Electrical characterization and modeling on mechanical strength of copper to copper bonds for three dimensional integrated circuits

I Made Riko

2011

I Made Riko. (2011). Electrical characterization and modeling on mechanical strength of copper to copper bonds for three dimensional integrated circuits. Doctoral thesis, Nanyang Technological University, Singapore.

<https://hdl.handle.net/10356/43639>

<https://doi.org/10.32657/10356/43639>

**NANYANG
TECHNOLOGICAL
UNIVERSITY**

**Electrical Characterization and Modeling on
Mechanical Strength of Copper to Copper Bonds
for Three Dimensional Integrated Circuits**

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**SCHOOL OF MATERIALS SCIENCE AND ENGINEERING
2011**

**Electrical Characterization and Modeling on
Mechanical Strength of Copper to Copper Bonds
for Three Dimensional Integrated Circuits**

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School Of Materials Science And Engineering

**A thesis submitted to the Nanyang Technological University
in fulfilment of the requirement for the degree of
Doctor of Philosophy**

2011

Abstract

Vertically stacking and bonding individual processed wafers with through-Si vias (TSV) to form three dimensional integrated circuits (3DIC) introduces the possibility of reducing signal propagation delay, a reduction in power consumption and heterogeneous device integration. Cu thermocompression bonding is seen as a general route to realize 3DIC, with bonded metals providing both mechanical adhesion as well as electrical interconnection.

Mechanical testing to assess the bond quality of bonded processed wafers can be very costly, particularly on production wafers which have multilayer devices designed in the chips. A new non-destructive characterization method based on measured resonance frequency is proposed. Capacitive and resistive characteristics of the contact interface are amplified and utilized with a designed external circuit that consists of an inductor and a resistor. This new measurement technique shows an improvement in sensitivity as compared to contact resistance measurement, as well as eliminates stray resistance effect from line resistance and probing contact resistance.

A 3D bonded Cu-Cu test structure that enables three methods of bond interface characterization, i.e. electrical contact resistance measurement, resonance-frequency characterization method and die shear test was designed and fabricated. The results verified the improvement in the electrical characterization with resonance frequency measurement, as well as showing the relation between electrical and mechanical characterization results that can be related through the true contact area and a proportional factor K , which can be empirically determined.

A true contact area model as a function of bonding load, bonding temperature, bonding duration, and surface roughness was developed for this purpose. The model also enables a construction of a true contact area map and an electrical bonding map which are useful for a fast estimate of the bonding quality, or determining the bonding process window given the required bond properties.

Post-bonding bond interface enhancement through thermal annealing and direct current stressing was also modeled and their implication discussed. Contact area growth during isothermal annealing process is modeled as sintering of contacting metal spheres. Simulation results show that it depends strongly on the temperature and the initial true contact area. A void free interface with $\sim 1\%$ of initial true contact area at an annealing temperature of 300°C or higher, provided that the Cu interface is maintained oxide free, can be achieved.

A similar principle was also being utilized to model the observed contact resistance reduction of Cu bonded interface under current stressing. Reduction in contact resistance implies a larger true contact area, which may lead to better bond integrity. The model has captured well the critical current dependence on the initial resistance value as observed by previous work.

Current stressing technique is particularly interesting for post-bonding bond enhancement as it requires no heating. It can be done at room temperature, as well as during device operation, which eliminates the stress buildup due to thermal expansion mismatch, as well as benefiting temperature sensitive device.

Overall, the thesis has provided a complete package for thermocompression bonding process. The true contact area model and the bonding map help one to achieve the desired interface contact resistance, and to optimize bonding condition to obtain optimal yield based on the equipment availability and capability. Non-destructive testing helps to identify a weak bonded die, which then can be repaired by thermal annealing in batch and locally by direct current stressing.

Acknowledgements

During my stay in NTU, I had the privilege of working with some brilliant minds. I would first like to thank my thesis advisor, Professor Gan Chee Lip, for accepting this novice researcher in his group and providing me with all the tools and the intellectual freedom to pursue the projects of my interest. Essentially, he had taught me how to perform research. I am grateful to Prof. Pey Kin Leong and Prof. Carl Thompson for the stimulating discussions and their valuable comments on the project. I am also grateful to my thesis committee members, Prof. Chen Zhong and Prof. Wong Chee Cheong, who have provided valuable key inputs in the early stage of my research as well as for the desertation. A very special thank to Prof Boey and Prof Subbu for their warm support for my PhD research in MSE

I acknowledge the contributions from all my collaborators, especially Dr Yang Liling, Dr Yoon Seung Wook and Prof. Lee Chengkuo whom had been providing time and guidance during my two years attachment in IME. Some of the key results in this thesis will not be possible without fabrication capability of IME.

