly, the presence of multiple layers of different materials has resulted in the mismatch of CTEs. Thus, during thermal loading, such as the solder reflow process, this problem is amplified and may lead to warpage and interfacial delamination and thereby affecting the circuit performance. Other challenges such as, the increase in sensitivity to microdefects introduced during handling and manufacturing processes due to the smaller system size.

Most of challenges encountered in 3D ICs affect the thermomechanical reliability of the IC package, and thus it is one of the major concerns in the semiconductor industry. Currently, it is noted that 65% of the total failures in microelectronics are thermomechanical-related failure (Van Driel *et al.*, 2006).

2.2 Failure in integrated circuits

As 3D ICs are used in many critical applications, such as aviation and automotive, their failure may have detrimental consequences in terms of safety or productivity. It is therefore important to ensure the integrity and reliability of the electrical components. As such, it is crucial to understand the failure modes and mechanism associated with 3D ICs so that failure can be predicted and mitigated to avoid future occurrence.

Failure analysis is the process of examining IC packages after failure by collecting and analyzing data using electrical, physical and chemical analysis techniques to determine the mode or mechanism of failure. It is an essential process in the improvement and development of the design of IC packaging. In a conventional failure analysis process, the first step is to identify the site of failure using inspection or electronic tools. Inspection tools, such as the optical microscopy and scanning acoustic topography, allow the analyst to observe for external or internal damages, such as delamination crack or burned marks. Electronic tools, such as the curve tracer, are used to check for possible leakages. After localizing the site of

failure, chemical etching can be carried out to allow visual access and further investigation of the failure. Next, experimental tools, such as scanning electron microscopy and Raman spectroscopy, can be employed to characterize the failure (Vallett, 1997). It is important to note that some of the experimental tools may be destructive, and thus at each investigation step, it is important to collect as much information as possible about the failure and any anomalies.

With the ability to characterize failure, the root cause of failure can be identified, and thus mitigation and prevention actions can be carried out to increase the reliability and integrity of the 3D ICs (Wagner, 1999). Furthermore, the knowledge gained by analyzing a certain failure can prevent similar failures from reoccurring and minimize the consequential effect. Therefore, the accuracy of failure analysis is vital and must be carefully conducted to establish the true cause of the error.

The functional performance of an IC package depends on the material properties of its components. Mechanical failure usually occurs when the 3D IC device is subjected to conditions that resulted in stresses beyond the threshold of the mechanical properties of its constituent materials. Some common mechanical failure modes observed in 3D ICs are (Ohring, 1998):

- Encapsulation failure
- Die attach failure
- Wire bond failure
- Silicon substrate failure
- Oxide layer faults
- Interfacial delamination

In general, these failures can arise from electrical, heat, chemical and mechanical stresses. Most of the failure modes in 3D ICs are attributed to thermomechanical stresses

(Van Driel *et al.*, 2006). Some examples of these failures include interfacial delamination and warpage induced by thermal cool down, resulting in silicon die crack and package cracking (Van Driel *et al.*, 2003; Yang *et al.*, 2007; Lu and Wong, 2009). Figure 2.3 illustrates a type of package crack occurring at the intermetallic layer. As a result of the thermal stress and mismatch of CTEs, the aluminum (Al) wiring material deforms and slides. When Al sliding occurs, cracks will form in the passivation film, which eventually causes corrosion, disconnection and electrical failures.

Figure 2.4 shows an example of the thermomechanical failure as a result of thermal cyclic stress. This thermal cyclic stress can cause mechanical stresses on the wires due to the differences between the CTEs and eventually wire fatigue, resulting in an open wire. Furthermore, wire deformation during molding can cause wires to come in contact with each other or with the edge of the chip at high temperatures, resulting in short circuit.

Figure 2.3. Crack resulting from the sliding mechanism of the Al layer. Courtesy of Infineon Technologies Pte Ltd.

Figure 2.4. SEM imaging of the cross-sectional grain structure of a copper-to-copper wire bond. Courtesy of Infineon Technologies Pte Ltd.

These failures are further compounded with the reduction of system size and increased vertical integration in the 3D ICs, as they lead to an increase in heat density due to the higher interconnection density and worsen the problem of mismatch of CTEs as more materials are added in (Marinissen and Zorian, 2009). Therefore, the proposed study will focus on the failures related to bulk Si material and interfacial delamination of dissimilar materials in the 3D ICs.

2.2.1 Cracking in silicon substrate

As previously mentioned, the functionality and performance of the 3D ICs are highly dependent on the integrity of its constituent materials. Due to its excellent semiconductor properties, Si is commonly used as the substrate material in the 3D ICs. Si has a diamond structure with a lattice constant of 5.43 Å. Like many crystalline materials, Si may have many intrinsic defects, such as grain boundaries (GBs), point defects and dislocations. It can also contain extrinsic defects, such as cracks, caused by mishandling, manufacturing and operating processes. These structural defects can alter the material properties of Si and significantly influence the deformation process and subsequent failure mechanism (Youssef *et al.*, 2012). The effects of these structural defects on the material properties are even more impactful at the nanoscale.

Generally, Si is considered as a brittle material and cracking in Si may occur due to various reasons. When high stresses are induced in the Si die during packaging, assembly and reliability testing, it could result in fracture in the die. Fracture may originate from the die attach or mechanical stresses experienced by the whole package. Die attach may contain imperfections, such as voids and incomplete fillet formation. As the die attach material has a greater CTE than the substrate material, during the thermal processes, these flaws serve as stress concentrators which exert large flexural stresses on the die and eventually results in cracks at the bottom side of the die.

Structural defects such as microcracks in/on the substrate can also result in fracture in the substrate. For example, an edge crack can result in crack propagation as observed on the Side D in Fig. 2.5a. These structural defects serve as stress concentrators and initiation points. When the die is subjected to stresses higher than the critical value, the atomic bonds begin to break and the elastic energy is released. Subsequently, a new surface is created as the crack propagates through the die (Fig. 2.6). The direction of crack propagation is almost perpendicular to the tensile loading direction and yields a relatively flat fracture surface which is also known as the cleavage plane. Inevitably, the mechanical properties of Si are degraded by these structural defects.

Figure 2.5. (a) SEM imaging of the systemic chip cracked without external damage on the surfaces as observed in the package and (b) the overview of the die after chemical decapsulation. Courtesy of Infineon Technologies Pte Ltd.

Figure 2.6. SEM imaging: (a) the planar view and (b) the tilted view of the crack chip corner. Courtesy of Infineon Technologies Pte Ltd.

Cracking becomes a more severe concern when the IC packaging is reduced to the nanoscale. Warpage may happen during assembly processes due to the differences in CTEs in the materials used. Even though the warpage level may be small, nevertheless, the stress states are more severe at such scale.

Crack propagation under mode I (opening mode) and mode II (sliding mode) demonstrated in Fig. 2.7 are the more common fracture modes observed in the cracking of Si, whereas mode III (tearing mode) is often neglected due to its inferior impact as compared to the other modes.

Figure 2.7. A schematic diagram of different fracture modes.

2.2.1.1 Crystallographic orientation

Crystalline Si is a strongly anisotropic material whose mechanical properties and fracture mechanisms depend on its crystallographic orientation. It is important to investigate the effect of crystallographic orientation of Si on its mechanical properties to obtain the optimal design of the 3D ICs (Kim *et al.*, 2001).

Many experimental studies have been carried out to understand the effect of the crystallographic orientation of Si (Fujii and Akiniwa, 2006; Uesugi *et al.*, 2013). Choi (2004) studied the influence of the polycrystalline size and anisotropy of Si on its effective elastic constants. The results showed that decreasing the polycrystalline size and increasing the anisotropy will result in a large scatter of elastic constants. Ando *et al.* (2004) measured the fracture strength and toughness of the single-crystal Si films with different crystal orientations under tensile loading. With a (100) surface orientation, when subjected to the $\langle 110 \rangle$ loading direction, the fracture toughness and strength are reduced by 40% and 10% respectively, as compared to the $\langle 100 \rangle$ loading direction.

Li. *et al.* (2005) also investigated the effects of notch and the crystal orientation on the fracture toughness and behavior of the single-crystal Si under tensile loading. The experimental results showed that the (100) plane has a higher fracture toughness as compared to the other low index planes, such as the (110) and (111) planes. Hence, it is more favorable for cracks to propagate in these low index planes. Moreover, the fracture behavior is influenced by the orientations of the crystal and notch front. When the notch front orientation is parallel to the low index planes, the possibility of crack propagation becomes even more dominant.

Bean and Gleim (1969) further explained that the (111) plane in Si has the maximum atomic density. As such, the forces between the adjacent planes were much weaker than those within the plane. Whereas for the (110) plane, the stresses were homogenous between the

adjacent planes and within the plane. For the (100) plane, the four-fold symmetry of the (111) planes intersect with the (100) slice surface and as a result, this plane was the least susceptible to fracture.

Even though, many have tried to analyze the effect of crystallographic orientation using experimental means, their findings are still limited by experimental difficulties when dealing with specimens in the nano- and microlevel scales.

2.2.1.2 Grain boundaries

For the polycrystalline Si, the arrangement of the grains leads to the formation of GBs. These structural defects cause alteration to the atomic bonding and formation of new surfaces. For instance, the formation of a vacancy breaks some bonds but also strengthens the neighbouring bonds through the redistribution of charge density (Xu *et al.*, 2006). As a result, the bond lengths and angles are altered and consequently the mechanical properties and deformation process of Si are affected.

The presence of GBs tends to affect the material properties as they serve as the sites for corrosion and precipitation of new phases from the solid. On the other hand, the GBs impede dislocation motion and help to improve the strength of polycrystalline material. The GBs are formed due to misorientation of two grains. Each grain has its own systemic packing of atoms, and thus it will have different orientation from the neighbouring grains and is separated by the GB.

The simplest characterization of GBs is that of the tilt GB, wherein the rotation axis is parallel to the boundary plane (Fig. 2.8a). Another basic type of GB is the twist GB whereby the rotation axis is perpendicular to the boundary plane (Fig. 2.8b). In real polycrystalline materials, GBs present are usually the mixed type so as to create the best fit between the

neighbouring grains. The angle of rotation θ between two grains can be determined as follows,

$$\theta = 2 \tan^{-1} \left(\frac{y}{x} \right) , \quad (2.1)$$

where (x, y) are the coordinates of the superimposed point in lattice “1” as shown in Fig. 2.9; x is measured parallel to the mirror plane.

Figure 2.8. The schematic representations of the (a) tilt grain boundary (b) twist grain boundary of a bicrystal.

The GB can be further characterized into the different coincidence site lattice (CSL), in which repeated grains are formed from points where two misoriented lattices happen to coincide. In the CSL theory, the degree of fit Σ between the structures of the two grains is described by the reciprocal of the coincidence sites to the total number of sites ratio (Ranganathan, 1966),

$$\Sigma = \begin{cases} 0.5(x^2 + y^2), & (x^2 + y^2) \text{ even} \\ (x^2 + y^2), & (x^2 + y^2) \text{ odd} \end{cases} . \quad (2.2)$$

Thus, high Σ GBs where the θ is more than 11° are expected to have higher energy as compared to low Σ due to the complexity of the structures involved. Hence, the larger angle GBs will have higher strength than the smaller angle GBs. Therefore, the different orientations of the grains will affect the mechanical properties of the polycrystalline materials (Hirth, 1972).

Figure 2.9. Determination of the Σ -values for rotation of the (100) plane in the cubic structure (Bollmann, 2012).

Some research has been conducted to understand the effects of structural defects on the mechanical properties of Si. For instance, Kuo *et al.* (2014) showed that the presence of the vacancy defects have marginal effect on the mechanical and fracture behaviour of the Si nanowires (NWs). However, as the cross-sectional of the NWs decreases, the vacancy defects can considerably weaken the ultimate strength of the NWs. Hence, this shows that even though these atomic defects may not have significant effect on the bulk material, however when the system size is reduced to the nanoscale, the effects of such defects may become dominant. Wu *et al.* (2013) found that the region of high dislocation density exhibit higher fracture toughness than the region of low dislocation density due to the crack tip shielding

that arises from the interactions of dislocations with an indentation crack. In spite of these previous works, little is known about the effect of the GBs on the mechanical properties of Si.

2.2.1.3 Defects

In IC packaging, a wafer is first grown from a single-crystal Si. During the crystal formation, the high melting temperature process facilitates the self-diffusion of Si atoms, resulting in the formation of vacancies and interstitial defects. When these thermal point defects condense, microdefects, such as dislocation loops, are formed (De Kock *et al.*, 1979).

Subsequently, the Si wafer is then grinded at the backside and cut into smaller dies. During the grinding process, grinding grooves are introduced on the surface of the backside of the die due to wafer thinning via coarse and fine grinding wheels. Consequently, the dicing process induces microcracks along the edges of the dies. Possible residual stresses are also built up along with the mentioned structural defects. Hence, when subjected to stresses during the assembly and operation processes, these defects serve as the potential sites for crack initiation and propagation and eventually lead to fracture. Some of the assembly processes include die attachment, epoxy curing, molding and post-mold curing. The wire bonding process onto the thin stack die could also result in fracture (Chong *et al.*, 2004).

Wu *et al.* (2003) found that the mechanical strength of Si is strongly influenced by the backgrinding patterns. The mechanical strength of the Si die is significantly degraded when the grinding mark is parallel with the loading axis. In contrast, the polished surfaces possess the highest mechanical strength due to minimum surface flaws and do not exhibit directional-dependent strength behavior. The authors also found that the geometrical factors have insignificant effect on the mechanical strength.

In addition, Si is purposefully doped with other elements, such as boron and phosphorous, to alter its electronic properties. The introduction of these foreign atoms results

in interstitial defects which may be a factor of the mechanical properties of Si. Recently, Ogawa *et al.* (2014) investigated the possible effect of the hydrogen charge on the mechanical properties of Si at the ambient temperature. The authors found that the addition of hydrogen has significant impact on both the mechanical and electronic properties of Si as it increases the deep local trapping of dislocation and facilitates plastic deformation near the surface.

Sumino *et al.* (1983) also studied the effect of nitrogen on the dislocation behaviour and mechanical strength of the Si crystals and found that the presence of the interstitial nitrogen atoms enhances the hardening of the Si crystals via the trapping of dislocations. Bhushan and Koinkar (1996) carried out the microtribological studies on the doped single-crystal Si and established that the lightly boron-doped Si has the lowest hardness as compared to the pure Si and phosphorous-doped Si. Lee *et al.* (1998) also showed that as the doping concentration increases, the Young's modulus of the phosphorous-doped polycrystalline Si film decreases.

From these previous studies, the effects of some of these individual intrinsic and extrinsic defects on the mechanical properties of Si can be understood. However, the coexistence of multiple types of defects is seldom considered and the coupling effect between environmental conditions and these defects are still not yet fully understood.

2.2.2 Interfacial delamination

Interfacial delamination in 3D ICs is caused by the thermomechanical stresses due to the presence of dissimilar materials. It is strongly related to the interfacial strength of two adjacent materials, which can be characterized by the energy release rate (Van Driel *et al.*, 2005). The mismatch of CTEs, thermal conductivities and intrinsic stresses of these layers contribute to the residual stresses in the 3D ICs. Interfaces near the free edge between dissimilar materials are the weakest link as they are susceptible to high stress gradients and

also internally, they are prone to crack initiations (Shkarayev *et al.*, 2001). As a result, when the strain energy exceeds the interfacial toughness between layers, delamination occurs.

The presence of residual stresses from the assembly processes and the changing thermal and humidity conditions also expedite interfacial delamination. Figure 2.10 illustrates a cross-sectional view of interfacial delamination between the dielectric layer and other metallic layers. Silicon nitride (Si_3N_4) is commonly used as an ultra-thin dielectric layer in these 3D ICs and also serve as a protective coating and gate insulator. It is deposited onto a Si substrate via chemical vapor deposition. During fabrication, both the mismatches in thermal properties and lattice structure between the Si_3N_4 and Si materials would introduce stresses at their interface, making it prone to crack initiations and sensitive to interfacial defects. Consequently, if these stresses exceed the bonding strength of the interface, interface fracture or delamination will occur and the functionality of the system will be jeopardized (Gall *et al.*, 2000; Gu *et al.*, 2001; Kay *et al.*, 2006; Rafii-Tabar *et al.*, 2006).

Figure 2.10. SEM imaging of the interfacial delamination between the dielectric and metallic layers. Courtesy of Infineon Technologies Pte Ltd.

Crack can be initiated at the surface due to high stresses or the presence of interfacial defects which may then propagate leading to the debonding of the interface and fracture within the adjoining materials. Interfacial defects can be introduced in the 3D ICs during the growth of their constitutive thin layers and the subsequent thermal annealing, resulting in the formation of voids at the interface and even within the layers as a consequence of thermal diffusion (Bachlechner *et al.*, 2006).

Furthermore, as the system size reduces to the nanoscale, the thin layers in 3D ICs become more sensitive to the interfacial defects, which can significantly influence their integrity and result in poor performance and even failure. The interfacial properties may be considerably different from those of the adjoining materials and can be further complicated by the presence of defects at or near the interface (Shilkrot and Srolovitz, 1998). Therefore, it is important to understand the effects of the defects on the fracture behavior of these multilayered thin films.

The prediction of interfacial delamination in the 3D multilayered IC packaging is vital for its stability and reliability. However, the characterization of the interfacial delamination in multilayered IC packaging is rather complex as it is challenging to quantify the critical energies of interfacial adhesion experimentally. Furthermore, the delamination failure mechanisms are not only dependent on the mechanical properties of the layers but also the chemical and bonding characteristics at the interface and the stress distribution generated by external loading during the assembly and operating processes.

Besides, it is also necessary to understand the stress distribution within the package and the adhesion energies between dissimilar materials, to predict and avoid the occurrence of such failure. Therefore, the fracture mechanics in the bi-material interfacial delamination problem has been of great interest and its theory has been widely used experimentally and numerically (Ho and Faupel, 1988; Mirman, 1991; Hutchinson and Suo, 1992; Nakamura and Kamath, 1992; Evans and Hutchinson, 1995; Jain *et al.*, 1995; Saitoh *et al.*, 1998, 2000;

Wang *et al.*, 2000; Barut *et al.*, 2001; Nicola *et al.*, 2002; Pang *et al.*, 2002; Zhong *et al.*, 2002; Zhang *et al.*, 2003; Panat and Hsia, 2004; Jiang *et al.*, 2007; Hallett *et al.*, 2008; Zhang *et al.*, 2012).

Many works have employed the conventional numerical and experimental approaches such as, linear elastic fracture mechanics (LEFM), finite element modeling (FEM), four-point bend test, nanoscratch test, nanoindentation test and laser spallation technique, to analyze and characterize the interfacial delamination failure (Vossen, 1978; Marshall and Evans, 1985; Sanchez *et al.*, 1999; Katipelli *et al.*, 2000; Volinsky *et al.*, 2002; Hughey *et al.*, 2004; Kandula *et al.*, 2008). The LEFM calculates the critical stress intensity factors and energy release rates at the crack tip material as singular and infinite, which is physically unrealistic. There will also be plastic deformation at the interface before fracture and thus LEFM alone is inadequate.

On the other hand, FEM uses the critical interfacial strengths of different materials as the governing criterion for failure and is commonly used to solve fracture mechanics problem for materials at the macroscale (Ortiz and Pandolfi, 1999). During thermomechanical loading, the interface behaves like a nonlinear material, undergoing damage initiation and delamination propagation which can be described by a nonlinear traction-separation law based on cohesive zone modelling. The material parameters required to be input into the traction-separation law are usually experimentally derived. However, during the sample preparation and the experimental process, there are bound to be errors and also defining the residual stresses in the thin films have always been a great challenge.

Furthermore, it becomes more challenging to accurately extract the material properties from experiments when the system size approaches the nanoscale. As the interfacial properties are dependent on the material properties such as the adhesion strength, reactivity and surface roughness, an accurate failure prediction of interfaces cannot be made unless

these material properties are well considered (Zhang *et al.*, 2012). Therefore, the FEM and experimental approaches are no longer adequate, more detailed methodologies are required to fully characterize the interfaces and predict interfacial delamination.

MD simulation serves as an excellent tool for the modeling of the interfacial properties at the atomistic level (Wang *et al.*, 2000; Fan *et al.*, 2001; Tanaka and Goettler, 2002; Gou *et al.*, 2004; Fan *et al.*, 2006; Van Driel *et al.*, 2006; Zhang *et al.*, 2006; Fan *et al.*, 2009; Fan and Yuen, 2010; Fan and Yuen, 2013), as it is able to account for the chemical interaction and bonding at the interface. With recent technological advancement, this tool is widely employed to investigate the failure mechanisms such as fracture and dislocations for a vast variety of materials (Abraham and Gao, 2000; Gerde and Marder, 2001).

Bachlechner *et al.* (2005) investigated the mechanical strength of the Si/Si₃N₄ interface by applying tensile strain parallel to the interface. The results showed that the binary system failed as the crack initiates and propagates in the Si₃N₄ layer, whereas in the Si layer, only dislocations were emitted. More recently, Yang *et al.* (2014) analyzed the crack propagation at the copper/silicon carbide interface under the mode I and mix mode loading conditions via MD simulation. They found that for the mode I loading, the crack propagates in an asymmetrical manner due to dislocations generated by lattice mismatch, whereas for the mixed mode loading, the crack propagation is dependent on the loading angle. Zhang *et al.* (2012) showed that the crack propagation leads to the formation of high temperature zone in the propagation direction. However, the effects of interfacial defects are seldom considered and the coupling effect of temperature and these defects are still not yet fully understood.