Several research staff have helped me with my experiments over the course of this work. I am indebted to Mastura Aidel, Heryani Binte Ahmad, Sandy Leong, whom had made the use to be Microelectronics lab to be more alive. I would like to thank Eric Tan Jok Boon whom keeping a watchful eye in MRC lab. I also acknowledge the help from Mr Lim Poh Chong from IMRE in using XRD.

I am thankful to all my fellow in MicroE grad-room, whom I have shared many scientific and philosophical conversation over the years. In particullar, Wardhana A. Sasangka and Mr. YY for insightfull and inspiring discussion, Gloria Cheng Yuhua, Yan Hua, Koh Li Buay, Dr Teh Lay Kuan, Dr Ang Xiao Fang and Eugene for memorable and inspiring conference trip, despite I missed the ski session. Chan Meying, Derick Ang and Yan Hua, you guys add some extra spices to our adventurous Bintan trip. Yip Chan Hoe, Lim Meng Keong for short course on MATLAB, Damar Yoga, Hendro Mario, Intan Ayu Perwitasari, Husein K, Dr Yudi Setiawan, Dr Tan Tam Lyn, because of you the grad room has the spark of life. I also thank the other Prof. Gan group members, Katherine Kor Hwee Boon, Cai Hui, Li Shaozhou, Liu Qing, Chun Shurong, and also Chia Hong Ling whom had help to provide important data for this thesis. My gratitude also to Steve Ong Hock Guan for a late night ride home in your little red car, Wenyi for the nice conversation at B2 staircase, Kwan Wee for the ever updated news coverage, GSWC committee for organizing events that kept from becoming insane.

My thanks stretch to friends that indirectly had help me maintain my sense of equilibrium through this sometimes bumpy ride. To Fatwa Firdaus Abdi, Pungky Pradoto, Kresna CW, Adhi Setiawan, Bekti, Gita, GiGi, Dana, Acay, Izhari, Batara Indra, Made Adi, Zamzani, Edo Posma that show me there is always hope in live. To my house mate, Yoga, Leni, Abi, Kadek Dharma, and especially little Kimi whom his late night cry reminded me that there is still life in the house.

Most importantly I would like to express my gratitude to my parents I Nyoman Murdika Wijaya and Ni Made Sulasteri, my brother I Wayan Eka Putra and my late grand mother, for their endless nagging and worries that turns into support and encouragement as the driving force for my studies. To my nephew Radha whom were a little gateway from the research work, until you are too big and too hard to handle. A special thanks goes to Ratih Oktarini whom had more than willing to accompany me in my late night work even though just via phone call, and still manage to give me an early morning wake-up call.

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Chapter 1

Introduction

1.1 Motivation for 3D-IC

Three dimensional integrated circuits / integration (3D-IC/Integration) refers to the broad concept of electronic system integration in the vertical direction, i.e. multiple active layers. Generally, it can be realized through 3D-IC packaging, 3D-monolithic integration, or wafer/chip level 3D-IC stacking with through substrate via. In 3D-IC stacking, individual wafers are first fabricated and then stacked vertically with through-Si vias (TSV) providing the interconnections between dice. IC-stacking can either be done at wafer-level or at die-level. Meanwhile, 3D-monolithic integration builds active semiconductor device layers sequentially up on the first IC layer [1].

A three dimensional architecture is first motivated by its potential to reduce the total chip size and shortening total interconnect length, hence reducing the signal propagation delay and its power consumption [2]. Traditionally, smaller feature sizes have dramatically improved device performance [3, 4]. However, the impact of this miniaturization and the performance of interconnect wires, had been less positive [5–8]. Smaller wire cross sections and smaller wire pitches have increased the resistance and capacitance of these lines respectively. As a result, signal propagation (RC) delay has increased significantly (see Figure 1.1). As interconnect scaling continues, the more RC delay becomes the dominant factor in determining the performance of advanced ICs [5–8]. Increasing in speed and functionality also

Figure 1.1: Interconnect and gate delays as a function of feature size in Al/SiO₂ and Cu/Low κ technologies [6, 10]. A three dimensional (3D) architecture is at first motivated by its potential to reduce the total chip size and shortening total interconnect length, hence reducing the signal propagation delay and its power consumption.

increase the complexity of chip design, which requires more and more transistors to be closely packed and connected [9]. As a result, chip size is continually increasing despite the reduction in feature size. Larger chip size affects the RC delays as it takes longer lines to transverse larger chips. Furthermore, there are physical limits to complementary metal-oxide-semiconductor (CMOS) transistor scaling.

As a workaround, designers are turning to multi-chip packages as a means to enhance system performance without fitting ever more devices on a single chip. Wire bonds are typically made from the edges of the chips to connect multiple chips. Because of growing circuit density and complexity, wire bonds have led to signal traffic bottleneck on the interconnects. Thus, wire bonds approach still presents latency, bandwidth, and power problems [2]. By having multiple active layers, the total chip size can be reduced and total interconnect length can be shorten, hence reducing the signal propagation delay and the power consumption. The 3D architecture also enable heterogeneous integration, placing different devices onto different layers. Since they are built on different layers, potential electromagnetic interference between such devices can be reduced. By fabricating such different technologies on separate

substrates followed by physical bonding, it can reduce the integration complexity significantly as well [2].

1.2 Monolithic 3D Integration

Monolithic is sometimes dubbed as the ‘bottom-up’ approach for 3D integration, where active silicon layers are built-up sequentially and separated from each other with interlayer dielectric. Although it is the most efficient way to integrate [1], there are still major technical challenges that need to be addressed. Probably, the most important process step of this approach is the formation of the single-crystal Si thin films on top of existing device layer. The easiest way possible to fabricate this film is to deposit polycrystalline Si (poly-Si) films or amorphous Si (a-Si) films as used in an active matrix liquid crystal display industry. However, building thin film transistor (TFT) on an a-Si or poly-Si is not applicable to the fabrication of ultrahigh density memory. Poly-Si or a-Si films have too many crystal defects that degrade carrier mobility and induce leakage current as well as other undesirable effects. Even if they can operate well as small-scale devices, such poor electrical characteristics cannot be tolerated for high density and highly reliable memory products. Currently, there are three popular techniques to achieve monolithic 3D integration, including beam recrystallization, silicon epitaxial growth, and solid phase crystallization.

1.2.1 Laser Beam Recrystallization

In this technique, a second active layer on an existing substrate is fabricated by first depositing a polysilicon layer followed by the fabrication of thin film transistors (TFTs) on top [11] as shown in Figure 1.2. However, transistors on polysilicon perform poorly, because they exhibit very low surface mobility and high threshold voltages. To improve the performance, an intense laser beam is directed towards the polysilicon layer to recrystallize and eliminate grain boundaries [12–20]. However, this is not practical for 3D devices because of the high temperatures, roughly

Figure 1.2: *Laser beam recrystallization [11]. Second active layer on an existing substrate is fabricated by first depositing a polysilicon layer followed by the fabrication of thin film transistors (TFTs) on top. An intense laser beam is directed towards the polysilicon layer to recrystallize and eliminate grain boundaries, hence improving device performance.*

around 1000°C, involved during melt. The high temperature will adversely affect the devices in the lower layers [21,22]. There has been on-going work to recrystallize polysilicon at lower temperatures [23,24], which can be tolerated better by lower layer transistors.

1.2.2 Silicon Epitaxial Growth

One of the techniques for forming additional Si layers is by first etching a hole in a passivated wafer. An epitaxially grown single-crystal Si is then seeded from an open window in the interlayer dielectric (ILD) as shown in Figure 1.3. The silicon crystal grows vertically and then laterally to cover the ILD [25]. The quality of the device can be as good as those fabricated underneath on the seed wafer surface, since the grown layer is single crystal with few defects [26]. However, the high temperatures (800°C) involved in this process cause significant degradation in the quality of devices on lower layers. Also, this technique cannot be used over metallization layers. Low-temperature silicon epitaxy using ultra-high-vacuum chemical vapor deposition (UHV-CVD) has been recently developed [27]. However, this process is not yet ready to be adopted in manufacturing.