As systems become integrated with new functionality, new materials will also be introduced. The lack of knowledge in understanding the interfacial delamination problem has impeded 3D ICs design and 3D technological advancement. Understanding the crack behaviors at the interface is helpful to lay the foundation to the knowledge of fracture

mechanisms involved in the multilayered chip devices and essential for materials selection and process control.

2.3 Methodologies for failure analysis

2.3.1 Molecular dynamics

MD simulation is an excellent and powerful simulation tool for modeling at the atomistic level. It involves solving a set of equation of motion for all the particles in the system governed by the Newton's 2nd law and allows the time evolution prediction of the interacting particles in a system. Consequently, MD simulation is able to provide an accurate description of the atomic interaction and does not require any assumption to be made, unlike that of FEM and experiments. These are especially essential with the complexity and miniaturization of 3D ICs and when experimental techniques can no longer determine the material properties accurately.

2.3.1.1 Fundamentals of MD simulation

MD simulation is a technique employed to investigate the structure, dynamics, and properties of many-body systems, by calculating the motion of the atoms in a molecular assembly based on the numerical integration of Newton's equation of motion:

$$m \frac{d^2 \vec{r}_i}{dt^2} = - \frac{\partial V}{\partial \vec{r}_i} \quad , \quad (2.3)$$

where m , $\vec{r}_i$ and V are the mass, position vector and interatomic potential of the i th atom respectively. The integration system used for Eq. (2.3) is the Verlet algorithm which predicts the position at $t + \delta t$ if given the position at the earlier time t and $t - \delta t$. In this algorithm, the Taylor expansion series of $\vec{r}_i$ at both $t + \delta t$ and $t - \delta t$ till the third order are developed as

$$\vec{r}_i(t + \delta t) = \vec{r}_i(t) + \vec{v}_i(t)\delta t + \frac{\vec{a}_i(t)}{2}\delta t^2 + \frac{\vec{b}_i(t)}{6}\delta t^3 + O(\delta t^4), \quad (2.4)$$

$$\vec{r}_i(t - \delta t) = \vec{r}_i(t) - \vec{v}_i(t)\delta t + \frac{\vec{a}_i(t)}{2}\delta t^2 - \frac{\vec{b}_i(t)}{6}\delta t^3 + O(\delta t^4). \quad (2.5)$$

The summation of Eqs. (2.4) and (2.5) produces the expression of the position $\vec{r}_i(t + \delta t)$ in terms of $\vec{r}_i(t)$ and $\vec{r}_i(t - \delta t)$ as

$$\vec{r}_i(t + \delta t) = 2\vec{r}_i(t) - \vec{r}_i(t - \delta t) + \vec{a}_i(t)\delta t^2 + O(\delta t^4). \quad (2.6)$$

Similarly, by using the Taylor expansion series of $\vec{r}_i$ at both $t + dt$ and $t - dt$ to the first order, the velocity $\vec{v}_i$ can be obtained as

$$\vec{v}_i(t) = \frac{\vec{r}_i(t + \delta t) - \vec{r}_i(t - \delta t)}{2\delta t} + O(\delta t^2). \quad (2.7)$$

Compared with other integration algorithm, the Verlet algorithm is simple, easy to implement, stable and time reversible, and thus has been widely applied.

One problem of the Verlet algorithm is that the estimation error of the position is in the order of $O(\delta t^4)$, but that of the velocity is in the order of $O(\delta t^2)$. To solve this problem, several improved Verlet algorithms have been developed and one of such algorithms is the Velocity Verlet algorithm which can be expressed as

$$\vec{r}_i(t + \delta t) = \vec{r}_i(t) + \vec{v}_i\delta t + \frac{\vec{a}_i}{2}\delta t^2, \quad (2.8)$$

$$\vec{v}_i(t + \delta t/2) = \vec{v}_i(t) + \frac{\vec{a}_i}{2}\delta t, \quad (2.9)$$

$$\vec{a}_i(t + \delta t) = \left(-\frac{1}{m}\right) \frac{\partial V}{\partial \vec{r}_i(t + \delta t)}, \quad (2.10)$$

$$\vec{v}_i(t + \delta t) = \vec{v}_i(t + \delta t/2) + \frac{\vec{a}_i}{2}\delta(t + \delta t)\delta t. \quad (2.11)$$

The Velocity-Verlet algorithm is simpler, faster and requires less computer storage space and has been more commonly used. Thus, this algorithm is adopted for this PhD study.

According to the principles of MD simulation, its general workflow can be divided into the following steps:

- (1) Initiating the positions and velocities of the atoms, i.e., setting $\vec{r}_i(0)$ and $v_i(0)$;
- (2) Choosing a suitable potential energy function and calculating the interatomic forces;
- (3) Solving the Newton's equations of motion to update the positions and velocities of the atoms, i.e., obtaining $\vec{r}_i(dt)$ and $v_i(dt)$;
- (4) Computing the quantities required and repeating steps 2 to 4 till the end of the simulation;
- (5) Analyzing the computed quantities to investigate the behaviors and properties of the entire system.

In this study, the MD simulation is performed by using the large-scale atomic/molecular massively parallel simulator (LAMMPS) package. It is a free and open-source classical MD code that models an ensemble of particles in a liquid, solid, or gaseous state. It can model atomic, polymeric, biological, metallic, granular, and coarse-grained systems using a wide variety of force fields and boundary conditions. It allows modification of its source codes according to specific simulation requirements. The simulation can be accelerated by running on multiple processors and the computational efficiency for large system size can be further improved with the use of high-performance computing clusters. Therefore, with its high efficiency and flexibility, this package is adopted in this study.

The MD approach is straightforward and can be easily implemented since the energy, stress and strain can be obtained directly from the computation of the classical quantities such as force, velocity and position. In addition, no significant assumption is made during the

calculation of the mechanical properties. The details of the MD simulation are provided in the following chapters.

2.3.1.2. Potential functions

The advantages of MD simulation lie in its high speed and simplicity, as well as in its flexibility and versatility in the choice of the atomic potential energy functions (or potentials in short). Generally, the total potential energy of a system can be broken down into

$$E = \sum_i V_1(\vec{r}_i) + \sum_{i<j} V_2(\vec{r}_i, \vec{r}_j) + \sum_{i<j<k} V_3(\vec{r}_i, \vec{r}_j, \vec{r}_k) + \dots \quad (2.12)$$

where the first term represents the total potential energy contributed by one-body and is usually related to an external field such as an electric or magnetic field. The second and third terms represent the two-body and three-body atomic interactions, respectively. The choice of the potential function usually depends on the problem, such as the type of the atomic structure and the atomic element. Next, the potential functions that are used in this PhD research are presented and briefly discussed.

(a) Stillinger-Weber potential

The Stillinger-Weber (SW) potential (Stillinger and Weber, 1985) is one of the first potentials that attempt to model a semiconductor with a classical model. The SW potential contains both the two-body and three-body interactions and can be expressed as

$$E = \sum_{i<j} V_2(\vec{r}_i, \vec{r}_j) + \sum_{i<j<k} V_3(\vec{r}_i, \vec{r}_j, \vec{r}_k), \quad (2.13)$$

with

$$V_2(\vec{r}_i, \vec{r}_j) = A_{ij} \left[B_{ij} \left(\frac{\sigma_{ij}}{r_{ij}} \right)^p - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^q \right] \exp \left(\frac{\sigma_{ij}}{r_{ij} - \sigma_{ij} a_{ij}} \right), \quad (2.14a)$$

$$V_3(\vec{r}_i, \vec{r}_j, \vec{r}_k) = \lambda_{ijk} \left(\cos \theta_{ijk} + \frac{1}{3} \right)^2 \exp \left(\frac{\gamma_{ij}}{r_{ij} - \sigma_{ij} a_{ij}} \right) \exp \left(\frac{\gamma_{ik}}{r_{ik} - \sigma_{ik} a_{ik}} \right). \quad (2.14b)$$

In the two-body term, the parameters σ_{ij} is the equilibrium interatomic distance, while a_{ij} denotes the cutoff distance. In the three-body term, θ_{ijk} is the angle centered on the i th atom. The remaining parameters A, B, p, q, λ and γ are varied to modify the two-body and three-body interactions according to the interatomic distances and angles.

The SW potential was mainly developed for the study of Si crystals. Since then, it has been widely used due to its simplicity and fairly realistic description of the atomic interaction of Si atoms. Its three-body term defines the equilibrium configurations based on the diamond-like tetrahedral lattice structure and uses only the geometrical quantities such as distances and bond angles as variables to establish potential functions. Based on these concepts, new SW potentials have been developed (Jiang *et al.*, 2013; Zhang *et al.*, 2014), with either new energy terms or new parameterizations, to be applicable for a wider range of materials.

(b) Tersoff potential

The Tersoff potential (Brenner, 1990) was developed with the focus on the covalent bonds in semiconductor systems. It is based on the concept of bond order which describes the bond strength between two atoms as a function of the local environment. In other words, the Tersoff potential considers the effect of all the nearest neighbors of an atom when calculating its interaction with other atoms, even though it only contains a two-body term.

The analytical form of the two-body term of the Tersoff potential is shown as follows

$$V_2(\vec{r}_i, \vec{r}_j) = f_c(r_{ij}) [f_R(r_{ij}) + b_{ij} f_A(r_{ij})], \quad (2.15a)$$

$$f_c(r_{ij}) = \begin{cases} 1, & r_{ij} < R - D \\ \frac{1}{2} \left\{ 1 - \sin \left[\frac{\pi}{2} \frac{(r_{ij} - R)}{D} \right] \right\}, & R - D < r_{ij} < R + D, \\ 0, & r_{ij} > R + D \end{cases} \quad (2.15b)$$

$$f_R(r_{ij}) = A \exp(-\lambda_1 r_{ij}), \quad (2.15c)$$

$$f_A(r_{ij}) = B \exp(-\lambda_2 r_{ij}), \quad (2.15d)$$

$$b_{ij} = \left(1 + \beta^n \zeta_{ij}^n \right)^{-\frac{1}{2n}}, \quad (2.15e)$$

$$\zeta_{ij} = \sum_{k \neq i, j} f_c(r_{ik}) g(\theta_{ijk}) \exp \left[\lambda_3^3 (r_{ij} - r_{ik})^3 \right], \quad (2.15f)$$

$$g(\theta_{ijk}) = 1 + \frac{c^2}{d^2} - \frac{c^2}{[d^2 + (\cos \theta_{ijk} - \cos \theta_0)^2]}. \quad (2.15g)$$

Here, $f_c(r_{ij})$ is the cutoff function which ensures only the nearest-neighbor interactions are taken into consideration and R and D are the cutoff distance parameters. The $f_R(r_{ij})$ and $f_A(r_{ij})$ functions represent the repulsive and attractive atomic interactions, respectively. The parameters A and B denote the cohesive energies, while λ_1 and λ_2 are the lattice parameters.

The parameter b_{ij} represents the bond orders and is determined by the local coordination of atoms around the centered i th atom. The introduction of the parameter b_{ij} is to account for the effect of the local environment on the atomic bond strength in the real systems, i.e., an atom with more neighbors forms weaker bonds than an atom with fewer neighbors. In the expression of b_{ij} , ζ_{ij} is the effective coordination number of the atoms, i.e., the number of the nearest neighbors, and takes into consideration the relative distance $r_{ij} - r_{ik}$ of two neighbors of the i th atom and the bond angle θ_{ijk} ; β and n are the adjusting parameters chosen to reflect the realistic lattice structure and physical properties of a specific material;

λ_3 is the cutoff parameter that determines the range for the calculation of ζ_{ij} . In the bond angle distribution function $g(\theta_{ijk})$, θ_0 is the equilibrium bond angle, and c and d are dimensionless parameters that determine the strength of the bond angle effect.

The Tersoff potential is first calibrated for Si systems and later for carbon (C) systems, and is validated by calculating their cohesive energy, elastic constants, phonon frequencies, defect energies and migration barriers. The results obtained with this potential were in good agreement with experiments and *ab initio* calculations. So far, the Tersoff potential can be applied to various different systems, including Si-C hybrids, Si-O oxides, and several other semiconductor systems such as germanium and gallium.

(c) Modified Embedded Atom Method (MEAM) potential

The MEAM potential is developed by Baskes (1992) and initiated from the covalent bonding in Si (Baskes, 1987). It is an extended form of the Embedded Atom Method potential obtained by considering the angle-dependent electron density in the semi-empirical formalism to model the bond bending effect. Consequentially, the shear behavior which includes effects such as the directionality of bonding and bond bending can be taken into account. Baskes further improved the formalism and applied it to a wide variety of materials and impurities, and thus the MEAM potential is capable of describing the elastic behavior and simple defect properties of materials (Baskes *et al.*, 1989; Baskes, 1992; Baskes and Johnson, 1994; Baskes, 1997).

In the MEAM potential, every atom is treated as an impurity embedded in a host lattice consisting of all other atoms. As a result, calculations can be done using the electron densities and the inclusion of impurities in structures that contain cracks, surfaces and alloying elements can be treated realistically. The electron densities are estimated by the linear

superposition of the spherically averaged atomic electron densities. The embedding energy of the atoms E_{total} depends on the local environment around the impurity and is given by

$$E_{total} = \sum_i \{F_i(\bar{\rho}_i) + \frac{1}{2} \sum_{i \neq j} \phi_{ij} r_{ij}\}, \quad (2.16)$$

where F is the embedding energy expressed as a function of $\bar{\rho}_i$ which represents the electron density of the host atom without atom i , and ϕ is the short-range electrostatic pair potential. The pair interaction is then summed over all neighbors j of atom i within the cutoff distance. Hence, the material properties such as the lattice constant and elastic constants can be obtained from Eq. (2.16).

The MEAM has been applied to many cubic metals such as the face-centered cubic and body-centered cubic metals, semiconductors and also diatomic gaseous elements. Simplification to the first nearest neighbors is also made possible to reduce the computational time. Currently, the MEAM has also been extended to the hexagonal close packing metals (Baskes and Johnson, 1994).

2.3.1.3 Applications

For cracking in Si substrate, MD simulation is able to introduce intrinsic defects, such as voids and GBs, and analyse their effect via the stress-strain relations. Furthermore, through the atomic visualization, the effect of the intrinsic defects on the failure mechanisms can be better understood. In terms of interfacial delamination, MD models are able to provide insights to the interfacial behavior of the localized region under different mechanical loading conditions, as MD simulation is able to take into account the chemical interaction of the atoms at the interface, such as bond affinity, defects formation and delamination propagation. Thus, MD simulation is able to simulate the stress distribution under an applied displacement during interfacial separation. At the same time, the effect of defects such as interfacial and

bulk material voids can also be investigated. Such defects may favour and expedite delamination process, resulting in shorting between layers and causing electrical failure in the 3D IC devices (Madenci *et al.*, 1998; Fan and Yuen, 2010).

Many researchers have also employed MD simulation to understand fracture and the material properties (Dahl *et al.*, 2009; Sun *et al.*, 2013). For instance, Zhang *et al.* (2012) created a hybrid model by integrating two-temperature model and used MD simulation to investigate the interfacial properties of the Cu/Al system under thermal flux conditions. The results showed that the interfaces of dissimilar materials are prone to crack initiations, leading to delamination at high temperature condition. Similarly, Yang *et al.* (2009) also used the same methodology as Zhang *et al.* and the simulation results revealed that the temperature distribution along the interface is non-uniform and at some regions, large temperature gradients and severe plastic deformation are present.

Recently, Sun *et al.* (2013) found that the presence of localized void defects significantly degrades the mechanical properties, such as Young's modulus and surface hardness, of Si. Dahl *et al.* (2009) studied the effect of grain growth on the mechanical properties of Si. Through experiments, the authors attributed the deviation of mechanical properties of the granular Si from the single crystal counterpart to the presence of grain boundary sliding.

Recent breakthroughs in methodologies and development of the empirical interatomic potentials have significantly increased the feasibility and the accuracy of MD models. Therefore, with proper formulation and appropriate use of boundary conditions, potential functions and simulation procedure, MD simulation is able to provide a good understanding of fracture at the fundamental level and play an essential role in guiding the design and optimization of materials used for 3D IC applications (Fan and Yuen, 2013). Hence in this work, MD simulation is conducted to study the fracture behaviours of bulk Si, bilayer and multilayer systems.

2.3.2 Finite element method

FEM is a numerical method and an excellent simulation tool that has been widely employed in failure analysis. It is able to solve problems with complicated geometries, loadings and material properties. Thus, it is commonly used to analyze and quantify the stresses induced in the package due to the assembly and operating processes. As the design geometry in 3D ICs is complex due to the presence of many layers of different materials, it is important to first understand the physical behaviors and define material properties of the materials used in 3D ICs, in order to obtain accurate results.

Previous FEM works have been performed to characterize failure in 3D ICs to help to overcome the design and their associated reliability problems. For instance, in the study of interfacial delamination failure, Chernin and Volokh (2004) conducted a qualitative analysis of the thin film delamination via FEM. The authors concluded that the dominant failure mode of the thermal delamination of the film is through shearing (Mode II) and the gradient of the thermal load and interfacial anomalies can influence the delamination process and the site of initiation (at the free edge or internal area) respectively. Wen and Basaran (2004), on the other hand, used an analytical procedure based on classical plate theory to calculate the interfacial shear and peeling stresses in the layered structure under thermal gradient.

Wiklund *et al.* (1999) studied the effect of the interface topography, coating thickness and elastic mismatch on the interfacial stresses via FEM. The authors found that the interface topography is more sensitive to the induced stresses as compared to thickness of the coating. At the critical coating thickness, the normal stress across the interface is comparable to the induced residual stresses. The effect of thickness of coatings on the interfacial stresses weakened as the thickness increases. The authors also carried out experiments to show that the localized fracture and delamination occur in ceramic materials that are subjected to high residual stresses. Fan *et al.* (2001) also tried to predict the likelihood of delamination at a

bimaterial wedge using maximum hoop stress criterion. The FEM model is built to define the corresponding parameters required for analytical calculation. The authors found that the opening stress intensity factor along the interface is vital in predicting the interfacial delamination failure.

2.3.2.1 Cohesive zone modelling

In the recent years, the CZM has been commonly used to simulate fracture in materials and structures. It is assumed that ahead of the physical crack tip, there exists a cohesive zone made up of the upper and lower surfaces held by a cohesive traction. When an external force is applied to the bilayer model, the upper and lower surfaces of the interface undergo separation. When the separation of these surfaces at the edges of the model exceeds a critical value, the interfacial crack will propagate. As such, energy flows into the fracture process zone for surface separation and the interfacial cohesive relation can be therefore governed by the traction-separation law.

The traction-separation law is well-described by the maximum cohesive strength, separation distance and energy release rate (Shet and Chandra, 2002). The energy release rate is associated with the bonding ahead and the plastic dissipation behind of the crack tip while the cohesive strength is dependent on the bonding at the interface and is affected by interfacial defects and residual stresses. Overall, the energy release represents the strain energy dissipation during crack propagation and the cohesive strength set the limit for the initial interfacial separation.

The advantage of using the traction-separation law is to eliminate the assumption that the interface is either fully-bonded, fully-debonded, or pre-cracked. Since the interfacial crack nucleation and propagation criteria are inherently included in the traction-separation law, its onset and propagation process can be captured and predicted. The CZM was initially

proposed to eliminate the crack tip stress singularity in mode I fracture (Barenblatt, 1962) but later, it is also applied to mode III fracture (Zhang and Deng, 2005). In order to eliminate the crack tip stress singularity, it is necessary for the cohesive traction to be a nonzero value at a very small separation displacement (Jin and Sun, 2005).

In addition, the fracture energy release mechanism is also required when the stress singularity at the cohesive zone tip is present. When the cohesive zone is very small, the fracture energy in the CZM is the same as the critical energy release rate in the linear elastic fracture mechanics. It is also necessary to predefine the direction of crack growth, i.e. crack growth at the interface (Fouk *et al.*, 2000). Although more accurate and real material system behaviours can be simulated with very complex CZMs, it is also more difficult for convergence to occur.

In the CZM, it is assumed that the tractions will gradually increase till a critical value before decreasing back to zero as the separation distance increases. The thickness of the interface during the unloaded state is also assumed to be zero. Tvergaard and Hutchinson (1993) introduced the traction-separation model as seen in Fig. 2.11 where the δ_n and δ_t are the normal and tangential components of the relative displacement of the respective surfaces across the interface in the cohesive zone.

Figure 2.11. The traction-separation relation governing the interfacial separation (Wei and Hutchinson, 1999).

Subsequently, a parameter λ is introduced to define the shape of the traction-separation relation and it is defined as

$$\lambda = \sqrt{(\delta_n / \delta_n^c)^2 + (\delta_t / \delta_t^c)^2} \quad . \quad (2.17)$$

The tractions are supposed to be zero when $\lambda = 1$. A potential form which the interfacial tractions in the separation zone are derived is expressed as

$$\Pi(\delta_n, \delta_t) = \delta_n^c \int_0^\lambda \sigma(\lambda') d\lambda' \quad . \quad (2.18)$$

And the normal T_n and tangential T_t components of the traction are given by

$$T_n = \frac{\partial \Pi}{\partial \delta_n} = \frac{\sigma(\lambda)}{\lambda} \frac{\delta_n}{\delta_n^c} \quad , \quad (2.19)$$

$$T_t = \frac{\partial \Pi}{\partial \delta_t} = \frac{\sigma(\lambda)}{\lambda} \frac{\delta_t}{\delta_t^c} \frac{\delta_n^c}{\delta_t^c} \quad . \quad (2.20)$$

In the case of Mode I fracture, T_t is assumed to be zero to achieve a purely normal separation. The maximum normal traction $\hat{\sigma}$ obtained during pure normal separation is also known as the interfacial strength and the work of separation per unit area of the interface Γ_0 is given by

$$\Gamma_0 = \frac{1}{2} \hat{\sigma} \delta_n^c [1 - \lambda_1 + \lambda_2] \quad . \quad (2.21)$$

The stress-strain relation for material is assumed to be:

$$\varepsilon = \sigma / E \quad \text{for } \sigma \leq \sigma_Y \quad . \quad (2.22)$$

The parameters required for the CZM are the elastic constants E , Poisson ratio ν and yield stresses σ_Y of the thin film and substrate and the Γ_0 and $\hat{\sigma}$ of the interface (Wei and Hutchinson, 1998). Since the mode I CZM only contains the opening failure mode, the traction-displacement relation can be expressed by

$$\sigma = \sigma_c f(\delta / \delta_c) \quad . \quad (2.23)$$

where σ_c is the peak traction; δ_c is the critical separation displacement and f is the dimensionless function which relates to the shape of the cohesive traction-displacement relation in Fig 2.11.

Since the introduction of the CZM in the FEM, many works have been performed to solve problems such as crack tip fracture and interfacial cracks in bilayer systems as it can avoid stress singularity at the crack-tip and represent the physics of the fracture process at the atomic scale (Yamakov *et al.*, 2006; Ural *et al.*, 2009; Wu *et al.*, 2016). Despite its advantages, the outcome of the CZM is still rather limited as its accuracy is highly dependent on the input cohesive parameters.

Moreover, for the interfacial delamination study, it is rather difficult to characterize these effects to describe the interface based on experimental and numerical means as they are not able to account for the chemical effect on the interfacial behaviour. So far, these parameters, which are experimentally obtained, lack quality with regards to the nanosized samples. Therefore, it is essential to establish these critical parameters which are temperature and size dependent.

2.3.2.2 Applications

Reliable failure analysis predictions of the root cause of delamination failure and its mechanism cannot be made accurately unless supported by the precise description of the interface through which the mechanical, electrical and thermal integrities of the ICs are achieved. Even though MD simulation is capable of providing an accurate description of the interfacial behaviors at the atomistic scale, it is only suitable to model thousands of atoms efficiently. The geometry of nano/microelectronic IC packaging are usually in several nanometers to micrometers or even larger. It is almost impossible to build a full model using MD simulation due to the costly computational time.

Furthermore, as the material properties are strongly influenced by the surface effect, rising concerns are noted with regards to the application and representation of properties derived from the small MD model as compared to the actual model. Therefore, it is also essential to bridge the gap between the different length and time scales by transferring the atomistic information from the atomic level to the continuum level to obtain a good description of the interfacial fracture behavior at the macroscale.

Hence, instead of using the conventional approach whereby the cohesive parameters are extracted from experiment, these parameters can be derived from MD simulation and input into the CZM to study the interfacial delamination response under external loading at the macroscale. Henceforth, the interface atomistic behavior governed by chemical interaction of atoms can be incorporated into the interface model in FEM and the potentials of the available simulation tools can be maximized.

Namilae and Chandra (2005) developed a hierarchical multiscale model to study the mechanics of interfaces in carbon nanotube-based composites. This model used MD simulation to derive the atomistic information of the interface and link it to the macroscopic scale via the cohesive zone traction-displacement relations. Later, Fan and Yuen (2010) also used the same model to bridge the gap between the atomic and continuum levels. Similarly, the constitutive relations derived from MD 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.

Therefore in this PhD work, a similar methodology is adopted for the interfacial delamination study of multilayered systems. The FEM is coupled with MD simulation to obtain more accurate material parameters, such as interfacial fracture energies, so as to study

delamination in the layered structure more effectively. Subsequently, the simulated model is validated with experimental findings. This approach based on MD and CZM-FEM is capable of transferring the atomic behavior at the interface to the continuum model to increase the accuracy of the FEM model. Essentially, experiments that are usually time-consuming and challenging are no longer required. Ultimately, the interfacial properties of different bi-materials systems derived from MD can be used to build a multilayered structure to predict interfacial delamination in the whole IC packaging under different operating conditions.

2.3.3 Experimental techniques

The process of failure analysis begins from a macroscopic visualization of the defect sample. The background of the sample and its effect of failure are first reviewed and numerous hypotheses are drawn while any anomalies on the defect sample are noted and recorded under a low magnification microscope or X-ray. It is vital to conduct a thorough understanding of the sample background to avoid creating artifacts or damage the failure site. Subsequently, when the site of failure is identified or narrowed down, sample preparation is performed for more detailed inspection and investigation so as to better characterize the failure and determine the true root cause.

Some of the techniques used in the sample preparation include, chemical decapsulation which is used to remove the mold compound that encapsulates the IC package, and cross-sectioning of the exposed package using the focused ion beam to allow visual access to the site of failure, especially if the failure happen within the package or at the substrate. After the sample preparation, the site of failure is ready for inspection. Some of the non-destructive 2D visual inspection and failure analysis experimental tools used for mechanical failures include;

- Scanning electron microscopy (SEM)
- Energy dispersive X-ray analysis (EDX)

- Transmission electron microscopy (TEM)
- Scanning acoustic microscopy (SAM)
- Raman spectroscopy

Through the visual inspection, the initiation and site of failure can be isolated and the extrinsic defects can be identified. Crack patterns and change in surface morphology can be analyzed with the fractography and raman spectroscopy respectively to deduce the root cause of failure. With technological advancement, these 2D tools are able to provide excellent details of the surface morphology of a sample. However, they are only able to deduce the cause of mechanical failure by observing the aftermath of failure. They are not able to provide information about the process of failure, chemical interaction among the layers, intrinsic properties and stress distribution of the materials, which is particularly important when dealing with thermomechanical type of failure. Therefore, as ICs approaches 3D, these techniques which are catered for the planar ICs are inadequate for the characterization of failure modes and mechanisms in 3D ICs.

Sometimes, failure may occur due to the inherent material properties which may weaken the integrity of the material. Furthermore, the deduction of the response using conventional experimental tools is very much influenced by the skills of the analyst and the data obtained are also subjected to human errors. The fractography of metals are very well-established, whereby the crack morphology is able to show the type of failure and its root cause. However, for brittle materials such as Si, the crack studies are not well-developed.

Many experimental works have been carried out quantify and characterize failure. Erich *et al.* (1999) conducted the ball shear test with thermal preconditioning to evaluate the fracture on the nickel/gold bond pads. After cross-sectioning, the fractography revealed interfacial failure in the IC packages. Through detailed metallography and SEM with EDX, two distinct types of interfacial failure mechanisms were characterized, namely due to the

precipitation of gold-tin intermetallic during isothermal aging process and the embrittlement at the interface between the nickel-tin intermetallic.

Koripella *et al.* (1989), on the other hand, attempted to characterize failure in ceramics. They purposefully created cracks in chips by subjecting the chips to thermal processes similar to that experienced in the manufacturing processes. The cracked chips were then analysed by fractographic methods to determine the cause of failure. The results presented many different types of crack patterns when subjected to different thermal loadings. The findings also revealed that internal flaws such as voids and interfacial defects between layers are the main cause of the fracture in the chips.

However, with the miniaturization of 3D ICs, handling of the nanosized specimens can be very challenging, and thus many of the experimental techniques are still underdeveloped due to lack in quality and poor reproducibility. Therefore, the theoretical simulation tools, such as FEM and MD, are required to provide validation and new insights to the mechanical properties and fracture behavior of brittle materials, and thus help to increase the accuracy of root cause determination of 3D IC failure.

2.3.3.1 Three-point bend test

The three-point bend test is a classical experiment in fracture mechanics that is capable of quantifying many fracture parameters such as the fracture toughness and fracture strength. It is carried out by applying load to the center of the specimen while supported at its ends (Fig 2.12).

Figure 2.12. Schematic diagram of a rectangular bar under three-point bending.

Based on the classical beam theory, when the load P is applied in the midspan of the specimen of length L , the stress distribution across the width of the specimen ($2c$) is shown in Fig. 2.13 and the stress is essentially zero at the neutral axis. Stresses pointing in the positive and negative x -direction represent tensile and compressive stresses respectively. Within the elastic region, the load-displacement curve of the brittle materials shows a linear relation where yielding occurs on a thin surface layer of the specimen at the midspan. Subsequently, crack will start to initiate at this region and eventually propagates and leads to failure. Hence, the three-point bend test is commonly used to determine the yield stress of brittle materials whose stress-strain curves shows a distinct linear-elastic behavior before failure.

Figure 2.13. Schematic diagram of the stress distribution of the xy -plane of a rectangular beam under bending.

Therefore in the linear-elastic region, the fracture stress σ_f of the brittle rectangular beam under bending is defined by

$$\sigma_f = \frac{3M}{2tc^2}, \quad (2.24a)$$

$$M = \frac{PL}{4}, \quad (2.24b)$$

where M is the bending moment; c is half the length of the specimen width (Fig. 2.13) and t is the thickness of the specimen.

The fracture stress of the specimen subjected to bending is also known as the bending strength. The yield strength of the material can be obtained by substituting the P at the yield point in Eqs. (2.24a and b). The bending strain is given by

$$\varepsilon = \frac{6wv}{L^2}, \quad (2.25a)$$

$$v = \frac{PL^3}{48EI}, \quad (2.25b)$$

$$E = \frac{L^3}{32tc^3} \left(\frac{dP}{dv} \right), \quad (2.25c)$$

where v is the maximum deflection of the beam from the center; I is the moment of inertia of the cross-sectional area of the rectangular beam and E is the elastic modulus of the material which can be obtained from the gradient of the load-displacement curve $\left(\frac{dP}{dv} \right)$ in the linear region.

The three-point bend test has been widely used to evaluate the strength of brittle materials such as Si which is rather difficult to quantify based on the simple uniaxial tensile test. Patwardhan *et al.* (2005) studied the effect of the flexural testing on the wafer level components mounted on a printed circuit board and concluded that the very small wafer level devices should not be placed at the regions where the maximum deflection is experienced so as to increase the reliability of the devices.

Seah *et al.* (2003) also studied the delamination failure mechanism in the IC caused by the warpage of a printed circuit board assembly using the three-point bend test and found that the delamination between the intermetallic layers and the vias results in a reduction in the stiffness of the printed circuit board and subsequently caused a sudden change in the gradient of the load-deflection curves. Chengalva *et al.* (2000) investigated the effect of the thickness of the Si die on the fracture strength and their results have showed that a thinner die bent more than a thicker die. Hence, considering the ease of sample preparation and testing procedures, the three-point bend test is employed in this PhD study to investigate the fracture limit of brittle materials and provide validation to the simulation approach described in the following chapters.

2.3.3.2 Indentation test

Indentation test is commonly used as an experimental technique to determine the mechanical properties of materials, in particular that of thin-film/substrate systems, at the submicron to nanometer scales. It has been widely accepted as an effective method to study delamination failure in multilayered systems as it is able to quantify the work of interfacial fracture by allowing deformation to occur in a controllable manner and subsequently generating interfacial cracks on a very small scale and localized site (De Boer and Gerberich, 1996a; 1996b; Zhang and Zhang, 2012).

Indentation technique and the fundamental analysis are first developed by Pethicai *et al.* (1983) and Doerner and Nix (1986) respectively. Later, Oliver and Pharr (1992) further improved the indentation technique and analysis of the load-displacement (P - d) curve. The classical form of the hardness calculation is given by

$$H = \frac{P_{\max}}{A_p} \quad , \quad (2.26)$$

where $P_{\max}$ is the maximum indentation load and A_P is the projected contact area of the indentation. For a perfect Berkovich indenter, the A_P is expressed as a function of the contact depth h_c and estimated to be

$$A_P = 24.5h_c^2 . \quad (2.27)$$

The elastic and plastic properties of the material and the indenter can be derived from the P - d curve. With a high depth-sensing resolution and a fast responsive speed, the indentation system can detect even the slightest fluctuations of the material properties, such as plastic deformation, phase transformation and crack initiation, which are indicated by the discontinuities observed in the P - d curve (Cross *et al.*, 2006). Such discontinuities in the loading and unloading curves are known as ‘pop-in’ and ‘pop-out’ respectively.

In a film/substrate system, the ‘pop-in’ effect is mainly due to elastic-plastic deformation of the thin film and substrate which results in the formation of cracks, while the ‘pop-out’ effect may be due to the debonding of layers as the indenter is retracted or phase transformation of Si substrate at increased contact pressure. These fracture behaviours can be validated with visual inspection to further analyse the interfacial delamination and crack propagation paths.

The shape of the P - d curve and failure mechanisms involved are not only dependent on the type of the materials (brittle or ductile), but also the type of indenters. The most commonly used indenter is the Berkovich which consists of a three-sided pyramid that has a centreline-to-face angle of 65.35° . The advantage of using the Berkovich indenter is that its contact area remains unchanged during the indentation process. The spherical indenter is also commonly used in the IC testing as it is able to replicate the ball bonding process to study the distribution of stresses and failure mechanisms involved.

During the loading process, the sample will undergo both elastic and plastic deformations. However, during unloading, there will only be elastic recovery in the sample which will result in a force experienced on the tip of the indenter as it retracts. Hence, the magnitude of the force recorded is able to relate to the amount of elastic recovery and the stiffness of the material. Therefore, the stiffness of the material can be derived from the load-displacement curve in the form:

$$S = \frac{dP}{dh} = \frac{2}{\sqrt{\pi}} E_r \sqrt{A}, \quad (2.28)$$

where h is the indentation depth and E_r is the reduced elastic constant of the material. Based on the model developed by Doerner and Nix (1986), the E_r can be obtained by the following equation:

$$\frac{1}{E_r} = \frac{(1-\nu^2)}{E} + \frac{(1-\nu_i^2)}{E_i} \quad (2.29)$$

where E is the modulus of the material, E_i is the modulus of the indenter, ν and ν_i are the Poisson ratio of the material and indenter respectively.

In addition, the differences in the loading and unloading processes may be attributed by the fracture phenomena observed in the deformed material. Such variances are often used to evaluate the energy dissipated due to the plastic deformation and fracture (Li *et al.*, 1997; Li and Bhushan, 1998; Malzbender and De With, 2000; Malzbender *et al.*, 2002). The work of indentation is usually defined by the area under the P - d curve and is significantly influenced by the indentation process. During the indentation process, this workdone can be transformed into elastic strain energy released during fracture, energy released due to plastic deformation and heat dissipation.

Li *et al.* (1997) studied the cracks and spallation of the hard coating subjected to indentation loading and the fracture process during loading is separated into three stages as

shown in Fig. 2.14a. In the first stage, the thin hard coating is compressed onto the substrate and crack is initiated due to the high contact stress by the indenter. In the second stage, the through-thickness crack and delamination are observed as the edges of the thin film buckle. Lastly, in the third stage, the thin film flexes and the elastic energy released contributes to the interfacial crack propagation. Eventually, the interfacial crack propagation will come to a stop due to the limitation of the through-thickness crack. Hence, the through-thickness crack and the buckling of the thin film will result in the ‘pop-in’ in the P - d curve as observed in Fig 2.14b. The energy dissipated can be computed from the area ABC.

Figure 2.14. The schematic diagrams of (a) the three stages of nanoindentation fracture for thin hard coatings coated system (Zhang and Zhang, 2012) and (b) the P - d curve and the fracture energy evaluation is based on previous works. (Li *et al.*, 1997; Li and Bhushan, 1998)

More recently, Lu and Huang (2015) characterized the interfacial energy release rate of the relatively tough SiN/GaAs film/substrate system via cyclic indentation loading. Their results show that the film experiences the hardening effect, and subsequently sufficient elastic strain energy is allowed to be accumulated and the interfacial delamination can be initiated. Hence, delamination is driven by the tensile stresses during the unloading process, attributed by the increased stored elastic strain energy of the film and the plastic deformed substrate.

Thus, for different types of film/substrate systems when subjected to indentation loading will result in different P - d curves due to the various failure mechanisms involved (Swain and Menčík, 1994). In order to characterize the interfacial fracture behaviour, the characteristics of the P - d curve and the fracture mechanics of the interface must be carefully evaluated and analysed.

2.4 Summary

The general failures seen in the 3D ICs are first reviewed. The two common types of failure, mainly the Si substrate cracking and interfacial delamination, which are the focus of this PhD study, are discussed in details. The factors that affect the fracture strengths and the failure mechanisms involved in these failures are reviewed. Lastly, the failure analysis methodologies are briefly discussed and those used for this PhD study are outlined in details. These methodologies are then combined to develop new failure analysis approaches to provide a multiscale understanding to the failure mechanisms involved in these 3D ICs.

Chapter 3. Modelling and Characterization of Fracture Behavior in Bulk Silicon

As fracture in Si is one of the common failures observed in IC packaging, it is essential to understand and explain the failure modes and mechanisms involved. In this chapter, the effects of crystallographic orientation, defects, grain boundaries, and temperature on the tensile properties and failure mechanisms of Si are first investigated via MD simulation, to provide a fundamental understanding to the types of failure modes and mechanisms. Then, the three-point bend experiment is conducted to validate and replicate failure modes observed in the MD simulation and in the real samples respectively. Lastly, a combined approach based on MD simulation, FEM and experiment is developed to deduce the root cause of failure of a Si die.

3.1 Methodology development

3.1.1 Simulation models

3.1.1.1 Molecular dynamics simulation

The fracture response of the bulk Si is first simulated via MD simulation to understand the effects of crystallographic orientation, defects and grain boundary on the fracture strength and failure mechanism of Si. Firstly, for the investigation of the crystallographic orientation effect, the dimensions of the computational cells are set as $15.4 \times 24.4 \times 44.5$ nm and the periodic boundary condition is applied in the x -, y - and z -directions to simulate the bulk Si. The $\langle 100 \rangle$ oriented and $\langle 111 \rangle$ oriented Si cells are considered and subjected to different loading directions to investigate the effect of crystallographic orientations and they are summarized in Table 3.1.

Table 3.1. The different loading directions for Si cells fracture simulation.

Die	Loading direction
$\langle 100 \rangle$	$[010]$ and $[001]$
$\langle 100 \rangle$	$[011]$ and $[0-11]$
$\langle 111 \rangle$	$[1-10]$ and $[11-2]$

For the investigation of the defect effect, the periodic boundary condition is applied in the y -direction and the free boundary condition is used along the x - and z -direction to simulate an infinitely long thin film. The defect is introduced on the yz - and xz -surfaces respectively to investigate the effects of backgrinding groove depth d and dicing notch length c on the fracture response of Si (see Fig. 3.1a and b).

Figure 3.1. The MD model of y -direction tensile loading for (a) backgrinding groove (b) dicing defect, where d and c are the depth and length, respectively.

Lastly, the fracture behavior for the notched single- and bicrystalline Si nanofilms with $\Sigma 25(001)\langle 001 \rangle$ twist GB or $\Sigma 25(710)\langle 010 \rangle$ tilt GB are investigated for the grain boundary effect (Fig. 3.2). The dimensions of the computational cells are set as $15.3 \times 3.8 \times 54.3$ nm and the GBs are arranged to be parallel to the xy plane (Fig. 3.2b). The grains of the bicrystals are of the same size. Based on the CSL model, the $\Sigma 25$ twist GB is constructed by rotating the upper and lower grains through the angles of $+8.13^\circ$ and -8.13° about the $[001]$ axis

respectively, as shown in Fig. 3.3a. Similarly, for the $\Sigma 25$ tilt GB, the upper and lower grains of the cell are rotated at the angles of $+8.13^\circ$ and -8.13° about the $[010]$ axis respectively (Fig. 3.3b).

A penetrating notch along the y -direction is introduced on the left surface (parallel to the yz plane) of the nanofilm and located on the same xy plane as that of the GB introduced. The notch has a depth of $2a$ where a is the lattice constant of bulk Si. The periodic boundary conditions are applied in both y - and z -directions, while free boundary condition is used along the x -direction to model an infinite large thin film. The simulation is conducted by using the large-scale atomic/molecular massively parallel simulator (LAMMPS) (Plimpton, 1995). The atomic interactions between the Si atoms are described by the SW potential (Stillinger and Weber, 1985).

Figure 3.2. The computational cells for notched (a) single-crystalline and (b) bicrystalline Si nanofilms before deformation.

Figure 3.3. The atomic configurations of the bicrystals with (a) twist $\Sigma 25$ GB along the (001) plane and (b) tilt $\Sigma 25$ GB along the (010) plane for the upper grain.

The initial structures are first relaxed to obtain the state with the minimum local potential energy. Afterwards, the system is equilibrated at constant 300 K and zero external stress by using the isothermal-isobaric (NPT) ensemble via the Noose-Hoover thermostat for about 40 ps. Upon achieving equilibration, the system is switched to the constant volume and temperature (NVT) ensemble and the uniaxial tensile strain is applied at a constant strain rate of 10^8 s^{-1} . The tensile strain on the Si cells is realized by deforming the simulation cell with the same strain rate along their respective loading directions. For the case of thin-film Si, as the free boundary condition is applied in the x -direction, the volume of the specimen may vary during the deformation process, despite the NVT ensemble being employed. Subsequently, the stress-strain curves are then obtained whereby the stresses are computed using the virial theorem (Shen and Atluri, 2004).