Figure 1.3: *Silicon Epitaxy Growth. A second Si layer is epitaxially grown, and single-crystal Si is then seeded from an open window in the interlayer dielectric (ILD) [11]*

1.2.3 Solid Phase Crystallization

Solid phase crystallization (SPC) is a relatively lower temperature technique to fabricate devices in 3D. The second silicon layer is first deposited in the form of amorphous silicon (a-Si) as shown in Figure 1.4. Amorphous silicon can be deposited at low temperature. Then the amorphous silicon is crystallized to form polysilicon [28–31]. Crystallization is induced by Ge seed [32,33] or Ni seed [34,35] implanted in a small patterned window at temperature <500 °C. Subsequent device layer is created by repeating this step. Some recent results show the feasibility of making better performing devices at lower temperatures [36–38]. Low processing temperatures makes this technique compatible with lower level metallization [39]. However, the electrical characteristics of these devices are inferior to those made on single crystal Si [11]. On-chip 3D integration technologies are still in research. The difficulty to build circuitry in 3D and its ability to integrate only a limited number of devices will probably enable its use to only highly specialized applications.

Figure 1.4: *Solid Phase Crystallization. The second silicon layer is first deposited in the form of amorphous silicon (a-Si) and subsequent crystallization is induced by Ge seed [32, 33] or Ni seed [34, 35], (a) Fabrication of amorphous device, (b) Use seeding for simultaneous crystallization and dopant activation [11].*

1.3 3D IC-stacking Using Through-Si Vias (TSVs)

3D IC-stacking with TSV as shown in Figure 1.5 may be considered as the ultimate interconnect concept. Stacked chips provide optimal functionality/volume and relatively low-cost heterogeneous integration of diverse technologies. Furthermore, this technology does not suffer from problems associated with 3D on-chip / monolithic integration. Low cost in 3D IC-stacking is achieved because each IC can be first made individually and then stacked together. This technique allows each of the layers in the stack to contain circuits with different voltage, performance and fabrication process requirements. Chip performance also improves as layers are connected with very short vertical interconnects (TSV), which reduce timings delays. 3D IC-stacking is a ‘top down’ approach.

Figure 1.5: Wafer stacking technology, the ‘vias first’ process involves fabricating vias before the ICs are bonded and the ‘via last’ process involves fabricating vias after the wafers/ICs are bonded. (a) 3D IC-stacking using the ‘via first’ process steps [40], (b) 3D IC-stacking using the ‘via last’ process steps [41].

An IC-stack can be done either at wafer-to-wafer [42], chip-to-wafer [43, 44] or chip-to-chip [45, 46] level. Wafer-level processing offers the most cost advantage, whereas chip-to-chip processing is high yielding because it allows the use of known-good-dice.

The process sequence will mainly depend on the approach taken for fabricating of the vias, i.e. ‘vias first’ and ‘vias last’. The ‘vias first’ process involves fabricating vias before the ICs are bonded and the ‘via last’ process involves fabricating vias after the wafers/ICs are bonded. The major process steps common to either of these processes are preparation of top and bottom wafers, wafer thinning, fabrication of through-Si vias, alignment and bonding [1]. Meanwhile there is also ‘vias middle’ where the vias are fabricated before the back end metalization (BEOL), thus it is subpart of ‘vias first’ [47].

1.4 ICs Stacking Technologies

Many different technologies of IC-stacking is currently being developed by different groups around the world. The main difference between the various technologies is on how the wafers/ICs are bonded. Other major steps like wafer thinning, fabrication of through-Si vias, and precision alignment do not vary much between different versions of the technologies. Wafer bonding can be classified into two broad techniques. First, in direct bonding where wafers are bonded without any intermediate layers. Second is indirect bonding, intermediate layers are added to enhance the bonding. In the latter case, the two most common intermediate materials used are metals and polymers. Figure 1.6 visualizes the differences among different bonding technology options.

1.4.1 Direct Bonding

Direct wafer bonding typically requires two mirror-polished wafers to be put into contact. The two wafers are held together at room temperature (RT) by adhesive

Figure 1.6: 3D IC-stacking technologies classification based on bonding mechanism used. (a) Direct Oxide Bonding, SiO_2 to SiO_2 , (b) Metal-to-Metal Bonding, (c) Adhesive Bonding, Polyimide(PI), Benzocyclobutene (BCB).

forces, without any additional materials [48,49]. Further annealing at higher temperatures enables covalent bonds to be formed, thus strengthens and secures the bond [34,50]. So far, direct bonding has been done on all combination of Si based materials, i.e. Si, SiO_2 , Si_3N_4 .