3.1.1.2 Finite element method

Past failure analysis have suggested that when the IC package is subjected to the temperature cyclic conditions, such as the reflow process, the Si die will undergo warpage due to the boundary conditions imposed by the mold compound, the die attach and other components in the IC package. When these induced thermomechanical stresses exceed the

fracture limit of the Si die, it will result in catastrophically fracture. Thus, FEM is carried out to provide a stress analysis of the warpage profile of the different oriented Si dies under temperature cyclic loading.

A high-order 3D FEM model of an IC package is built via the ANSYS full 3D static structure simulation (Fig. 3.4). The configuration of the model is based on a failed IC package which contains two differently oriented Si dies (<100> and <111> Si dies) where the <100> Si die is observed to be fractured into two parts. In the simulation, the <100> and <111> Si dies are assumed to be homogeneous and linearly elastic with the young moduli of 130 and 168 GPa and Poisson ratio of 0.064 and 0.262 respectively (Kim *et al.*, 2001). The FEM model is then subjected to five different stages of temperature loading, (i) 448 K, (ii) 296K, (iii) 233 K, (iv) 523 K and (v) 296 K. The stress distribution of the dies during the heating and cooling processes are then obtained and analyzed.

Figure 3.4. The ANSYS simulation model of the IC package under thermal cyclic loading.

3.1.2 Experimental method

The three-point bend test is performed on the bare Si dies with different orientations to validate the MD simulation findings, investigate the failure modes involved and determine the fracture strengths of bare Si dies of different crystal orientations under bending at the

microlevel. The die specimens have the orientation of $\langle 100 \rangle$ and $\langle 111 \rangle$ and they are prepared by dicing the Si wafers in the specific crystallographic orientations.

A notch with a size of $1/50$ of the length of the die is also introduced to study the effect of notch defect on the fracture response of the bare Si dies (Fig. 3.5a). The die specimen has a dimension of $10 \times 10 \times 0.5$ mm. A load-controlled bending test is performed via an INSTRON 8848 tester using 500N load cell (Fig. 3.5b). The specimens are subjected to a loading rate of 0.01 mm/s and a load span of 8 mm is also used to ensure that specimen is subjected to pure bending only. The fracture strengths and the failure modes are obtained and analyzed.

Figure 3.5. (a) A through-notch introduced at the edge of the die, and (b) the set-up of the three-point bend test.

3.2 Fracture strengths and failure mechanisms

3.2.1 Crystallographic orientation effect

The single-crystal Si cells with different crystallographic orientations are simulated under tensile loading via MD simulation. Figure 3.6 shows the stress-strain relations obtained at 300K for single-crystal Si with different crystallographic directions subjected to different

loading directions. For the $\langle 100 \rangle$ Si die, subjected to loading in $[010]$, $[001]$, $[011]$ and $[0-11]$ direction are denoted by $\langle 100 \rangle/[010]$, $\langle 100 \rangle/[001]$, $\langle 100 \rangle/[011]$ and $\langle 100 \rangle/[0-11]$ respectively. For the $\langle 111 \rangle$ Si die, subjected to loading in $[1-10]$ and $[11-2]$ are denoted by $\langle 111 \rangle/[1-10]$ and $\langle 111 \rangle/[11-2]$ respectively.

Figure 3.6. The stress-strain relations for the single-crystal Si nanofilms of different crystallographic directions subjected to uniaxial tensile loading at 300 K.

It is observed that the $\langle 100 \rangle/[010]$ and $\langle 100 \rangle/[011]$ Si cells have similar fracture strengths of about 31 GPa. This is because the (010) and (001) belong to the same family of $\{100\}$ crystallographic planes, and thus when subjected to tensile loading in the $y[010]$ and $z[001]$ directions, their fracture strengths and elastic moduli are similar.

On the other hand, the $\langle 100 \rangle/[011]$ and $\langle 100 \rangle/[0-11]$ Si cells have similar fracture strength of about 29 GPa. Similarly, as the (011) and $(0-11)$ fracture planes are from the same family of $\{011\}$ crystallographic planes, the different loading in the y - and z -direction will not have much influence on the fracture strength and elastic modulus.

The fracture strength for the $\langle 100 \rangle$ Si with the crystal orientation of $x[100]/y[011]/z[0-11]$ is slightly lower than that of the $\langle 100 \rangle$ Si with the crystal orientation of $x[100]/y[010]/z[001]$. This slight difference in fracture strength is due to the difference in the failure mechanism

involved. When the tensile loading is applied to the $x[100]/y[010]/z[001]$ oriented $\langle 100 \rangle$ Si cell, fracture occurs in the $\langle 110 \rangle$ direction through sliding dislocation instead of brittle fracture in the $\langle 100 \rangle$ direction, as shown in Fig. 3.7a. Hence, since both of the different oriented $\langle 100 \rangle$ Si cells undergo similar fracture behaviour in the $\{110\}$ plane (Figs. 3.7a and b), their fracture strengths are found to be comparable. Experimentally, Ando *et. al.* (2004) reported that the average fracture strengths of $(100)/\langle 010 \rangle$ and $(100)/\langle 011 \rangle$ single-crystal Si are also comparable with the values of ~ 5.36 GPa and ~ 4.82 GPa respectively. Hence, the MD observations are coherent with the experimental findings.

For the $\langle 111 \rangle$ single-crystal Si, the fracture strength is lowered by $\sim 30\text{-}50\%$ as compared to the earlier cases of the $\langle 100 \rangle$ Si cells, regardless of the loading direction. Zhang *et. al.* (2001) explained that the energy required for cleavage is proportional to the bond density, i.e. the number of bonds per unit area. When sufficient stress is applied to the single-crystal Si, it will cleave along a plane or fracture in a direction that involves the least number of atomic bonds to be broken. The relative bond densities across the planes of $\{111\}$, $\{110\}$, $\{112\}$ and $\{100\}$ of Si are in the ratio of $1:\sqrt{1.5}:\sqrt{2}:\sqrt{3}$ (Zhang and Zhang, 2001; Cook, 2006). Hence, when the Si cells are subjected to the tensile loading in the $\langle 110 \rangle$ and $\langle 112 \rangle$ directions, lower stresses are required for cleavage along the $\{110\}$ and $\{112\}$ planes as compared to the $\langle 100 \rangle$ directions (Figs. 3.7b and c).

Figure 3.7. The atomic configurations of (a) $x[100]/y[010]/z[001]$, (b) $x[100]/y[011]/z[0-11]$ and (c) $x[111]/y[1-10]/z[11-2]$ oriented Si cells subjected to tensile loading in the y-direction at different strains. Atoms are highlighted in red to illustrate the direction of fracture

Furthermore, many theoretical studies have also shown that when Si is subjected to mechanical stresses at ambient temperature, it will cleave in the planes with the low bond densities into the $\{111\}$ plane which is the most preferred cleavage plane before propagating in the $\langle 110 \rangle$ or $\langle 112 \rangle$ directions (Sherman, 2006; Kermode *et al.*, 2008; Danilewsky *et al.*, 2013). Therefore, the orientation of the planes will influence the fracture strength due to the difference in their bond densities.

In addition, from the stress-strain curves in Fig. 3.6, the elastic moduli E of $\langle 100 \rangle/[011]$ and $\langle 111 \rangle/[1-10]$ Si dies are obtained to be about 124 and 129 GPa respectively, while the E of $\langle 100 \rangle/[010]$ Si die is found to be slightly lower about 101.5 GPa. From the literature (Hopcroft *et al.*, 2010), the elastic constants of $\langle 100 \rangle$ and $\langle 110 \rangle$ bulk Si at 298 K are 130 and 169 GPa respectively. The deviation of values from the literature is due to size effect, whereby the reduction of size increases the surface effect, and thus affecting the mechanical properties of Si.

However, the differences in E for the different oriented Si cells can be explained by the interplanar spacing of the different fracture planes. The elastic modulus is proportional to the second derivative of the potential energy curve with respect to the interplanar spacing of crystallographic plane, whose normal is parallel to the axial loading direction. Based on Bragg's law, the interplanar spacing d_{hkl} is obtained by Eq. (3.1),

$$d_{hkl} = \frac{a^2}{\sqrt{h^2 + k^2 + l^2}} \quad , \quad (3.1)$$

where a is the crystal lattice constant and h , k and l are the miller indices. Hence, for the $\{010\}$ fracture plane has the d_{010} of 29.4, whereas for the $\{110\}$ fracture planes have a d_{011} of

20.8. This implies that the {100} fracture plane have lower resistance (higher d) to deformation as the adjacent planes are further apart, and thus a lower E is expected. Fujii *et al.* (2006) also reported that the E of the thin-film Si subjected to the [100] loading direction is lower than that of the [111] loading direction.

Therefore, the MD results show that the fracture strengths and elastic moduli of the single-crystal Si nanofilms are dependent on the surface crystallographic orientation and loading direction respectively. Overall, the MD findings are very promising as it is able to provide the theoretical explanation for the effect of the different crystallographic orientations on the fracture strengths and mechanisms involved in Si.

Subsequently, the three-point bend test is performed to validate the MD simulation findings, investigate the failure modes involved and determine the breaking strength of the different oriented bare Si die under bending at the macrolevel. From the experiment data obtained in Fig. 3.8, it is observed that the same family of planes with the same bond densities have relative similar fracture strengths which is coherent to that of the MD findings. It is noted that the $\langle 100 \rangle$ Si die subjected to bending in the $\langle 100 \rangle$ directions have the highest fracture strength of ~ 730 MPa while for the rest of cases, the fracture strengths are ~ 450 MPa.

The crack propagation paths of the different oriented Si dies subjected to bending in the different directions and the crack fractography of the $\langle 100 \rangle$ /[0-11] case are shown in Figs. 3.9 and 3.10 respectively. The deflection of the crack propagation path can be explained by the fracture energies of the different crystal planes. It is observed that for the $\langle 100 \rangle$ die when subjected to loading in the [0-11] direction, crack propagates along the preferred (110) crack plane without deflection. From the crack fractography analysis, the high impact stress induced by the bending load caused distinct unstable kinked crack fractography at the top part of the die while a smooth crack fractography is observed at the lower part of the die. This

observation is also consistent with the experimental results obtained by Sherman (2009) as shown in Fig. 3.11. When subjected to high bending stress, crack is first initiated at the contact point before undergoing fast crack propagation. Subsequently, in the presence of this pre-crack, crack will continue to propagate in a stable manner, resulting in the smooth crack surface finishing.

Figure 3.8. The maximum fracture stresses of the dies subjected to bending in the different directions are plotted for comparison. The good dies are represented by solid lines while, the notched dies are represented by dotted lines.

Figure 3.9. Crack propagation paths of the different oriented Si dies subjected to loading in different directions. The crack propagation paths are outlined in red.

Figure 3.10. Crack fractography analysis of the $\langle 100 \rangle$ die subjected to $[0-11]$ loading direction.

Figure 3.11. The optical and schematic presentation of the deflection phenomenon: specimens with relatively long notches cleave along the (110) cleavage plane (a), while those with shorter notches cleaved along the (111) cleavage plane (c). The crack in specimens with intermediate notches' length propagated first along the (110) plane, and thereafter the crack was deflected to (111) plane (b). The crack direction is from left to right (Sherman, 2009).

Overall, the MD and experimental results are very promising as the MD findings are able to provide an understanding of the difference in fracture strengths and failure modes observed in Si dies with different crystal orientations and explain the true failure response observed in the experiment. The fracture strengths determined by the experiment are able to provide the fracture limit of the good Si die sample at the macrolevel. In the next sub-section, the effect of defects on the fracture strength and failure mechanism of Si is investigated.

3.2.2 Defect effect

The effects of backgrinding groove and sawing notch defects on the fracture behavior of the different oriented single-crystal Si nanofilms are investigated via MD simulation. Figure 3.12 shows the stress-strain relations of the different crystallographic orientation of Si nanofilms with different groove depths and notch lengths. Generally, the presence of these stress concentrators will result in the reduction in the fracture strengths of Si nanofilms. It is observed that the presence of these structural defects has the most detrimental impact on the fracture strength of the $\langle 100 \rangle / [010]$ Si nanofilm as compared to the $\langle 100 \rangle / [011]$ and the $\langle 111 \rangle / [1-10]$ single-crystal Si nanofilms.

In addition, the presence of the dicing notch defect has more adverse impact on the fracture strength than that of the groove mark. For example, it is observed in the $(100) / [010]$ Si nanofilm that with a groove depth of 10% with respect to the thickness, the fracture strength is reduced by $\sim 11\%$, whereas with a dicing notch length of 10% with respect to the length of the nanofilm, the fracture strength is reduced by 30% (Figs. 3.12a and d).

For the $\langle 100 \rangle / [001]$ Si nanofilms, the earlier MD investigation of the crystal orientation effect on the fracture strength of Si nanofilms has revealed that Si nanofilms can fail via brittle fracture or sliding dislocation and that the $\{100\}$ planes have the highest fracture strength. Hence, even when the notch is introduced, the crack did not initiate at the crack tip nor propagation along the (010) plane, but instead it fails via sliding dislocation in the $\langle 110 \rangle$ direction (Fig. 3.13). Furthermore, despite the fact that the $\{111\}$ planes are the most energetically favored cleavage planes, sliding dislocation occurs in the $\langle 110 \rangle$ direction. This is explained by Zhang *et al.* (2001) that for the $\langle 100 \rangle$ Si wafer, the (111) and (110) planes are at an angle of 54.75° and 90° to the (100) plane respectively, and thus it is easier for sliding dislocation to happen in the $\langle 110 \rangle$ direction due to the bond density. The increase in

the length of the notch with respect to the length of the film has insignificant effect on the failure mechanism.

For the $\langle 111 \rangle / [1-10]$ Si nanofilms, the smooth single-crystal Si without defect undergoes brittle fracture. When a notch length of 5% of the length of the nanofilm is introduced in the xy surface, crack propagation occurs at the notch tip as expected. However, the crack propagation was subsequently arrested due to the lattice trapping observed at the tip of the notch (Fig. 3.14a). As a result of the lattice trapping, the stress required for further crack propagation is higher than that required to break Si-Si bond in a perfect $\{110\}$ plane. Eventually, the nanofilm fails via brittle fracture along the (111) plane of the Si nanofilm away from crack tip. Similarly, when the notch length is increased to 10% of the length of the nanofilm, crack propagation along (111) plane occurs to a small extent and then arrested as a result of the extensive lattice trapping at the tip. Subsequently, it is observed that the course of propagation has been diverted in the $\langle 110 \rangle$ direction (Fig. 3.14b). This phenomenon occurs because the lattice trapping at the notch tip increases the stress required for crack propagation along (111) plane, and thus the next energetic favorable plane would be the (110) plane. Hence, the crack is observed to propagate in that direction. Similar deformation process is also observed for the $\langle 100 \rangle / [011]$ Si nanofilm.

Figure 3.12. The stress-strain relations for the (a) $\langle 100 \rangle / [010]$, (b) $\langle 100 \rangle / [011]$ and (c) $\langle 111 \rangle / [1-10]$ Si nanofilms containing groove mark defect and (d) $\langle 100 \rangle / [010]$, (e) $\langle 100 \rangle / [011]$ and (f) $\langle 111 \rangle / [1-10]$ Si nanofilms containing dicing notch defect, when subjected to uniaxial tensile loading along y-direction. Curves for smooth single-crystalline Si nanofilms of different orientations are also plotted for comparison.

Figure 3.13. The atomic visualization of the failure mechanism of the $\langle 100 \rangle / [010]$ Si nanofilms with the (a) 5% and (b) 15% sawing defect notch length at different strains.

Figure 3.14. The atomic visualization of the failure mechanism of the $\langle 111 \rangle / [1-10]$ Si nanofilms with the (a) 5% and (b) 10% sawing defect notch length at different strains.

For the $\langle 100 \rangle / [011]$ and $\langle 111 \rangle / [1-10]$ Si nanofilms, when a groove line defect is added on the yz surface, in the z -direction, lattice trapping is also observed when the tensile loading is applied. As the groove line stretches in the z -direction, the concentration of lattice trapping is much higher than that seen in the sawing notch defect. Hence, the crack propagation only happen to a small extent and the ultimate failure mechanism is still via the brittle fracture along the perfect $\{011\}$ and $\{111\}$ planes within the nanofilms instead of at the groove tip. The increase of groove depth up to 20% of the nanofilm's thickness has insignificant effect on the failure mechanism but generally weakens the fracture strengths of the nanofilms.

For the $\langle 100 \rangle / [010]$ Si nanofilm, the groove depth of 10% of the film thickness has insignificant influence on the failure mechanism. The nanofilm still fails via sliding dislocation in the $\langle 110 \rangle$ direction at some region away from the groove defect, similar to that of a smooth specimen without defects (Fig. 3.15a). As the depth of the groove line increases, it is observed that cracks propagated initially along the (010) plane to a small extent and then undergo sliding dislocation in the $\langle 110 \rangle$ direction (Figs. 3.15b and c). The sliding dislocation at the groove tip shows that the presence of stress concentrator weakens the integrity of the Si nanofilms, and thus fracture occurs at the tip as the critical stress required is lower as compared to other regions away from the defect.

Therefore, the presence of structural defects in the different oriented Si nanofilms results in the different failure mechanisms when subjected to tensile loading. These MD results are helpful in providing insights to the failure mechanisms involved in Si nanofilms and also identifying the type of defects that has a more dominant effect on the fracture strength of the Si nanofilms and the crystal orientation of Si that is more sensitive to the defects.

Figure 3.15. The atomic visualization of the failure mechanism of the $\langle 100 \rangle / [010]$ Si nanofilms with the groove depths of (a) 10%, (b) 15% and (c) 20 % with respect to the thickness of the nanofilms, at different strains.

Lastly, the three-point bend test is performed to validate the MD simulation findings, investigate the failure modes involved and determine the breaking strength of bare die in the

presence of defects at the macrolevel. From the experiment data obtained in Fig. 3.8, it is observed that the fracture strengths for all the notched Si dies are significantly reduced to the range of 150 to 250 MPa as compared to the good Si dies, regardless of their orientation. The results also indicate that the $x[100]/y[010]/z[001]$ oriented die is more sensitive to the microdefects. Similar phenomenon is also observed in the MD results whereby the presence of an edge notch results in the substantial decrease in the fracture strength such that the fracture strengths for all the different oriented Si cells become comparable (Figs 3.12d, e and f).

The crack propagation paths of the different dies subjected to bending in the different directions are shown in Fig. 3.16a and they are found to be similar to that of the MD results (Fig. 3.16b). For the $\langle 100 \rangle/[001]$ case, both the experimental and MD simulation results show that the crack propagates in the $\langle 110 \rangle$ direction instead of the $\langle 100 \rangle$ direction. Similarly for the $\langle 100 \rangle/[0-11]$ case, both paths prove that the crack propagate via the preferred cleavage direction of $\langle 110 \rangle$. However, for the $\langle 111 \rangle/[112]$ case, the crack first propagate in the $\langle 112 \rangle$ direction before deflecting to $\langle 110 \rangle$ and $\langle 111 \rangle$ directions.

Therefore, this combined analysis of the MD and experiment results has shown that the MD findings are able to provide a theoretical and fundamental understanding and explanation to the fracture response of bulk Si at the macroscale. In the next sub-section, the effect of grain boundary on the fracture response of Si is investigated.

Figure 3.16. Crack fractography of (a) the notched dies of different orientations subjected to loading in different directions and (b) MD atomic configurations of the notched Si cells under tensile loading are also obtained for comparison. The crack propagation paths are outlined in red.

3.2.3 Grain boundary effect

In this investigation, the fracture behavior for the notched single- and bicrystalline Si nanofilms with $\Sigma 25(001)\langle 001 \rangle$ twist GB or $\Sigma 25(710)\langle 010 \rangle$ tilt GB are considered for the grain boundary effect. Figure 3.15 shows the stress-strain relations obtained at 300 K for both the single- and bicrystalline Si nanofilms with and without notch. The stress-strain curves for the single-crystalline and bicrystalline nanofilms are depicted by lines without and with symbols respectively.

It is found that for the smooth (without notch) single-crystalline nanofilm, the fracture strength is approximately 11.8 GPa which is close to that for the monocrystalline Si thin film subjected to [011] loading (~ 13 GPa) (Umeno *et al.*, 2005). The strength of the smooth bicrystalline nanofilm with the tilt GBs is slightly lower (~ 10 GPa), while the fracture strength of the smooth nanofilm with twist GBs is comparable to that of the smooth single-crystalline nanofilm. This is due to the fact that for the bicrystalline nanofilm with twist GBs and single-

crystalline nanofilm, the (001) plane is perpendicular to the loading direction, in spite of the change in the crystallographic orientation of the grains due to the twist GB.

Figure 3.17. The stress-strain curves for the Si nanofilms containing twist, tilt GBs, with and without notch, when subjected to uniaxial tensile loading along the z -direction. The curves for the single-crystalline Si nanofilms are also plotted for comparison.