For a good bond, careful preparation of mating surfaces is required. The mating surfaces should be pore-free or have high oxide density. Furthermore, the surface has to be smooth, flat, clean and with surface reactivity [42,51]. To avoid degradation of active devices, oxides are typically grown at relatively low temperature ($<450^\circ\text{C}$). However, oxides grown at such temperature normally are not dense enough for forming a good bond. Presence of fine pores can trap gas and absorbed OH^- ions. Gases and water molecules evolutions during post-bond annealing can cause bond-line voids and defects. Therefore, the oxides are usually densified by annealing in a N_2 atmosphere at 350°C for 5 h prior to bonding.

On the other hand, oxide densification can increase the oxide roughness by up to 8 nm - rms. To achieve a good bond, sub-nanometer roughness is required. Fortunately, subsequent chemical mechanical polishing (CMP) process is able to reduce the surface roughness. In the case of wafer to wafer bonding, the bond quality also depends on other factors such as wafer bow, warpage and patterning of the wafers [52]. Wafer bow of $<25\ \mu\text{m}$ over 6" wafers can have adverse effects on bonding. Furthermore, bow caused by materials deposition of oxide or any other materials during semiconductor processing can contribute additional $10\ \mu\text{m}$ to wafer

bow [1]. In order to reduce the bow, a force typically of 1 kN is applied during bonding and post-annealing.

Direct bonding has a very stringent requirement on surface cleanliness. Dry cleaning with oxygen plasma, followed by wet cleaning of RCA [53] or with piranha ($\text{H}_2\text{O}_2:\text{H}_2\text{SO}_4$) and a final rinse with deionized water [51] was found to be effective to get a good bond. The cleaning step removes possible foreign contaminant, and at the same time activates the mating surfaces. During the cleaning step, oxide surface terminated with OH groups initiate wafer bonding. The initial bonds at room temperature are weak, as they are based on Van der Waals attractive forces and hydrogen bonds. Subsequent annealing at higher temperatures will make these bonds stronger. The reaction at higher anneal temperature converts the weak Si-OH-Si bond to a stronger Si-O-Si bond, with the reaction $\text{Si-OH} + \text{OH-Si} \rightarrow \text{Si-O-Si} + \text{H}_2\text{O}$. This reaction is enhanced at higher temperature. However, the plasma is expected to roughen the surface as shown by Gui *et al.* [54], which is detrimental to bond quality.

Direct bonding of Si-Si or Si-SiO₂ is generally followed by an annealing treatment to enhance the bond quality, though the annealing temperature could be unacceptably high. However, a lower annealing temperature is also possible. An hour long post-bonding anneal between 200°C and 400°C resulted in higher (almost twice) bond energy compared to bonding without annealing [55].

Anodic bonding was introduced by Wallis and Pomerantz in 1969 [56]. As an enhancement of direct bonding, this method uses electrostatic attraction to pull the bonding surfaces together. It is a method commonly used to bond silicon or metals with glass. A typical glass-silicon bonding consists of applying an electric field of 100-1000 V across the structure, at temperatures between 300 – 400°C [57, 58]. By holding the substrate in positive potential with respect to the glass, the mobile sodium ions are driven away. The charge separation on the interfaces creates an electric field that pulls the surfaces together by electrostatic forces. Whether a seal (formation of SiO_x between Si and O atoms from opposite surfaces) will form

subsequent to contacting will depend on the bonding temperature and length of time the surfaces remain in contact. Anodic bonding is less sensitive to surface roughness or particulates than direct bonding. However, the coefficient of thermal expansion of the materials must be closely matched to minimize residual stresses. The glasses can also outgas at room temperatures. Hence for applications that require hermetic sealing, the glass must be outgassed at elevated temperature prior to bonding, to ensure reliability [59].

1.4.2 Polymer Adhesive Bonding

In adhesive wafer bonding, the polymer adhesive bears the forces involved to hold the surfaces together. The main advantage of using polymer adhesive for bonding is the high tolerance to surface topography. Ultra-smooth surface is not required as adhesive coating can smooth out any microscopic unevenness in the surface. The low bonding temperatures ensure the compatibility with standard integrated circuits wafer processing. Furthermore, it has the ability to join different types of wafers [60].