With the addition of a notch, the fracture strength of the single-crystalline nanofilm decreases significantly by 40%, resulting in a much lower strength as compared to the bicrystalline cases. For the notched bicrystalline nanofilms with twist GBs, their fracture strength is reduced by ~20%, while the fracture strengths of the notched nanofilms with tilt GBs stay almost unaffected. In other words, the presence of a notch in the bicrystalline Si nanofilm with twist GBs is more detrimental to its strength than that with tilt GBs.

Interestingly, the slope of the stress-strain curve, i.e., the Young's modulus E , of the single-crystalline nanofilm decreases dramatically with the presence of notch and becomes lower than those of the bicrystalline nanofilms. Similar phenomenon has been observed in the

MD simulation of fracture behaviours of Si nanofilms with micronotches (Fujii and Akiniwa, 2006). This significant reduction in E is probably due to the effect of surface inhomogeneity induced by the defects, such as a notch. It is previously found that the elastic constants of Si thin films are lowered by the effect of inhomogeneity near the surface and the resulted change in the internal atomic displacement (Izumi *et al.*, 2004).

For the validation of the above simulation results, the Young's moduli E for the single crystalline and bicrystalline samples are calculated using a theoretical model and compared with the E obtained from the MD simulation. Theoretically, the E of bulk single crystalline Si is calculated by (Hopcroft *et al.*, 2010)

$$\frac{1}{E_{hkl}} = s_{11} - 2[(s_{11} - s_{12}) - \frac{1}{2}s_{44}](m^2n^2 + n^2p^2 + m^2p^2). \quad (3.2)$$

The terms m , n and p are the “direction cosines”: the cosine of the angle between the direction of interest $[hkl]$ and the X -, Y - and Z - axes while the term s_{ij} represents the compliance constant. The values of s_{ij} are obtained from Ref. (Hopcroft *et al.*, 2010).

Based on the elastic Hook's law, the ‘effective’ modulus of the bulk bicrystalline structure is estimated by (Berbenni *et al.*, 2013)

$$\mathbf{E}_{eff} = f\mathbf{E}^I(\mathbf{E}^*)^{-1}\mathbf{E}^{II} + (1-f)\mathbf{E}^{II}(\mathbf{E}^*)^{-1}\mathbf{E}^I, \quad (3.3)$$

where f is the volume fraction of each grain in the computational cell and $\mathbf{E}^* = (1-f)\mathbf{E}^I + f\mathbf{E}^{II}$. Here, the matrices $\mathbf{E}^I$ and $\mathbf{E}^{II}$ denote the elastic moduli for the upper and the lower grain respectively, and is calculated by Eq. (3.2).

For the single crystalline nanofilm, the E in $[001]$ direction obtained from the stress-strain relation in Fig. 3.17 is found to be ~ 105.5 GPa, while using Eq. (3.2), the bulk single crystal has E_{001} of 130 GPa. For the case of a bulk bicrystalline Si with twist $\Sigma 25$ GB, the calculated effective E_{001} is 115 GPa, while the E of the nanofilm with twist GB obtained

from the curve is 97.7 GPa. Similarly, for the case of a bulk bicrystal with the tilt $\Sigma 25$ GB, the calculated E_{001} is 118 GPa while the MD result demonstrates an E of 96.4 GPa.

These simulated values for the nanofilms are slightly lower than the E calculated for the bulk samples. This discrepancy is probably due to the surface effect and GBs which is not taken into account in Eq. (3.3). Similar discrepancy has also been found by Fujii *et al* that the stiffness for Si thin film obtained via MD is much smaller than that calculated using the FEM analysis as the surface has a significant effect on the deformation behaviour which is not included in the latter method (Fujii and Akiniwa, 2006). In general, the elastic moduli of the nanofilms obtained from the MD simulation in this study are close to the theoretically calculated values, and thus validating the tensile behavior observed for the Si nanofilms.

For all the nanofilms studied, it is observed that the tensile stress increases linearly with the strain before fracture. Generally, Si is classified as brittle material at room temperature and its plastic deformation is seldom observed in experiments. However, the simulation reveals that at the atomic scale, the single-crystalline Si subjected to tensile loading undergoes plastic deformation near its elastic limit through dislocation sliding mechanism along the fracture plane (Fig. 3.18a).

Similar plastic behavior has been reported in several MD simulation of Si and this behavior is mostly attributed to the empirical potentials used (Kang and Cai, 2007). One key mechanism for the occurrence of the plastic behaviors is the lattice trapping which is the energy barrier that can arrest crack propagation motion. If the lattice trapping is sufficiently large, failure mechanisms, such as dislocation nucleation and plastic deformation, could become active before brittle fracture can occur. Bernstein and Hess (2003) addressed the significance of the lattice trapping in the mechanical behavior of Si and showed that much

popular potentials, such as SW, tend to produce a large lattice trapping and often lead to a ductile-like fracture behavior.

Despite the plastic deformation, the crystal order in the Si nanofilm is relatively high, unlike that of ductile metals, whereby the generation of dislocations is much more extensive resulting in low crystal order (Komanduri *et al.*, 2001). Moreover, the plastic deformations in ductile metals are much slower as compared to that in brittle semiconductors and these metals usually exhibit considerable necking during the plastic deformation. However, in the case of single-crystalline Si, sliding occurs at a much faster rate and no necking is observed. Hence, the plastic-like behaviour is weakly reflected in the stress-strain curves and does not affect the fracture strength greatly. This may also be the reason that in many experiments it is observed that the Si fractures in a brittle manner and does not show plasticity.

Moreover, as the temperature increases, Si tends to transform from brittle to ductile. Thus, the plastic-like fracture behaviors observed in the MD simulation may provide useful information for studying Si at high temperatures.

Figure 3.18. The stress distribution at different strains for the (a) single-crystalline nanofilm and (b) bicrystalline nanofilm with tilt GBs at deformation temperature of 300 K.

Similar to the case of single-crystalline Si nanofilms, plastic deformation happens through dislocation sliding in the bicrystalline nanofilms with both types of GBs. High crystal order is preserved and no considerable necking is observed either. However, in contrast to the

single-crystalline nanofilms whose failure initiates within the grain, the failure of bicrystalline nanofilms initiates at the GBs, as exemplified by the case of tilt GBs in Fig. 3.18b.

Based on the fracture behavior analysis of both the single- and bicrystalline Si nanofilms, the lower fracture strength and strain of latter can be explained by the strong anisotropic nature of the covalent bonds directionality and different crystallographic orientations (Pérez and Gumbsch, 2000; Ivashchenko *et al.*, 2007; Kim and Windl, 2007). The directionality of covalent bonds defines the strength and stiffness of covalent compounds. Si is generally brittle because of the directional nature of their covalent bonds, which strongly affects the shearing motions associated with plastic flow. However, the introduction of the GBs changes the crystallographic orientations, resulting in different arrangements of covalent bonds and at the same time, the GBs can hinder dislocation motion. Hence, the bicrystalline samples fracture at a lower stress and strain. Simultaneously, the atomic discrepancy at the GB can facilitate the dislocation generation, and thus accounting for the high strain obtained for the nanofilm with twist GBs without notch.

The stress distributions in Fig. 3.18 show that before the dislocation sliding, atoms with high and low stresses are randomly distributed in the single-crystalline Si nanofilms; whereas in the bicrystalline nanofilms, the atoms generally have high stresses and they fill the grains in a homogenous manner. Therefore, these account for the differences occur in the fracture strength and elastic modulus between the single- and bicrystalline nanofilms. Overall, it is concluded that the presence of the GB weakens the nanofilms, lowering their strengths and stiffness as compared to single-crystalline sample.

Besides GBs, the notch effect on the deformation processes and mechanical properties of the Si nanofilms is also studied by investigating their structure at different strains as shown in Fig. 3.18. It is noted that for the notched single-crystalline nanofilm, fracture does not initiate

from the notch as expected, the failure mechanism is through dislocation sliding which starts from the surface of the nanofilm (Fig. 3.19a). This phenomenon is due to the fact that the critical stress for the opening and propagation of the notch is higher than that for the dislocation sliding. Similar phenomenon has also been reported by Thaulow *et al.* (2011) that the failure of single-crystalline Si with a crack on the surface occurs through $\langle 111 \rangle$ dislocation sliding.

From the stress distribution of the notched single-crystalline nanofilm, no stress concentration near the tip of the notch is observed and the stresses are randomly distributed throughout the nanofilm. However, when the notch depth is increased to $3a$, the simulation results (not presented here) show that stress concentration appears near the tip and dislocation sliding starts exactly at the tip and propagates in the $\langle 111 \rangle$ direction. This indicates that the depth of the notch has a significant effect on the site of sliding initiation and its presence is detrimental to the tensile strength of the single-crystalline Si nanofilm.

Figure 3.19. The stress distribution at the different strains for the notched nanofilms subjected to tensile loading at 300 K: (a) single-crystalline, (b) with twist GBs and (c) with tilt GBs.

For the notched bicrystalline Si nanofilms with both tilt and twist GBs, they undergo brittle fracture and no apparent plastic deformation is observed (Figs. 3.19b and c). As the stress exceeds the fracture strength, the Si-Si bonds near the notch tip first break, and the

elastic energy is released in this region as indicated on stress distribution map by the blue color. Afterwards, the notch penetrates inside the nanofilm along the GB, resulting in cleavage fracture of the nanofilm without plastic deformation. This fracture behavior is distinct from the dislocation sliding that observed in both the notched single-crystalline and smooth bicrystalline Si samples. Such distinction is caused by the presence of GBs which alters the crystallographic orientation with respect to the applied loading direction, and thus impedes dislocation movement. Consequently, the critical stress for the opening of the notch becomes lower than that for the dislocation sliding. Thus, in the presence of a stress concentrator, such as a notch at the edge of the GB, it is more probable that fracture initiates at the tip of the notch and propagates along the GB inside the nanofilm. Therefore, the failure of the notched bicrystalline nanofilms occurs through the cleavage mechanism and their fracture strength and strain are reduced.

Lastly, the effect of temperature on mechanical properties of both the notched single- and bicrystalline Si with twist and tilt GBs are investigated. Simulation is performed at 600 K and the results are compared to that obtained at 300 K as shown in Fig. 3.20. As temperature increases from 300 to 600 K, all the nanofilms become less stiff (the slope of the curves decreases) and their fracture strengths are significantly reduced.

For the notched nanofilms with GBs, similar deformation behavior is observed regardless of the temperature, whereby brittle fracture occurs through crack propagation along the GBs and no plastic deformation is observed. For the notched single-crystalline nanofilm, the failure is still via dislocation sliding. However, the fracture strain increases considerably and the plastic response is more visible from the stress-strain curve, as compared to the other nanofilms. These results show that the temperature has a strong influence on the stiffness and fracture strength of Si nanofilms, but does not change their failure mechanism.

Figure 3.20. The stress-strain curves for the notched single- and bicrystalline Si with twist and tilt GBs under tensile loading at 300 and 600 K.

3.4 Case study

A combined failure analysis approach based on the simulation and experimental results obtained in the earlier investigation is developed to characterize the fracture of the Si die found in a failed IC package (Fig. 3.21). The first phase of analysis contains two Si dies of different crystal orientations; mainly the $\langle 100 \rangle$ and $\langle 111 \rangle$ Si dies. It is found that the $\langle 100 \rangle$ Si die has fractured into two parts, while the $\langle 111 \rangle$ Si die located on the other end of the package remains undamaged.

The first phase of analysis consists of the conventional FA techniques to provide an overview of the site of failure. However, based on visual inspection, there is no apparent crack initiation point and crack fractography information is limited in this case. As such, the prediction of the root cause of failure is rather challenging. In the second phase, MD simulation is incorporated to understand the fundamental fracture mechanics for the particular die crack failure and give new insights to the fracture behavior of Si at the atomistic level. Since no apparent crack initiation point is found and failure only occurs in the

$\langle 100 \rangle$ die but not in the $\langle 111 \rangle$ die, it is hypothesized that failure may be stress driven and the failure mode is probably due to the weakness in the crystallographic planes. Hence, MD simulation will be performed to understand the effect of crystallographic orientations on the stress-strain relation and failure mechanism of the single-crystal Si cell. The stress-strain relations are then obtained and analyzed to provide an insight to the fracture strength and failure mode of the Si die of different orientations.

In the third phase, FEM will be performed to provide the stress distribution of the Si dies at the package level when subjected to temperature cyclic loading, and also investigate the influence of other components of the package on the dies. Consequently, the stress states of the dies at the different thermal loadings can be evaluated and determined if the thermomechanical induced stresses are below the fracture limit of the Si dies. As such, the critical condition that causes the failure can be identified and mitigation can be carried out to prevent similar failure from occurring. Lastly, in the fourth phase, the simulation results will be validated with experiment findings qualitatively. Three-point bend test is designed to understand the fracture strengths and modes involved at the macroscale. The experiment results can be observed under SEM to examine for similar crack fractography and failure mode that are seen in the damaged die. As such, the Si die crack failure and its failure mechanism can be fully characterized and understood at both the molecular and package level.

Therefore, in the first phase of the failure analysis (FA) approach, the failure mode and crack fractography are first observed via the SEM. A smooth (011) fracture plane that is parallel to the long side of the $\langle 100 \rangle$ Si die is observed with no apparent initiation (Fig. 3.22). Under the X-ray inspection, a significant void is observed in the die attach of $\langle 100 \rangle$ Si die. The failed $\langle 100 \rangle$ die has an orientation of $x[100]/y[011]/z[0-11]$. From the crack

fractography, the fracture surface is relatively flat, which is believed to be the cleavage plane of Si.

Figure 3.21. Schematic diagram of the four phases of the combined approach for fracture characterization of Si die crack.

Figure 3.22. SEM imaging of the crack surface of the damaged $\langle 100 \rangle$ Si die. Courtesy of Infineon Technologies Pte Ltd.

In the second phase, MD simulation is incorporated to provide the fundamental understanding and new insights to the fracture mechanics and fracture behavior of Si at the

atomistic level respectively. The earlier MD simulation of the effects of crystallographic orientation and defects on the fracture strength and failure mechanism of single-crystal Si have shown that $\{110\}$ and $\{112\}$ planes have lower fracture strengths due to their low bond densities as compared to the $\{100\}$ planes. Hence $\{112\}$ and $\{110\}$ planes are known to be the preferred cleavage planes of the single-crystal Si.

Generally, the structural defects which serve as stress concentrators weaken the strength of Si. It is found that dicing defect has more adverse impact on the integrity of Si as compared to groove line defect caused by backgrinding process. Simulation results also revealed that the integrity of the $\langle 100 \rangle$ Si subjected to tensile loading in $[010]$ direction is more sensitive to these structural defects.

Therefore, with these simulated findings, the fracture response of this particular crack in the Si die is explained. It is known that the fracture plane of the $\langle 100 \rangle$ die is the (011) plane. Theoretically, the (011) fracture plane has the highest atomic packing and contains the most number of nearest-neighbor atoms, and thus more atomic bonds in that plane are satisfied. Subsequently, it will also have the least number of dangling bonds after fracture, resulting in a mirror-like crack fractography as observed in the damaged die.

Furthermore, despite the fact that the (111) plane is the standard cleavage plane in the single-crystal Si due to its lowest bond density, fracture occurs along the (011) plane rather than the (111) plane. As explained in the earlier MD discussion, for the $\langle 100 \rangle$ Si die, the (111) plane is 54.75° to the (100) plane. At this angle, the (111) plane contains the same number of bonds as that of the (110) plane. However, in the presence of a microdefect, such as backgrinding groove line introduced to the (110) plane, the number of bonds in the (110) plane is slightly reduced (less bonds than (111) plane). Then, the cleavage along the (110) plane is more energetically favorable.

In addition, from the first phase analysis based on the SEM visual inspection, it is observed that the side walls of the die subjected to dicing do not have any apparent defect. However, the limited fractography of the crack surface shows signs that the crack propagation may have initiated from the bottom side of the die due to the backgrinding groove lines. Hence, from the combination of the visual and MD findings, it is deduced that the cause of the failure may be due to the backgrinding groove defect that coincides with the $\{110\}$ plane and consequentially reduces the strength of the Si die significantly. Thus, when subjected to high stress, the crack will propagate and cleave along the $\{110\}$ plane resulting in failure.

Therefore, in the next level of failure analysis, the FEM simulation is carried out to provide a stress analysis of the IC package to understand the range of the induced stresses on the Si dies due to the other electrical components present in the IC package and the conditions at which the IC package is subjected to before failure. Figure 3.23 shows the stress paths retrieved from the thermal cyclic stress analysis obtained from the FEM simulation, according to the vertical lines indicated in Fig. 3.4. The difference in the stress profiles is due to the anisotropic properties of the different oriented Si dies. It is noted that the stress profile for the $\langle 100 \rangle$ die is much wider as compared to that of the $\langle 111 \rangle$ die, indicating that the $\langle 100 \rangle$ die is subjected to a greater degree of warpage during the thermal cyclic loading.

Conversely for the $\langle 111 \rangle$ die, the stress profiles for the different thermal loadings remain close to the neutral axis. The difference in the stress variation between the $\langle 100 \rangle$ and $\langle 111 \rangle$ dies is more apparent in Fig. 3.23a and c. Besides the stress profiles, the FEM results also provide the range of thermomechanical stresses experienced by the dies during the assembly process, particularly the reflow process.

Hence, even though the MD results have shown that the $\langle 111 \rangle$ Si die has a lower fracture strength as compared to the $\langle 100 \rangle$ Si die, the FEM simulation is able to provide

further insights to the occurrence of failure in the $\langle 100 \rangle$ die instead of the $\langle 111 \rangle$ die despite its higher fracture strength. These FEM findings also show that the design and process application of the IC package may contribute to the failure of the Si die.

Figure 3.23. The stress paths of the $\langle 111 \rangle$ and $\langle 100 \rangle$ Si dies during the (a) cooling from 448 to 296 K, (b) cooling from 296 to 233 K, (c) heating from 233 to 523 K and (d) cooling from 523 to 296 K of the IC package.

In the last phase of failure analysis, the experimental results from the three-point bend test are able to explain and replicate the failure modes and determine the fracture limit of the bare die involved at the macroscale. The simulation results have shown that the thermomechanical stresses induced by the assembly processes are well below the fracture limit determined by the experimental means. However, the experimental results indicate that the presence of a notch at the edge of the specimen greatly reduces the experimental fracture strength regardless of the orientation. Hence, this indicates that a microdefect, such as an edge notch, must be present and aligned to the weakest fracture plane to result in such a failure.

Therefore, with the combination of the simulation and experimental findings, the failure modes and mechanisms involved is explained and understood at both the atomistic and macrolevel. It is concluded that the failure of the $\langle 100 \rangle$ Si die is mainly due to the presence of backgrinding groove defect which is of a significant depth and is aligned to the weakness of the (011) crystallographic plane. As a result, the intrinsic strength of the Si die is greatly reduced and when the thermomechanical stresses induced during the reflow process are sufficiently high, the crack is able to propagate easily through the (011) plane to achieve the mirror-like crack surface as observed. This combined approach show the capability and practical failure analysis application of MD. Henceforth, with this new combined approach, the accuracy of root cause deduction and characterization of the fracture in Si die is improved and the failure modes and mechanisms involved are better understood.

3.5 Summary

The effects of crystallographic orientation and defects on the fracture strengths and failure mechanisms of Si are first investigated via MD and experiment. The experimental results are coherent with those obtained from the MD simulation. It is concluded that the $\langle 100 \rangle$ Si die has the highest fracture strength but is also the most sensitive to structural defects. The structural defects, such as the sawing notch and the backgrinding groove, serve as stress concentrators and weaken the strength of Si nanofilms regardless of their crystallographic orientation and may also alter their failure mechanism. Moreover, the dicing defect is found to have a more adverse impact on the integrity of Si nanofilms as compared to backgrinding groove defect. Generally, the MD results show that Si can fail via brittle fracture or dislocation sliding mechanisms and the fracture response is affected by the

weakness of the crystallographic planes and the extensive lattice trapping at the tip of the defect.

Next, the grain boundary and temperature effects on the fracture strengths and failure mechanisms of Si nanofilms are studied via MD simulation. The results show that the fracture strengths of smooth Si nanofilms with both tilt and twist GBs are lower than that of the smooth single-crystal Si nanofilms as the introduction of GBs alter the crystal orientations. At 300K, both the single- and bicrystalline nanofilms subjected to tensile loading undergo dislocation sliding failure mechanism. When an edge notch is added to the nanofilm, the fracture strength of the single-crystalline nanofilm is reduced by ~40% while that of the bicrystalline sample with twist GBs is reduced by ~20%. All the notched bicrystalline nanofilms undergo brittle fracture through cleavage mechanism instead of dislocation sliding regardless of the types of GBs. However, the fracture mechanism for the notched single-crystalline nanofilm does not change. The increase in temperature reduces both the stiffness and fracture strength of nanofilms but has insignificant effect on their failure processes.

It is noted that the SW potential used in the study overestimates the lattice trapping barrier that impedes the brittle fracture of Si nanofilms and tends to predict their ductile fractures. In spite of this fact, brittle cleavage fractures are still observed in the notched bicrystalline Si nanofilms, indicating that the weakening effect of the GBs and notches is even stronger in real cases. It is reported that at ~850K silicon exhibits an abrupt transformation from brittle fracture to ductile flow. Since the results presented in this work show that the same plastic-like fracture behaviours are observed for Si nanofilms at high temperatures, these results may well reflect the plastic properties of Si nanomaterials.

Eventually, a combined FA approach, based on these simulation and experimental findings, is developed to characterize the root cause of the Si substrate crack found in the IC

package. In the first phase of analysis, the visual inspection is carried out to gain information of the failure mode involved. It is observed that the failed IC package contains two Si dies, the $\langle 100 \rangle$ and $\langle 111 \rangle$ oriented Si dies, where the former has fractured into two parts and the latter remains undamaged. Subsequently, the MD simulation and experimental results obtained earlier are able to provide some fundamental understanding of the fracture responses of the different oriented Si dies containing the structural defects that are introduced by the manufacturing process.

Then, FEM is performed to analyse the stress profiles of the different oriented Si dies subjected to the boundary and temperature conditions due to the other components in the IC package and the reflow process respectively. The FEM simulation results show that the thermomechanical stresses induced during the reflow process are well below the fracture limit of the Si die determined experimentally at the macroscale. However, a larger stress profile is obtained for the $\langle 100 \rangle$ Si die as compared to the $\langle 111 \rangle$ die due to the IC design and anisotropic properties of the Si, and thus it is more probable for the $\langle 100 \rangle$ Si die to undergo failure despite its higher fracture strength. Henceforth, it is concluded that only in the presence of the structural defects, the fracture limit of the $\langle 100 \rangle$ Si die is significantly reduced such that when subjected to the relatively high thermomechanical stresses, the $\langle 100 \rangle$ Si die undergo fracture along the (110) plane resulting in a mirror-like crack as observed.

Therefore, this case study shows that the fracture behaviour of Si is not only dependent on intrinsic factors but also external factors such as the IC design and processes. The combined FA approach has shown the capability to support and validate the deduction and characterization of the true failure response, and thus is useful in the determination of root cause. Overall, this study is helpful in understanding the mechanical behaviour of Si and providing useful information for 3D ICs design and applications.

Chapter 4. Modelling and Characterization of Interfacial Delamination in a-Si₃N₄/Si Bilayer Systems

It is challenging to understand and predict interfacial delamination in multilayered IC packaging due to the difficulties in experimentally quantifying the interfacial adhesion energies. In this chapter, the effects of voids and temperature on the interfacial fracture behavior and mechanisms of a-Si₃N₄/Si bilayer systems are first investigated via MD simulation. Subsequently, a combined approach based on MD and FEM simulations is adopted to characterize and predict delamination in a-Si₃N₄/Si bilayer systems. Lastly, the nanoindentation test is conducted to provide validation to the approach.

4.1 Methodology development

4.1.1 Simulation models

4.1.1.1 Molecular dynamics

MD simulation serves as an excellent tool for the modeling of the interfacial properties at the atomistic level (Wang *et al.*, 2000; Tanaka and Goettler, 2002; Van Driel *et al.*, 2006; Fan and Yuen, 2013), 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 (Abraham and Gao, 2000; Gerde and Marder, 2001). Hence, this study investigates the effects of voids and temperature on the interfacial fracture behavior and mechanisms of a-Si₃N₄/Si bilayer systems via MD simulation.

Figure 4.1a shows the computation cell of the perfect (without voids) a-Si₃N₄/Si bilayer system, while Figs. 4.1b and c show the systems with a void in the Si layer near the interface

and with a void at the interface respectively. The dimensions of the systems are set as $140 \times 130 \times 58 \text{ \AA}$. The void size is approximately $2a$ long along the y -direction and a thick along the x -direction, where a is the lattice constant of Si. The void in the Si layer is located approximately $2a$ distance away from the interface while the void at the interface is created symmetrically about the interface, with half of the void lying in the Si layer and the other half in the Si_3N_4 layer. The periodic boundary conditions are applied in the y - and z -directions, while the free boundary condition is used along the x -direction to model an infinite large thin film. The simulation is conducted using the large-scale atomic/molecular massively parallel simulator (LAMMPS) (Plimpton, 1995). The atomic interactions between both the Si-Si and Si-N atoms are described by the Tersoff potential (Billeter *et al.*, 2006).

Figure 4.1. Computational cells of the α - Si_3N_4 /Si system (a) without defects, (b) with a void in the Si layer and (c) with a void at the interface.

The crystalline Si and Si_3N_4 layers with the dimensions of $70 \times 130 \times 58 \text{ \AA}$ are 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 NPT ensemble via the Noose-Hoover thermostat for about 40 ps. Upon achieving equilibration, each layer is switched to the NVT ensemble.

The α - Si_3N_4 layer is obtained by melting and quenching the crystalline Si_3N_4 layer under the NVT ensemble following the procedures reported in Ref. (Liao *et al.*, 2011). The structural properties of the α - Si_3N_4 are influenced by the melting temperature and duration, and the quenching rate (Vollmayr *et al.*, 1996; Ippolito and Meloni, 2011). The similar annealing process is also carried out by de Brito Mota *et al.* (1998) using the same force field presented in this work and they have shown that the structural properties of α - Si_3N_4 are coherent with experimental results. The melting and quenching processes are achieved by heating crystalline Si_3N_4 to 8000 K via the Langevin thermostat in 20 ps, to allow the atoms to overcome the minimum local energy. Subsequently, it is rapidly cooled down to the temperature of 3000 K in 10 ps and then held at this temperature for 500 ps. Finally, the Si_3N_4 layer is further cooled to room temperature (300 K) in 10 ps. After the α - Si_3N_4 layer is obtained, it is further equilibrated at constant 300 K for 10 ps.

The structural information of the equilibrated crystalline Si and α - Si_3N_4 layers are then imported into a new simulation model as show in Fig. 4.1. Initially, the α - Si_3N_4 layer is deposited on top of the Si layer with a separation distance of 6 Å. Such a large interface distance of 6 Å is chosen to allow ample time for the atoms at the periodic boundaries to rearrange and relax themselves, particularly for the α - Si_3N_4 layer, where high-stresses sites may present at the boundaries due to its amorphous phase. Afterwards, the two layers are moved towards each other in steps of 0.05 Å followed by relaxation of 0.5 ps until the separation distance of 2 Å, to form the interface. The separation distance of 2 Å is selected as the average of the Si-Si and Si-N bond lengths which are ~ 2.35 and ~ 1.70 Å, respectively. With the 2 Å separation distance being held, the bilayer system is allowed to relax under the NVT ensemble for 10 ps to allow the system to attain a globally stabilized structure. Subsequently, as high-stress sites at the interface may be present due to the formation of new bonds and lattice mismatch, energy minimization is then performed to ensure low local

energy state at the interface is obtained. For the inclusion of voids, some atoms are deleted and the NVT is further applied to achieve an equilibrated structure.

Upon the realization of the equilibrated structure, the tensile (mode I) and shear (mode II) loadings is applied. To apply the tensile (shear) loading, 5 Å-thick layers of a-Si₃N₄ atoms at the top and Si atoms at the bottom are fixed respectively, and then a small displacement is applied to the top fixed a-Si₃N₄ layer in the x -direction (y -direction) each simulation step. The deformation process is realized at a strain rate of 0.002 ps⁻¹ until fracture occurs. The corresponding interfacial stress-strain relations are then obtained, whereby the interfacial stresses are computed using the virial theorem (Shen and Atluri, 2004) and subsequently the interfacial fracture energy is computed. The effect of the strain rate is not taken into account in this study as its effect on the work of the interfacial fracture is negligible.

4.1.1.2 Finite element method

At the continuum level, the CZM has been widely used to study the interfacial fracture process as it can avoid stress singularity at the crack-tip and represent the physics of the fracture process at the atomic scale (Yamakov *et al.*, 2006; Ural *et al.*, 2009; Wu *et al.*, 2016). The interface can be described by the interfacial constitutive relation governed by the traction-separation law (Needleman, 1987). This law is well described by the maximum cohesive strength, energy and separation distance (Shet and Chandra, 2002). The advantage of using the CZM is to eliminate the assumption that the interface is either fully-bonded, fully-debonded, or pre-cracked. Since the interfacial crack nucleation and propagation criteria are inherently included in the traction-separation law, its onset and propagation can be captured and predicted.

A high-order 3D FEM model of the a-Si₃N₄/Si system is built using the ANSYS software to simulate the nanoindentation process and determine the work of interfacial fracture. The

system is divided in three substructures, mainly the a-Si₃N₄ thin film, Si substrate and the interface (Fig. 4.2). Both the a-Si₃N₄ film and Si substrate are modeled as isotropic elastic-plastic materials and their material properties are obtained from MD simulation (Nakano *et al.*, 1995). The mixed-mode bilinear CZM is employed to simulate the interfacial delamination process during nanoindentation.

The cohesive parameters, mainly the maximum stresses and the strains of the interface before any damage occurs and the interfacial fracture energies in the mode I and II directions, are derived from MD simulation and input into the CZM to study the interfacial delamination response. Thus, the interface atomistic behavior governed by chemical interaction of atoms can be incorporated into the interface model in FEM.

For simplicity, the indenter is modeled as a rigid body with a flat tip radius of 150 nm as the curvature of the berkovich tip model has led to severe convergence issue. The simulation model boundary condition is constrained using fixed boundaries. The modal meshing is based on the regional meshing method whereby the meshing refine quality is controlled and smooth transition from the contact area to the far-field area is ensured. The transient static simulation is used for the delamination assessment. Friction force between the indenter and the a-Si₃N₄/Si system will not be considered in this study and small sliding conditions are adapted. The maximum indentation depth during indentation is 400 nm. The brittle cracks in the thin film and substrate and the residual stress in the thin film are also not considered for simplicity. The load-displacement curve is then obtained and the work of fracture is computed.

Figure 4.2. Initial configuration of a high-order 3D FEM model of the a-Si₃N₄/Si system.

4.1.2 Experimental method

The nanoindentation test has been widely accepted as an effective method to quantify the work of interfacial fracture as it enables deformation to occur in a controllable manner by generating interfacial cracks on a very small scale and localized site (De Boer and Gerberich, 1996a; Zhang and Zhang, 2012). Hence in this study, the nanoindentation test is conducted to provide validation to the work of interfacial fracture predicted by the CZM.

The 300 nm-thick a-Si₃N₄ films are deposited using the plasma-enhanced chemical vapour deposition on a 500 μm-thick (100) Si wafer. The displacement-controlled nanoindentation experiments are carried out at ambient temperature using the Nanotest 550, with a loading rate of 2 mNs⁻¹. A Berkovich indenter with a tip radius of 150 nm is used to measure the interfacial adhesion strength of a-Si₃N₄/Si bilayer. The sample is subjected to a constant indentation depth of 400 nm, performed over 20 indent points.

The maximum stress and work of interfacial fracture are then computed from the *P-d* curve. After indentation, the samples are placed under focused-ion beam (FIB) to make a cross-sectional cut so that the microstructure of the bilayer at the indented region can be revealed. Subsequently, the SEM and TEM are used to observe for the failure modes involved and the presence of phase transformation in Si and also to measure the radial crack length and delamination diameter.

4.2 Tensile loading

The thermodynamic interfacial adhesion energy W is first calculated to validate that the appropriateness of an interface separation distance of 2 Å for the interface formation between the Si and a-Si₃N₄ layers. The W of the a-Si₃N₄/Si system is calculated from (Nagao *et al.*, 2003)

$$W \equiv (E_{\text{Si}} + E_{\text{Si}_3\text{N}_4} - E_{\text{Bi}}) / A, \quad (4.1)$$

where E_{Si} , $E_{\text{Si}_3\text{N}_4}$ and E_{Bi} are the energies of the isolated Si layer, the a-Si₃N₄ layer and the combined a-Si₃N₄/Si bilayer respectively, and A is the interface area. It is found that the W of the a-Si₃N₄/Si bilayer system is 1.41 J/m². Since the W for a given metal/ceramic pair is typically a small value of ~0.5-2 J/m², it is concluded that the a-Si₃N₄/Si interface is well-established (Khanna, 2010).

4.2.1 Temperature effect

Figure 4.3 shows the stress-strain relations obtained for a perfect a-Si₃N₄/Si bilayer subjected to tensile loading in the x -direction, at temperatures ranging from 300 to 600 K. Generally, as the temperature increases from 300 to 600 K, the fracture strength of a-Si₃N₄/Si system is lowered by ~20%. Moreover, a significant drop in the fracture strength is observed when the temperature increases from 500 to 600 K. This drop can be explained by the weakening of the strength of the a-Si₃N₄ layer at higher temperatures.

At 300 and 400 K, when the applied strain results in stress exceeding the critical value, the atomic bonds at the interface are broken and fracture occurs at the interface as shown in Fig. 4.4a. However, as the temperature increases to 500 and 600 K, the fracture strength of a-Si₃N₄ is greatly reduced and becomes lower than that of the interface, resulting in fracture occurring in the a-Si₃N₄ layer instead of at the interface (Fig. 4.4b). Similar temperature

dependence on the strength of the α -Si₃N₄ layer has been previously reported by Liao *et al.* (2011) that for an applied strain rate of 0.0025 ps^{-1} , the yield stress of α -Si₃N₄ decreased by 16% as temperature increases from 300 to 600 K, which was also found to be consistent with experimental results (Qian *et al.*, 2005).

Figure 4.3. The stress-strain relations of the α -Si₃N₄/Si systems under tensile loading, at temperature ranging from 300 to 600 K.

At 600 K, fracture occurs near the top region due to the fixed boundary conditions applied during deformation and the asymmetric bilayer structure (Fig. 4.4b). As the few layers of atoms at the top are fixed, the atoms near the fixed layers experienced high constraint as compared to the atoms in the region far away. As a result, atoms near the fixed layers do not have sufficient freedom of space to either rearrange themselves or undergo relaxation, and thus fracture occurs at the top region. It is also noted that at the strain of 0.21, the Si layer shrinks back to its initial size after fracture. This is because upon the fracture, part of the stored elastic energy in the Si during the deformation process is released, and thus the Si layer appears to return back to its initial size.

Figure 4.4. The atomic configurations of the $a\text{-Si}_3\text{N}_4/\text{Si}$ bilayer systems at the different strains, under tensile loading perpendicular to interface, at (a) 300 K and (b) 600 K.

4.2.2. Void effect

The effect of voids on the fracture behavior of the $a\text{-Si}_3\text{N}_4/\text{Si}$ systems subjected to tensile loading, at different temperatures of 300 and 600 K are then investigated. As illustrated by the stress-strain relations in Fig. 4.5, the existence of a void in the Si layer near the interface at 300 K does not have much effect on the fracture strength and mode of the bilayer when subjected to uniaxial tensile loading perpendicular to the interface.

Figure 4.6 shows the stress distributions of $a\text{-Si}_3\text{N}_4/\text{Si}$ system with a void in the Si layer at the different strains at 300 K. It is evident that at the strain of 0.177, high stresses are observed at the edge of the void in the Si layer (colored in red) whereas the Si atoms surrounding the void are at lower stresses (colored in green). Meanwhile, the stresses at the interface at a certain distance away from the void also appear to be low as compared to those

at the edge of the void. Therefore, instead of crack initiation at the interface, fracture is observed to initiate from the void which then branch out to the interface and eventually leads to interfacial separation.

Figure 4.5. The stress-strain relations of the α - $\text{Si}_3\text{N}_4/\text{Si}$ systems with voids in the Si layer near the interface and at the interface, under tensile loading, at 300 and 600 K. The stress-strain relations for the perfect α - $\text{Si}_3\text{N}_4/\text{Si}$ systems at the specific temperatures are also included for comparison.

As the temperature increases to 600 K, the coupling effects of temperature and void in Si layer near the interface have resulted in apparent reduction of both the fracture strength and the fracture strain of the bilayer (Fig. 4.5), though the fracture mode remains as interfacial failure. However at 600 K, instead of brittle crack propagation from the edge of the void, dislocation emission is apparently observed near the edge of the void. The dislocation emission subsequently becomes more extensive and eventually the high dislocation density formation leads to the crack initiation at the interface, as exemplified by the atoms highlighted in green in Fig. 4.7. This fracture behavior is also different from that of the

perfect a-Si₃N₄/Si system at 600 K whereby fracture happens in the a-Si₃N₄ layer due to its weakening at high temperatures.

From the high stress concentration and plastic deformation observed at the edge of the void, regardless of the shape of the void, similar high stress concentration is observed at the edge of the void. Furthermore, the void also loses its shape during deformation (Fig. 4.7), and thus its shape will not have significant influence on the failure mechanism involved.

Figure 4.6. The stress distribution map of the a-Si₃N₄/Si systems under tensile loading perpendicular to interface, with a void in the Si layer at the strain of (a) 0 and (b) 0.177, at 300 K.

The presence of high dislocation density region near the interface accounts for the nonlinearity observed in the stress-strain relations before the fracture (Fig. 4.5). In addition, the formation of dislocations also causes the interface to be imperfect, which eventually weakens its interfacial strength. Kendall (2001) has previously revealed that the adhesion of the interface is dependent on numerous factors such as surface roughness, contamination and interfacial bonding. Therefore, at 600 K, the dislocations induced near the interface by the void in the Si layer will deteriorate the interfacial strength such that it becomes weaker than that of the strength of a-Si₃N₄ layer, resulting in fracture occurs at the interface instead of in a-Si₃N₄ layer. Since the fracture of the interface is brittle as compared to that of the a-Si₃N₄

layer, a lower fracture strain is reflected in the stress-strain curve for the $a\text{-Si}_3\text{N}_4/\text{Si}$ system with void in the Si layer.

Figure 4.7. The atomic configurations of the $a\text{-Si}_3\text{N}_4/\text{Si}$ systems with a void in the Si layer at the different strains, under tensile loading, at 600 K.

The atomic configurations of the $a\text{-Si}_3\text{N}_4/\text{Si}$ systems during the deformation process at 600 K also demonstrate that the crack initiates at one end of the interface and then propagates along it (Fig. 4.7). Afterwards, the crack dips into the void before propagating along the interface again. When the crack encounters the void, the whole system fractures rapidly, affirming the fact that at high temperature of 600 K, the presence of void is detrimental to the interfacial strength. After fracture, a ‘bridge’ of atoms is observed around the void. This phenomenon can be explained by the large plasticity evident by the large dislocation emission at the strain of 0.167 and the existence of free surfaces within the void.

As such, the atoms around the void are able to deform freely and continue to deform plastically even though the bonding in the other regions along the interface have been broken, resulting the formation of the ‘bridge’ observed at the strain of 0.173. Additional simulation has been performed for the different locations of the void in Si layer. It is found that the void in the Si layer must be sufficiently near the interface to have an effect on the fracture behavior of the $a\text{-Si}_3\text{N}_4/\text{Si}$ system.

When the void is located at the interface, under the tensile loading, the interface strength of a-Si₃N₄/Si system is weakened by ~20% and fractures at the interface regardless of the temperature (Fig. 4.5). The reduction of the fracture strength is mainly due to the presence of void at interface which reduces the number of interfacial bonds between the two dissimilar materials, and thus lowers the interfacial fracture strength. Since the reduced interfacial strength becomes lower than the fracture strength of the a-Si₃N₄ layer, the bilayer system fractures at the interface in a brittle manner instead of the ductile failure in the a-Si₃N₄ layer even at high temperatures. This difference of fracture mode is also reflected in the stress-strain curve where a sharp drop of the stress is observed immediately after the maximum stress point for the a-Si₃N₄/Si system with an interfacial void is attained.

Therefore, it is concluded that the presence of void at the interface is more detrimental to the interfacial fracture strength than having voids in the Si layer near the interface, particularly at room temperature of 300 K. When located in the Si layer near the interface, the void does not have much effect on the interfacial strength at low temperature but the strength is significantly reduced as the temperature increases.

On the other hand, if voids are present at the interface, the interfacial strength is weakened regardless of the temperature. Further investigation has been carried out to examine the effect of the coexistence of these two void types on the fracture behavior of a-Si₃N₄/Si systems. When the void in the Si layer near the interface is sufficiently far away from the other defect, i.e., the interfacial void, the effect of the interfacial void dominates the fracture behavior of the a-Si₃N₄/Si system. However, if both defects lie close together, both defects will contribute to the weakening of the interfacial strength and failure.

4.3 Shear loading

4.3.1 Temperature effect

The effect of temperature on the fracture response of a-Si₃N₄/Si systems under shear loading in the *xy*-plane is considered. The stress-strain relations obtained for the different temperatures and void locations are plotted in Fig. 4.8. It is observed that at 300 K, during the initial deformation (denoted as Region I), the stress increases linearly with strain, indicating an elastic deformation process. However, as strain increases, the stress-strain curves exhibit non-linearity (denoted as Region II). In Region II, this non-linearity is due to strong contribution of plastic flow of the a-Si₃N₄ layer, as the atoms undergo rearrangement (Ivashchenko *et al.*, 2007).

Figure 4.8. Stress-strain relations of the a-Si₃N₄/Si systems with voids in the Si layer near the interface and at the interface, under shear loading at 300 and 600 K. The curves for the a-Si₃N₄/Si systems at the specific temperatures are also included for comparison.

At the end of Region II, the stress reaches its maximum value and then enters into Region III. In Region III, the stress first decreases and then changes in a fluctuating manner. The fluctuation is more apparent at lower temperature. Upon reaching the maximum stress state, the interatomic bonds of the atoms at the interface between Si and a-Si₃N₄ are broken,

resulting in the relative slip of the two layers with respect to each other, and thus the stress decreases. During the interfacial sliding process, the Si crystalline structure undergoes relaxation. Subsequently, as the shear strain is applied continuously, new bonds between atoms of the two layers are formed and the system undergoes further shear deformation as in region II again. When the critical stress is reached again, the interfacial sliding occurs again, leading to the fluctuating behavior of the stress.