The most commonly used adhesives are polymer dielectrics, namely Polyimide (PI) or Benzocyclobutene (BCB). Polymers in liquid form that dissolved in a solvent are spin coated on either one of the mating surfaces or both. Spin-coated wafers are then aligned and bonded. Then, the polymer in the bonded wafers is cured in N_2 at $250^\circ C$ or at $300 - 400^\circ C$ for BCB and PI, respectively. Care needs to be taken during bonding, as adhesive bonding will tend to have entrapped voids [60,61]. The source of the voids can come from entrapped contaminants, out-gassing solvents or air [43,62].

1.4.3 Metal Eutectic Bonding

Solder/Eutectic bonding processes are fairly low temperature processes depending on the use of bonding materials that form eutectic alloys at specific temperatures. Like anodic bonding, they are also less sensitive to surface roughness and particulates than direct bonding [63]. In addition, eutectic alloys can be chosen that are

conductive, which provide an electrical connection between the devices and package. Examples of these materials are Au-Sn, Au-Ge and Au-Si, which have eutectic temperatures of 280°C, 361°C and 363°C, respectively [64]. As solder/eutectic bonding involves the formation of eutectic alloys, there must be good wetting between the bonding materials and substrate at the eutectic temperatures. However, oxide formation on any component will hinder proper wetting, which leads to poor bonding [64,65].

1.4.4 Copper-Thermocompression Bonding

For the reasons of better electrical performance, Cu has replaced Al as the interconnect material in modern IC. In 3D-IC stacking, Cu has the advantage as both the bonding material as well as interconnect material. However, Cu is known to oxidize under ambient conditions and even worse in that its oxide is not self-passivating [66]. It has been demonstrated that the presence of Cu oxide results in significantly lower Cu-Cu bond strengths compared to bonding of clean Cu surfaces (without oxide). Hence, it is imperative to remove this layer of oxide prior to bonding. It has been reported that samples that had gone through an acetic acid pre-clean followed by a reducing gas purge in the bond chamber yielded the highest bond toughness [67]. HCl has also been used to remove Cu oxide layer, and Chen *et al.* reported that small amount of oxide that forms in the interval time between HCl treatment and bonding does not appear to affect the bond quality [68].

Other factors that can affect the bond quality include thickness of the Cu layer, the geometry and size of the patterns, and the different types of surface pre-bond cleaning. In the case of wafer bonding, the quality of the bond has been shown to be tolerant to wafer bow [67]. It was demonstrated that wafer bows of up to 100 μm (tensile and compression) on 100 mm diameter substrates did not cause any reduction of the toughness of thermo-compression Cu-Cu bonds, compared to wafers bonded with nominally zero bow. This is mainly due to the the applied pressures that are sufficiently high to elastically deform the bowed wafers. For

bonding of Cu layers with different thicknesses, the Cu-Cu bond toughness has been shown to increase with Cu thickness, due to increased plastic dissipation in thicker films [69, 70]. The Cu-Cu bond toughness is also known to vary with pattern size and geometry of the bonding layer, due to differences in plastic energy dissipation and orientation of the features with respect to the loading direction [67].

Bonding chamber environment is another important factor to obtain good bonding. The chamber ambient should be in a vacuum environment with the pressure kept as low as possible. There are two reasons that vacuum is good for bonding. First, vacuum chamber can dramatically reduce particles in the atmosphere adhering to the surface. Solid particles on the copper surface may hinder the bonding process. The second reason is that oxygen in the atmosphere can be reduced. Presence of oxygen during the bonding process can lead them to react with copper atoms and form oxides. The existence of copper oxides has been shown to be deleterious to bonding quality [71, 72]. The commercial EVG bonder was designed to pump the chamber down to a minimum pressure of about 5×10^{-4} Torr, whereas a higher vacuum of about $10^{-6} - 10^{-8}$ Torr is required to prevent Cu surface oxidation. Hence, the unavailability of high vacuum commercial wafer bonders is a serious limitation.