The atomic-bonds breaking and reforming behaviors at the interface during the shear deformation process is further evident by the atomic configuration of the $a\text{-Si}_3\text{N}_4/\text{Si}$ interface at the different strains, as exemplified with the case for perfect bilayer system at 300 K (Fig. 4.9). The marker highlighted in red revealed that an elastic shear deformation is induced in both layers (Figs. 4.9a and b) at initial deformation stage. As the shear strain increases, the interfacial sliding occurs and a thin amorphous layer of Si is formed near the interface (Fig. 4.9c). For the $a\text{-Si}_3\text{N}_4$ layer, during shear deformation, it undergoes plastic flow as a result of structural (atomic) rearrangement whereby bonds are broken and reformed. Similar shear deformation behavior is observed when the temperature is increased from 300 to 600 K.

Figure 4.9. The atomic configurations of the $a\text{-Si}_3\text{N}_4/\text{Si}$ systems during shear loading in the xy -plane at the strain of (a) 0, (b) 0.055 and (c) 0.19 at 300 K. A thin column of atoms are highlighted in red to illustrate the deformation process.

4.3.2 Void effect

The effect of voids either in the interface or in the Si layer near the interface on the interfacial fracture strength of the α -Si₃N₄/Si system under the shear loading is also investigated. It is found that the existence of these voids reduces the interfacial strength but does not influence the interface fracture behavior. The coupling effect of the voids and high temperatures causes the stresses required for interfacial sliding to occur to be reduced by ~ 25% due to lower activation energy of the atomic rearrangement and weaker interfacial bonds (Fig. 4.8). Furthermore, the significant fluctuation of atoms in the imperfect interfacial region at high temperature will also attribute to lower energy and stresses required for the interfacial sliding to occur.

4.4 Indentation loading

In the earlier MD investigation, the stress-strain relations for the perfect α -Si₃N₄/Si bilayer systems subjected to tensile and shear loadings in the x - and y -direction at 300 K respectively are obtained. Strain is applied incrementally till the stress exceeds the critical value. At this critical stress, the atomic bonds at the interface are broken and fracture occurs at the interface. The maximum stresses, the fracture strains and total fracture energy for mode I and II are derived, providing the cohesive parameters for the CZM in FEM (Table 4.1).

Table 4.1. Cohesive parameters obtained from MD simulation.

	Max stress (GPa)	Fracture strain	Total fracture energy (mJ/mm ²)
Mode I	20	0.18	0.0497
Mode II	12	0.19	

Based on the cohesive parameters derived by MD as shown in Table 4.1, the nanoindentation simulation is performed via CZM-FEM. Figure 4.10a shows the P - d curve obtained and the change in the slope from A to C corresponds to the delamination failure process observed in the simulation. This is because energy is released during the initiation and propagation of an interface crack. Figure 4.10b shows the deformation during indentation containing an interfacial crack, during the loading process at the indentation depth of 180 nm. At this depth, some of the cohesive elements have completed the damage evolution progress, indicating that the crack has initiated.

Figure 4.10. (a) The P - d curve of the α - $\text{Si}_3\text{N}_4/\text{Si}$ system obtained from the FEM simulation and (b) the deformation during the indentation loading containing an interfacial crack, at the indentation depth of 180 nm.

The delamination length a obtained from the FEM is $\sim 7.558 \mu\text{m}$. From the curve, the energy required to create the interfacial crack is obtained by the area ABC. Line AB is the extrapolation of the initial loading curve in the event if no delamination is present. Hence, extrapolating the curve up to the point B and the difference in the area is the work done to drive the interfacial crack. The work of interfacial fracture is then calculated to be 0.11 J/m^2 .

Next, the nanoindentation test is performed to provide validation to the simulation results. Figure 4.11 shows the P - d curve of a particular indent on the sample under a constant

indentation depth of 400 nm. During loading and unloading, various small displacement bursts and a large significant burst are observed in the curve respectively. Such discontinuities in the loading and unloading curves are known as ‘pop-in’ and ‘pop-out’ respectively. The ‘pop-in’ effect is mainly due to deformation of the thin film which results in the crack formation in the thin film, while the ‘pop-out’ effect may be due to the debonding of layers as the indenter is retracted or phase transformation of Si substrate at increased contact pressure.

Figure 4.11. The P - d curve of a particular indent on the sample under constant indentation depth of 400nm.

During the initial indentation, high localized mechanical deformation and stresses are introduced on the surface of the $a\text{-Si}_3\text{N}_4$ thin film, resulting in the elastic-plastic deformation of the thin film. The small ‘pop-ins’ observed in the P - d curve indicate that cracks are formed in the thin film. This is because the increase in loading will cause the amorphous thin film to deform elastically until it cracks. Consequentially, the energy released due to the formation of the crack surfaces are indicated in the P - d curve as the ‘pop-ins’ where no significant increase in the loading force is observed despite an increase in the indentation depth.

As the loading increases, high in-plane stresses are also induced along the interface of the $a\text{-Si}_3\text{N}_4/\text{Si}$ bilayer. At point A, with a displacement of ~ 350 nm, a significant discontinuity is observed and this is mainly due to the complete fracture through the thickness of the thin film (Fig. 4.12b). The through-thickness fracture is exacerbated by the bending stresses which arise once plastic deformation of the substrate occurs and the thin film bent into the impression.

Figure 4.12. SEM imaging: (a) the top view of the indent in the sample and FIB cut location and (b) the cross-sectional view after FIB cut.

Beyond point A, the sufficiently high contact stress causes the substrate to undergo plastic deformation and phase transformation (Hu *et al.*, 1986; Bradby *et al.*, 2001; Zarudi *et al.*, 2005; Rao *et al.*, 2007). This is evident in Fig 4.13a, whereby the slip bands and the different phases are observed in the Si substrate. It is also known that under high contact pressure of 11.3-12 GPa, the crystalline Si (Si-I) can transform to a metallic β -tin phase (Si-II) under pure hydrostatic conditions. In addition, during unloading, the unstable Si-II can further transform to either an amorphous phase (a-Si) or to other polymorphs of Si (Si-III or Si-XII) depending on the experimental conditions (Bradby *et al.*, 2000; Zarudi *et al.*, 2005).

As such, the phase transformation will cause a change in the volume and density of the substrate during unloading process.

Figure 4.13. TEM imaging: (a) the cross-sectional overview of the sample after indentation, indicating compressive plastic deformation around indent region, substrate crack, slip bands and Si phase transformation and (b) the detailed micrograph on the phase transformation zone and the presence of a median crack in the Si substrate.

When the indenter reaches the maximum indentation depth, it slowly undergoes the unloading process. During this process, the indented region of the Si substrate that has been plastically deformed and undergone phase transformation can no longer return back to its original form. The $a\text{-Si}_3\text{N}_4$ layer around the indented region experiences more elastic recovery than the Si substrate in the same region, due to the decrease in the stiffness of the thin film. As a result of this difference, localized tensile stresses and high stress concentrations are induced at the interface and near the edge of the indenter respectively, and these stresses increase as the indenter retracts. Furthermore, the redistribution of the elastic and plastic strains may occur. The stored elastic energy in the crack thin film is released during unloading, and thus in the further deformation, this part of thin film may be elastically deformed rather than plastically. Any membrane stress is also released (Chen and Bull, 2007).

The phase transformation of Si can also be noted in the P - d graph, whereby a distinct ‘pop-out’ is observed at a depth of ~ 260 nm of the unloading profile. This is because the Si phase transformation has resulted in the change in volume and density of the Si substrate, and thus the contact stress acting on the Si substrate is reduced during unloading and the substrate relaxes in a single burst rather than progressively. However, the ‘pop-out’ does not correspond to the onset of delamination nor phase transformation but rather indicates that such phenomenon have taken place. Particularly, when conducting nanoindentation on the Si substrate with a Berkovich indenter, the P - d curve is unable to indicate the onset of delamination failure distinctively (Whitehead and Page, 1992; Whitehead and Page, 1993; Hainsworth *et al.*, 1996).

At the depth of ~ 210 nm of the unloading curve, a sudden change in slope of the P - d curve is observed. This indicates that the indenter is retracting faster than expected. This phenomenon is most likely due to the debonding of the layers as the a-Si₃N₄ thin film that has undergone through-thickness crack bends and flexes. Hence, coupled with the high-induced tensile stresses, the interfacial adhesion strength is overcome and the bonding between the a-Si₃N₄ layer and Si substrate is suddenly broken, resulting in the nucleation of the interfacial crack.

The interfacial crack quickly propagates as the a-Si₃N₄ thin film releases its elastic strain energy due to bending (Whitehead and Page, 1992). As the interfacial crack propagation is limited by the through-thickness crack of the thin film, it will eventually come to a stop when the system reaches equilibrium. This is evident from the TEM image in Fig. 4.13b, which shows that the crack propagated for a distance r of ~ 4.69 μ m, resulting in the interfacial delamination. This occurrence is similar to the two-dimensional version of Obriemoff’s classic fracture mechanics experiment (Lawn, 1993) and also observed in the experiment carried out by Hainsworth *et al.* (Hainsworth *et al.*, 1998). The experimentally obtained

delamination length is found to be lower than the simulated length of 7.558 μm . This is mainly due to the fact that the experimental work done by the indenter is not only used to create the interfacial crack but also surface and through-thickness cracks.

As the indenter detaches from the surface, localized chipping of the α -Si₃N₄ thin film is observed near the indented region due to the delamination process, causing the localized spallation as shown in Fig. 4.12a. Furthermore, the stress applied by the indenter is non-uniform, and thus the film delaminated from the substrate in a leaf-like pattern (Chang and Huang, 2007).

Based on the energy approach described by Hainsworth *et al.* (Hainsworth *et al.*, 1998) and the Obriemoff's experiment, the work of interfacial fracture G_c^i is estimated. From the post-indentation analysis, it is assumed that delamination failure only occurs during the unloading process as no significant discontinuity is observed during the loading process of the P - d curve (Harea and Aifantis, 2014) and therefore, the total energy of the system U containing an interfacial crack of radius, r , is given by

$$U = W_c + W_m + W_f \quad , \quad (4.2)$$

where W_c is the work done to create the interfacial crack; W_m is the mechanical work done against the indenter by the flexure of thin film, which is represented by the shaded area in Fig. 4.11; W_f is the stored elastic energy of the flexed thin film which is released as it unflexes. The work done W_c is given by

$$W_c = \pi r^2 G_c^i \quad , \quad (4.3)$$

where r is the radius of the crack area (see Fig. 4.12b). The work done W_m is directly derived from the shaded area of the P - d curve. The energy W_f is given by

$$W_f = \frac{2\pi Et^3 (\Delta\delta)^2}{3r^2} \quad , \quad (4.4)$$

where $\Delta\delta = \delta_B - \delta_{res}$; E and t are the elastic constant and thickness of the a-Si₃N₄ thin film respectively. Thus, when the system containing the interfacial crack reaches equilibrium (no crack growth) and the minimum energy configuration of the system is obtained, the differential of Eq. (4.2) with respect to r is set to zero. It is assumed that the work done against the indenter by the flexure of thin film does not vary significantly with the interfacial crack growth and thus is ignored. Henceforth, G_c^i is calculated to be 0.085 J/m².

The experimental derived estimated work of interfacial fracture obtained is close to 0.11 J/m² obtained by FEM simulation. The slight deviation in this value is most probably due to the presence of interfacial defects such as voids and contaminants present at the interface of the real system, which will degrade the interfacial properties of bilayer system. The residual stresses in the thin film which are neglected in the calculation may also help to drive the interfacial crack. Furthermore, as the frictional effect is neglected in the FEM simulation, the work done by the indenter to overcome friction is ignored which may cause the work of interfacial calculated to be a slight overestimation. Hence, these factors will contribute to the lower work of interfacial fracture that is obtained experimentally.

4.5 Summary

The effects of temperature, voids at or near the interface on the interfacial fracture behavior of the a-Si₃N₄/Si bilayer systems under the tensile and shear loadings are first investigated via MD simulation. Under the tensile loading, the fracture behavior of the perfect a-Si₃N₄/Si system is found to be temperature-dependent. At 300 K, the interfacial

strength of the bilayer system without voids is ~22.5 GPa and it undergoes brittle fracture at the interface. However, at 600 K, failure occurs in the a-Si₃N₄ layer in a ductile mode.

With the existence of void in the Si layer in the a-Si₃N₄/Si system, crack initiates at the void and propagates towards the interface at 300 K. As the temperature increases to 600 K, the same bilayer system undergoes brittle fracture at the interface at a significantly lowered interfacial strength. However, for the bilayer system containing an interfacial void, the system fractures at the interface with a deteriorated strength regardless of the temperature. This is because the number of interfacial bonds is reduced, making it easier for crack propagation to happen at the interface. The existence of voids near or at the interface results in imperfect interface formation and consequently, leads to interfacial fracture at lower fracture strengths as compared to that of the a-Si₃N₄/Si system with perfect interface. Moreover, the simulation results show that the presence of an interfacial void has a more adverse impact on the interfacial strength than having a void in the Si layer.

Under the shear loading, the bilayer system deforms in three stages: elastic deformation, plastic flow in the a-Si₃N₄ layer and interfacial sliding. The presence of voids and the increase in temperature lower the stress required for interfacial sliding but they do not have significant effect on the shear deformation process. Overall, these simulation results provide an insight to the fracture behavior of a-Si₃N₄/Si system at certain operating conditions at the atomistic level.

Subsequently, a direct and effective combined approach which is capable of bridging microscopic and macroscopic structures via MD and CZM-FEM simulations is adopted to characterize and predict delamination in the a-Si₃N₄/Si bilayer system at the microlevel. In the approach, the material parameters that are required to be input into the CZM constitutive relation are derived from MD simulation rather than experiment. The work of interfacial

fracture obtained from both the MD-FEM simulations and the nanoindentation experiment show very good agreement.

Thus, the approach has proven to be a more accurate and effective characterization method as the reduction of system size has made it very challenging to extract the interfacial properties from experiments. The results obtained from the FEM simulation can be further improved by employing the extended-FEM so that a more accurate and closer modelling of the real state can be obtained.

This work is helpful for the understanding of deformation and failure in the multilayered structures. The atomistic investigations of the effect of defects in the a-Si₃N₄/Si system can supplement experimental research to gain fundamental understanding of possible failure mechanisms in 3D ICs. Essentially, other bi-materials systems can be analyzed via MD-FEM modeling, and thus the interfacial properties of the interlayers can be determined more accurately. In the next chapter, the interfacial properties of different bilayer systems are obtained from MD and incorporated in FEM to build a multilayered structure, so that the interfacial delamination in the whole IC packaging can be predicted under different operating conditions.

Chapter 5. Modelling and Characterization of Interfacial Delamination in Multilayer Systems

In this chapter, the above approach is further extended to characterize the interfacial energies and predict delamination in the Cu/Ti/SiO₂/Si multilayered system. Such a system is chosen as it is a common 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. 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 multilayer 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 modelling results. Henceforth, the interfacial fracture energy and delamination in the whole IC packaging can be characterized and predicted under different operating conditions respectively.

5.1 Methodology development

5.1.1 Simulation models

In this study, MD simulation is first performed to extract the interfacial properties in the Cu/Ti/SiO₂/Si multi-layered system to provide the cohesive parameters needed for FEM simulation. Figure 1 shows the computation cell of the Cu/Ti bilayer 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 for the SiO₂/Si bilayer is also built. However, as no suitable interatomic potential is available to model the atomic interactions at the Ti/SiO₂ interface, and thus the interfacial properties are adopted from the literature (Cordill *et al.*,

2004). The interactions among the Si-Si and Si-O atomic pairs and those among the Ti-Cu, Ti-Ti and Cu-Cu atomic pairs are described by the Tersoff (Tersoff, 1988) and the MEAM potentials (Baskes, 1987; Baskes and Johnson, 1994) respectively. Periodic boundary conditions are applied in the x - and y -directions, while free boundary condition is used along the z -direction to model an infinite large thin film. The simulation is conducted using the large-scale atomic/molecular massively parallel simulator (LAMMPS) (Plimpton, 1995).

Each material layer in the bilayer 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 NPT ensemble via the Noose-Hoover thermostat for about 40 ps. Upon achieving equilibration, the system is then switched to the NVT ensemble. The structural information for each layer is then imported into a new simulation model to form the bilayer system as shown in Fig. 5.1.

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 relaxation of 0.5 ps until they are ~3 Å distance apart. At the short separation distance of ~3 Å, the bi-layer system is allowed to relax under the NVT ensemble for 10 ps to allow the interfacial bonds to form and for the system 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 lattice mismatch, energy minimization is then performed to ensure that low local energy state at the interface is obtained.

Upon the realization of the equilibrated structure, the tensile loading is applied by fixing the top and bottom layers of the system, each with a thickness of ~10 Å and then displacing the top fixed layer along the z -direction at each simulation step. The deformation process is

conducted at a strain rate of 0.002 ps^{-1} until fracture occurs. The corresponding interfacial stress-strain relations are then obtained, whereby the interfacial stresses are computed using the virial theorem (Shen and Atluri, 2004). The effect of the strain rate is not taken into account in this study as its effect on the thermodynamic work of adhesion is negligible.

Figure 5.1. Computational cells of the Cu/Ti system.

Subsequently, these cohesive parameters derived from MD simulation are input into the CZM to study the interfacial delamination response under external loading at the macroscale. The FEM model of the Cu/Ti/SiO₂/Si multilayered system is built using the ABAQUS software to model the indentation test based on a quasistatic approach without considering time effect. The 50 μm -diameter sphericoconical diamond tip indenter is used for the indentation process as illustrated in Fig. 5.2. The system is divided into four substructures, mainly the 1 μm -thick Cu layer, 60 nm-thick Ti layer, 1 μm -thick SiO₂ layer and 20 μm -thick Si, which are separated by a 1 nm-thick interface between each layer. All the individual material layers are modeled as isotropic elastic-plastic materials while the interfaces are modeled using cohesive elements whose constitutive relation is governed by the interfacial traction-separation law (Needleman, 1987). The necessary parameters required in this law are: the maximum stresses, the maximum separation of the interface and the interfacial

fracture energy. The mixed mode bilinear CZM is employed to simulate the interfacial delamination process during the indentation loading.

Due to the symmetric of the system, axisymmetric elements are used for the substructures and interfaces. The vertical motion of the bottom surface is constrained. For simplicity, the indenter is modeled as a rigid body and its vertical displacement is specified as the reference point. The regional meshing method is used for the modal meshing whereby the meshing refine quality is controlled and the transition from the contact area to the far-field area is smoothened out. Transient static simulation is used for the delamination assessment. The friction force between the indenter and Cu/Ti/SiO₂/Si system will not be considered in this study and small sliding conditions are adapted. The maximum indentation depth during indentation is 2 μm which is the same as that performed in experiment. The cracks in the thin film and substrate and the residual stress in the thin film are also not considered for simplicity. Ultimately, the focus of this study is on the prediction of interfacial delamination.

Figure 5.2. Initial configuration of the FEM model of the Cu/Ti/SiO₂/Si system

5.1.2 Experimental method

Lastly, the indentation damage test is conducted to provide validation to the interfacial fracture energy predicted by the CZM. The multilayered sample is prepared using the standard wafer fabrication process on a 100 mm-diameter wafer. The 1 μm -thick SiO_2 dielectric layer is first deposited onto the 500 μm -thick Si wafer via the plasma-enhanced chemical vapour deposition. Next, the 1 μm -thick Cu/Ti metallization layers are then sputtered onto the SiO_2 dielectric layer. Lastly, the wafer is diced into a small die size of dimension 10×10 mm for experimental analysis.

The indentation damage experiments are carried out at ambient temperature using the microindentation system integrated with an acoustic emission (AE) sensor. The indentation process is performed using a 50 μm -diameter spherical diamond tip indenter and the P - d response and the AE signal are recorded simultaneously. When a crack event occurs, an ultrasonic wave will be emitted and detected by the AE sensor and consequently be reflected as a spike in the output voltage. Subsequently, the first AE signal detection will prompt the system to stop the loading process and the unloading process will ensue.

After the indentation test, the samples are placed under the FIB to make a cut to reveal the cross-sectional microstructure of the multilayered structure at the indented region. Subsequently, the SEM is used to provide insights to the cause of the AE signals and also conduct measurement of the delamination crack length for the quantification of the interfacial energy, thus providing validation to the simulation results.

5.2 Interfacial adhesion energy characterization

The cohesive traction-separation relations obtained for each bilayer system subjected to tensile loading in the z -direction at 300 K via MD simulation are shown in Fig. 5.3. Strain is

applied incrementally, till the stress exceeds the critical value. At this critical stress, the atomic bonds are broken and fracture occurs. The maximum cohesive traction $\sigma_{\max}$, separation distance $D_{\max}$ and fracture energy G can be obtained from the curves. The thermodynamic work of adhesion W of each bilayer is calculated from $W = (E_A + E_B - E_{AB})/A$ where E_A , E_B and E_{AB} are the total energies of the first material layer, second material layer and the combined bi-layer system respectively, and A is the interface area (Nagao *et al.*, 2003). All the MD parameters computed are summarized in Table 5.1.

Figure 5.3. Cohesive traction-separation relations of the Ti/Cu and SiO₂/Si systems under tensile loading at 300 K.

Table 5.1. Cohesive parameters derived from MD simulation.

Interfaces	$\sigma_{\max}$ (GPa)	$D_{\max}$ (nm)	G (J/m ²)	Stiffness (10 ¹⁰ MPa/mm)	W (J/m ²)
Cu/Ti	8.16	0.776	3.09	1.07	59.2
Ti/SiO ₂ (Cordill <i>et al.</i> , 2004)	1.7	1.18	1	0.193	-
SiO ₂ /Si	16.9	3.35	29	0.546	7.25

Theoretically, the G includes the W and the energy dissipated by the materials due to plastic deformation and other inelastic contributions, and thus the value of G should be larger than W . However, it is observed that the G for the Cu/Ti system (3.09 J/m^2) is significantly lower than its W (59.2 J/m^2) (Table 5.1). This is because the Cu and Ti layers are very well adhered, and thus when tensile loading is applied, fracture did not happen exactly at the interface but an atomic layer away from the interface (Fig. 5.4b). Hence, this indicates that the Ti-Cu interfacial bonds are not broken and therefore the G calculated is lower than W . Nevertheless, this interfacial fracture energy obtained is realistic as the experimentally derived G for the Cu/TiW system is $\sim 1.5\text{-}2.5 \text{ J/m}^2$ (Furuya and Ohshita, 1998). The experimentally derived G is slightly lower than that of the simulated value as the interface in the real system has certain surface roughness and may contain interfacial defects or impurities.

Figure 5.4. The atomic configurations of the Cu/Ti systems under tensile loading at the separation distance D of (a) 0 and (b) 2.79 nm.

For the SiO_2/Si system, its G (29 J/m^2) is significantly larger than its W (7.25 J/m^2). This is expected as interfacial fracture occurs at the SiO_2/Si interface and large plastic deformation is observed before fracture, as shown in Figs. 5.5b and c. The W obtained is in good

agreement with the experimentally measured fracture energy of W/SiO₂/Si system which is ~5.5-9.0 J/m² (Volinsky *et al.*, 2002).

Subsequently, these cohesive parameters derived from MD simulation are used to describe the cohesive traction-separation relation for the indentation damage model in FEM and this relation is assumed to be bilinear. The W is used as the main fracture criterion in the CZM as it is independent of the system geometry and applied strain rate.

Figure 5.5. The atomic configurations of the SiO₂/Si systems under tensile loading at D of (a) 0, (b) 3.25 and (c) 3.28 nm.

5.3 Indentation damage modelling and testing

The indentation damage simulation is then performed and the deformation evolution process is illustrated in Figure 5.6. At the indentation depth of 725 nm, it is observed that some of the cohesive elements have completed the damage evolution progress, indicating that the interfacial delamination has occurred. The delamination length a obtained from the FEM is measured to be ~ 9.57 μm . Figure 5.7 shows the P - d curve and its corresponding damage dissipation energy graph of the Cu/Ti/SiO₂/Si system are obtained from the CZM-FEM

simulation. During the indentation loading, the external work done by the indenter is equal to the internal energy of the system which consists of namely the plastic energy dissipation, the stored elastic strain energy and the energy released when damage occurs, i.e. damage dissipation energy. Since the only failure mechanism involved in the indentation damage model is the delamination failure at the SiO_2/Si interface (Fig. 5.6), the energy released due to the damage is used to drive the interfacial crack.

However, it is noted that no apparent discontinuity is observed in the P - d curve despite the occurrence of the damage. This is most probably due to the fact that the damage dissipation energy due to the delamination failure is of a very small magnitude of $\sim 2.67 \mu\text{J}$ (Fig. 5.7b). Hence, the damage energy loss is not apparently reflected in the P - d curve. Most of the work done by the indenter is converted to plastic energy dissipation in the bulk Si substrate and stored elastic strain energy in the system. Thus, from the a and damage dissipation energy, the G is calculated to be $\sim 8.23 \text{ J/m}^2$.

Figure 5.6. (a) The von Mises stress distribution and (b) the corresponding damage state of the deformed model during at the indentation depth of 725 nm.

Figure 5.7. (a) The P - d curve of the Cu/Ti/SiO₂/Si system and (b) the corresponding damage dissipation energy graph obtained from the FEM simulation.

Next, the indentation damage test is performed to provide validation to the MD-FEM simulation results. Figure 5.8 shows the time history graph and the corresponding P - d curve of a particular indent on the Cu/Ti/SiO₂/Si sample under indentation loading. During the loading process, the AE signal is first detected at the indentation depth of 2000 nm which also corresponds to the first ‘pop-in’ as shown in Fig. 5.8b. This is because when the sample is subjected to indentation loading, localized mechanical deformation and stresses are introduced in the thin films and substrate, resulting in the elastic-plastic deformation.

As the loading increases, high in-plane stresses are also induced along the interface and dislocations are emitted in the Si substrate. Subsequently, the interaction of the high-density dislocation formation may result in the substrate cracks as observed in Fig. 5.9b (Li *et al.*, 2014). Stresses are released as the dislocation formation are emitted and this attributes to the ‘pop-in’ observed in the P - d curve whereby no significant increase in the loading force is observed despite an increase in the indentation depth. Similarly, the formation of such cracks will also emit an ultrasonic wave which is then detected by the AE sensor and result in a spike in the voltage output (Fig. 5.8a).

Figure 5.8. (a) Time history graph and (b) the $P-d$ curve of a particular indent on the Cu/Ti/SiO₂/Si sample.

After the first AE signal is detected, the system undergoes the unloading process. No discontinuities in the unloading curve are observed. During this process, the indented region of the Si substrate that is plastically deformed can no longer undergo complete elastic recovery. On the other hand, the thin-film layers around the indented region are able to experience greater elastic recovery as compared to the Si substrate due to their lower stiffness. As a result of this difference, localized tensile stresses and high stress concentrations are induced at the interface and near the edge of the indenter respectively, and these stresses increase as the indenter retracts.

The FIB cut along the cross-sectional of the indented region in the post indentation analysis (Fig. 5.9b) shows that one of the substrate cracks formed during the loading process has propagated to the interface boundary. The presence of this crack near the interface boundary will result in high stress concentration at that region, leading to a significant increase in the localized tensile stresses. Subsequently, when the stored elastic energy in the deformed thin-film layers is released during unloading process, the interfacial adhesion strength between the SiO₂/Si layers is easily overcome and the crack will propagate along the

weak interface instead of penetrating through the SiO_2 thin film, resulting in the interfacial crack.

When the system reaches equilibrium, the interfacial crack propagation will eventually stop. This is evident in Fig. 5.9b whereby the interfacial crack is observed to be initiated from the substrate crack at $8.76 \mu\text{m}$ away from the center of indentation and propagated for a distance of $2.02 \mu\text{m}$. This failure mode is similar to that of the constrained blister test whereby an annular delaminated region is observed. At the end of the unloading process, the second AE signal is detected. This signal is detected in all the indents regardless of the presence of an interfacial crack, and thus it is most likely to be attributed by the removal of the indenter from the surface of the sample. Neither the AE sensor nor the P - d output curve is able to provide any insights to the onset of interfacial delamination.

Figure 5.9. SEM imaging: (a) the top view of the indent and (b) the cross-sectional view of the indented region after FIB cut.

The work of interfacial fracture G can be estimated from the fracture mechanics analysis model proposed by Wan and Dillard (Wan and Dillard, 2003), which is derived based on the linear elasticity and energy balance approach. In the model, a circular thin film without initial

residual stresses is fixed at its circumference and adhered to a cylindrical indenter that has the same diameter as the film. When the indenter is pulled up, a membrane stress is induced in the film and the indenter-film interface undergoes partial delamination, leading to the ‘pull off’ phenomenon, as shown in Fig. 5.10. Thus, this fracture model is able to represent the delamination failure mode observed in this indentation damage test whereby part of the circular imprinted area remains adhered to the substrate while delamination occurs at a certain distance away from the center of the indentation.

Figure 5.10. Schematic diagram of the adherence between the flat cylindrical punch and a thin circular film fixed at its perimeter.

In this proposed model, an external upward force is applied quasistatically to the cylindrical indenter onto a thin circular film fixed at its circumference, to separate and drive delamination at the indenter-film interface. The thin film has the properties of an elastic modulus E , Poisson’s ratio ν , thickness t and radius R . When the system reaches equilibrium, the contact area will reduce from initial radius R to $(R-r)$ and an opening crack displacement c is obtained (Fig. 5.10). Based on the energy balance approach, the total energy of the system during the unloading process is defined as,

$$U = W_c + W_m + W_f \quad , \quad (1)$$

where $W_c = A.G$ is the work done to create the interfacial annular crack of area $A = 2\pi r(R - r)$; $W_m = Fc$ is the mechanical work done by the indenter load F and W_f is the stored elastic energy of the annular membrane which is given by

$$W_f = \frac{4\pi E' t}{(1 - \zeta) \log \zeta \log \zeta} \left(\frac{c^4}{4} \right) . \quad (2)$$

where $\zeta = \left(\frac{R - r}{R} \right)^2$ and $E' = \frac{E}{1 - \nu}$.

During delamination, the prestress is not released due to the constraints at the circumference. A quasistatic equilibrium is then achieved when $\frac{dU}{dA} = 0$, and from the differential energy balance of Eq. (1), the G can be expressed as

$$G = \frac{3(2 - 2\zeta - \zeta \log \zeta)}{\zeta(1 - \zeta)^2 [\log(1/\zeta)]^3} \left(\frac{E' t c^4}{R^4} \right) . \quad (3)$$

Henceforth, the G is calculated to be $\sim 9.79 \text{ J/m}^2$. This experimentally derived G is close to that obtained by the FEM simulation above ($\sim 8.23 \text{ J/m}^2$). This slight deviation of 16% is most likely attributed by the error from the estimation of the crack area which may not be perfectly annular. Furthermore, the residual stress which is present in the real thin-film stack is neglected in the calculation, and thus the experimentally derived G to be slightly overestimated. Nevertheless, the experimental and simulation results are in good agreement.

5.4 Summary

A direct and effective combined approach based on MD and CZM-FEM simulations is adopted to characterize the interfacial energies and predict delamination in the Cu/Ti/SiO₂/Si multi-layered system. In the approach, the necessary material parameters that are required to be input into the CZM constitutive relation are derived from MD simulation rather than

experiment. Ultimately, the W is used as the failure criterion for the FEM simulation as it is independent of the system geometry and applied strain rate.

The interfacial fracture energy of 8.23 and 9.79 J/ m² obtained from both the MD-FEM simulations and the indentation damage experiment respectively, are in good agreement. The approach has proven to be a more accurate and effective method as the reduction of system size made it very challenging to extract these parameters from experiments. The simulation results can be further improved by considering the effect of substrate cracks via extended-FEM so that a more accurate and closer modelling of the real failure state can be achieved. Experimentally, the residual stresses of the thin films can also be taken into account to obtain a more realistic G . Henceforth, the current approach can be utilized to predict interfacial delamination in 3D ICs packaging under different operating conditions, thereby improving reliability of such devices.

Chapter 6. Conclusions and Recommendations

In this last chapter, the main conclusions for the works conducted in this PhD study are drawn and future works are recommended.

6.1 Conclusions

Si is commonly used as a substrate material in the IC packaging but yet its fracture behavior theoretical framework is still not well-developed. Data on the fracture in the single nanocrystalline Si is limited due to the difficulties in performing precisely controlled experiments. Hence, MD simulation is first performed to investigate the effects of crystallographic orientation, defects, GBs and temperature on the fracture behavior of the bulk Si subjected to uniaxial tensile loading, to provide fundamental understanding to the failure mechanisms involved.

Subsequently, FEM is performed at the global package level to provide the stress profiles of the Si die when subjected to constraints due to other package components and also thermal cyclic conditions such as the reflow process. These combined simulation findings are then used to substantiate and explain the fracture behavior of bulk Si subjected at the macroscale. Such a new combined failure approach has provided a better understanding to the fracture behavior of Si and improvement in the accuracy of the failure root cause deduction.

Next, 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 IC packaging. Furthermore, the mismatch in the CTEs between dissimilar materials induces thermomechanical stresses, leading to problems such as thermal warpage and eventually resulting in interfacial delamination failure.

Understanding and predicting interfacial delamination failure in the multilayered IC packaging are rather challenging due to the difficulties in experimentally quantifying the interfacial adhesion energies. As such, similar MD investigation is first extended to the a-Si₃N₄/Si bilayer systems to understand the effects of voids and temperature on their interfacial fracture behavior. MD simulation is capable of characterizing the interfacial properties, i.e. interfacial adhesion energies, as it is able to take into account the chemical and bonding characteristics of the interface. Thus, the interfacial properties derived by MD simulation are used as the input parameters for the CZM in FEM for the modelling of interfacial delamination failure at the macrolevel. Thereafter, experiments are performed to validate the results obtained from the combined MD-FEM approach. The work of interfacial fracture obtained from both the MD-FEM simulations and the nanoindentation experiment are in good agreement.

Based on the above approach, MD simulation is further performed on the different bilayer systems to extract their interfacial properties, and subsequently these MD-derived properties are incorporated into CZM-FEM model to predict the interfacial delamination of a multilayered structure. The simulation and experimental results are in good agreement. Ultimately, through this combined simulation approach, interfacial delamination in the global IC packaging can be predicted under different operating conditions so as to improve the reliability of the 3D IC packaging, leading to increase in their production yield and lower costs.

The major conclusions that can be drawn from all these investigations are listed as follows:

- The investigations of the crystallographic orientation and defect effects on the fracture strengths and failure mechanisms of Si based on MD simulation and experiment concluded that the $\langle 100 \rangle$ Si die has the highest fracture strength but

is also the most sensitive to structural defects. The structural defects, such as the sawing notch and the backgrinding groove weaken the strength of Si nanofilms regardless of their crystallographic orientation and may also alter their failure mechanism. Moreover, the sawing notch defect is found to have a more adverse impact on the integrity of Si nanofilms as compared to backgrinding groove defect. Generally, the MD results show that Si can fail via brittle fracture or dislocation sliding mechanisms and the fracture response is affected by the weakness of the crystallographic planes and the extensive lattice trapping at the tip of the defect. The experimental results are coherent with those obtained from the MD simulation.

- The investigations of the grain boundary and temperature effects on the fracture strengths and failure mechanisms of Si nanofilms via MD simulation show that the fracture strengths of the Si nanofilms with both tilt and twist GBs are lower than that of the single-crystal Si nanofilms as the introduction of GBs alter the crystal orientations. At 300K, both the single- and bicrystalline nanofilms subjected to tensile loading undergo dislocation sliding failure mechanism. When an edge notch is added to the nanofilm, the fracture strength of the single-crystalline nanofilm is reduced by ~40% while that of the bicrystalline sample with twist GBs is reduced by ~20%. All the notched bicrystalline nanofilms undergo brittle fracture through cleavage mechanism instead of dislocation sliding regardless of the types of GBs. However, the fracture mechanism for the single-crystalline nanofilm remains unchanged regardless of the presence of the notch. The increase in temperature reduces both the stiffness and fracture strength of nanofilms but has insignificant effect on their failure processes.

- Based on the simulation and experimental findings above, a combined FA approach is developed to characterize the root cause of the Si substrate crack found in the IC package. It is observed that the failed IC package contains two Si dies, the $\langle 100 \rangle$ and $\langle 111 \rangle$ oriented Si dies, where the former has fractured into two parts and the latter remains undamaged. The MD simulation and experimental results obtained earlier are able to provide some fundamental understanding of the fracture responses of the different oriented Si dies containing the structural defects. The FEM results show that the thermomechanical stresses induced are well below the fracture limit of the Si die determined experimentally at the macroscale. However, as a larger stress profile is obtained for the $\langle 100 \rangle$ Si die as compared to the $\langle 111 \rangle$ die due to the IC design and anisotropic properties of the Si, it is more probable for the $\langle 100 \rangle$ Si die to undergo failure despite its higher fracture strength. Henceforth, it can be concluded that in the presence of the structural defects, the fracture limit of the $\langle 100 \rangle$ Si die is significantly reduced such that when subjected to the relatively high thermomechanical stresses, the $\langle 100 \rangle$ Si die will undergo fracture along the (110) plane resulting in a mirror-like crack as observed. Therefore, this case study shows that the fracture behaviour of Si is not only dependent on the intrinsic factors but also the external factors such as the IC design and processes.
- The investigations of the temperature and void effects on the interfacial fracture behavior of the a-Si₃N₄/Si bilayer systems via MD simulation show that under tensile loading, their fracture behaviors are found to be temperature-dependent. At 300 K, the interfacial strength of the bilayer system without voids is ~22.5 GPa and it undergoes brittle fracture at the interface. However, when the temperature is increased to 600 K, failure occurs in the a-Si₃N₄ layer in a ductile

mode. With the existence of void in the Si layer in the a-Si₃N₄/Si system, crack initiates at the void and propagates towards the interface at 300 K. As the temperature increases to 600 K, the same bilayer system undergoes brittle fracture at the interface at a significantly lowered interfacial strength. However, for the bilayer system containing an interfacial void, the system fractures at the interface with a deteriorated strength regardless of the temperature. The simulation results also show that the presence of an interfacial void has a more adverse impact on the interfacial strength than having a void in the Si layer. Under the shear loading, the bilayer system deforms in three stages: elastic deformation, plastic flow in the a-Si₃N₄ layer and interfacial sliding. The presence of voids and the increase in temperature lower the stress required for interfacial sliding but they do not have significant effect on the shear deformation process.

- A combined simulation approach based on MD and CZM-FEM simulations is adopted to characterize and predict delamination in the a-Si₃N₄/Si bilayer system at the microlevel. The material parameters that are required to be input into the CZM constitutive relation in FEM are derived from MD simulation. The work of interfacial fracture obtained from both the MD-FEM simulations (0.11 J/m²) and the nanoindentation experiment (0.085 J/m²) are in good agreement. Thus, the approach has proven to be a more accurate and effective characterization method as the reduction of system size has made it very challenging to extract the interfacial properties from experiments.
- The above approach is extended to characterize the interfacial energies and predict delamination in the Cu/Ti/SiO₂/Si multilayered system. The thermodynamic work of adhesion W derived from MD simulation is used as the

failure criterion for the FEM simulation as it is independent of the system geometry and applied strain rate. The interfacial fracture energy of 8.23 and 9.79 J/m² obtained from the MD-FEM simulations and the indentation damage experiment respectively, are in good agreement.

6.2 Recommendations

In this PhD study, the current combined approach is direct and effective as it is based on the thermodynamic work of adhesion derived from MD simulation to bridge the gap between the atomistic and continuum level. However, the bridging between the MD and FEM simulations is still limited and challenged due to the different length and time scales involved. It would be desirable to explore into multiscale modelling so as to achieve a closer bridging between the atomistic and continuum levels, and thus the interfacial delamination of the multilayered IC packaging can be captured and predicted more accurately.

In this multiscale modelling of a bilayer system, their interface and subsurface regions can be generated by the atomic arrangements from MD simulation and the continuum finite element mesh in FEM respectively. The atomic and continuum regions are then coupled through an overlap region in which the constitutive equations of mechanics in both regions are solved. Thus, each region is able to provide the boundary conditions for the other at the edge of the overlap region. Consequently, this overlap region is able to bridge the atomic and continuum regions and transfer the localized deformations in both regions during the deformation process. The structural equilibrium of the bilayer can be achieved by iteratively solving the constitutive equations of mechanics in the different regions. Hence, the contact forces at the interfacial area are dominated by the atomic interactions, and the distribution of the interfacial area and strain are determined by the elasto-plastic response of the material

properties at the continuum level. Therefore, the interfacial delamination failure in the multilayered system can be better understood.

In addition, the current work only considers the interfacial delamination failure in the multilayered systems in which each layer is homogenous. Inevitably, in the real multilayered system, the materials are heterogeneous as they contain cracks and voids that may degrade the interfacial properties. Inclusions may also be purposefully added to enhance the functionality of the multilayered system. Thus, the presence of these inhomogeneities may cause surface deformation and eventually affect the localized interfacial stress field, resulting in unpredicted failure (Zhou *et al.*, 2011; Dong and Zhou, 2015; Dong *et al.*, 2015). It will be interesting to investigate the effect of the coexistence of the inhomogeneities, such as inclusions and cracks, on the interfacial fracture behavior of the multilayered systems via the multiscale modelling. A pre-existing crack may result in stress singularity at the crack tip and propagate along a weak interface or within the material which will eventually lead to failure in the IC packaging. Besides, the interactions of these inhomogeneities can further complicate the interfacial delamination failure prediction in the multilayered IC package. Therefore, it is essential to investigate the effect of the coexistence of the inhomogeneities on the interfacial fracture behavior of the multilayered system so as to obtain a better correlation with the real system.

The fatigue life prediction of 3D IC packaging is also crucial to its reliability and failure analysis. The IC packaging is often subjected to thermal cyclic loading. The fluctuation of the induced thermomechanical stresses will lead to the crack initiation and eventually the uncracked section can no longer support the continuous loading, resulting in fatigue damage. The Paris law has been utilized widely to predict the fatigue life of layered materials in the macroscale. Hence, the multiscale model can be further extended to investigate the growth and direction of cracks and predict the fatigue life of the multilayered IC packaging

under low-magnitude cyclic loading. This may be helpful in understanding the relation between the crack growth path and fatigue life of 3D ICs.

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