A higher bonding temperature gives copper atoms in two bonded layers more energy to diffuse and allows grains to grow. Therefore, a high bonding temperature improves the bonding quality. For example, the diffusivity of Cu atoms at 400°C is much larger than that at room temperature. This finding also explains why it is difficult to bond at room temperature. However, in order not to degrade other materials in the device, the bonding temperature cannot be increased without limitation. In general, based on the bonding condition of 30 min bonding with an optional 30 or 60 min nitrogen anneal, 300°C is necessary to achieve a reliable bonding quality but with a distinguishable bonding interface [73]. A temperature of 350°C or 400°C with a longer anneal duration is necessary to achieve a strong bonding with no distinct bond interface. In addition, according to the previous study, there are no degradation effects on other materials under these bonding temperatures [74].

Sufficient bonding pressure can bring the two surfaces to be bonded close enough and let the atoms from the two layers interdiffuse in the initial stage of the bonding process. Therefore, sufficient bonding pressure is a necessary parameter for the success of bonding. The optimal pressure of EV AB1-PV bonder is 4,000 mbar (4000 N on 4" wafer) and offers enough contact for two wafers to process the bonding [75].

Bonding duration is another key to the completeness of the bonding process. It is especially important when the bonding temperature is not high enough. A long duration of bonding offers enough time for copper atoms and grains to complete bonding, although their energies are low. In this research regime, 30 min of bonding is the optimal duration for bonding processes above 300°C. Chen *et al.* [76] have shown that the Cu-Cu bond quality can be enhanced with an anneal step of about 30 minutes, after the application of the load, allowing further grain growth, atomic diffusion and recrystallization to occur. Chen *et al.* also observed various morphologies of non-distinct, zigzag, and distinct interfaces in the Cu bonded layer. It was proposed that these morphologies indicate a strong relationship between the roughness of surfaces and the initial steps of bonding [76].

Suga *et al.* [77,78] have shown that under a high vacuum of about 10^{-10} Torr and with surface activation using Ar beam bombardment (Surface Activation Bonding: SAB), Cu-Cu bonding at room temperature is possible. The Ar beam bombardment had done two things to the Cu surface. First, as indicated by X-ray photoelectron spectroscopy (XPS) analysis, Cu surface after CMP was covered by 2-3 nm of contamination and hydro-oxide, and 7-8 nm of CuO and Cu₂O. Ar beam bombardment removes these contaminants. Second, even though Ar of only less than 10^{13} dose/cm² was irradiated to sputter the Cu surface, several tens of nano-meter materials thickness was removed, which is more than the thickness of the surface oxide. Ion beam bombardment for activating the surfaces to be bonded may induce a large amount of lattice defects in the areas. The defects induced at the surface may enhance the diffusion at the contact area to contribute an ultimate contact for bonding [72].

Alternatively, the same concept of maintaining the cleanliness of the Cu surface

can be achieved by means of surface passivation [79]. On the other hand, maintaining Cu surface by means of oxide growth retardation had not been done before. In theory, low temperature storage can retard the surface oxidation rate. Oxide growth is temperature dependent, therefore lowering down the storage temperature may reduce its growth rate significantly.

1.5 Bond Strength Measurement Methods

In order to relate the bonding process parameters to the bond quality, a suitable measurement technique must be developed to quantify the bond strength of the bonded interfaces. The technique must be robust and sensitive enough to capture any effects due to changes in the bonding process. There are several techniques used to measure bond strength and a brief overview of each will be discussed. A comprehensive review of several bond-strength measurement methods is given by Vallin *et al.* [80].

1.5.1 Razor Blade Test

The razor blade test was first described by Maszara *et al.* [81] in which the insertion of a razor blade into the bonded interface, as shown in Figure 1.7, results in a crack length opening that is estimated from IR imaging. The crack length is related to the surface energy γ by [81]

$$\gamma = \frac{3}{8} \frac{Eh^3y^2}{L^4} \quad (1.1)$$

where E is the Young's modulus, h is the thickness of the wafer, y is half the blade thickness and L is the measured crack length. Another measurement parameter is the critical strain energy release rate G_C , which for brittle fracture is closely related to γ and simply differ by a factor of two [69], where

$$G_C = 2\gamma. \quad (1.2)$$

Figure 1.7: Schematic illustration of the razor blade test [81]

This method is advantageous for its simplicity in equipment and does not require any pre-test preparations of the bonded samples. However, there are several shortcomings to this method. First, the blade cannot be forced in between interfaces with high bond strengths and it is difficult to keep the blade perfectly perpendicular to the interface so that the crack front is straight and parallel to the interface. Both cases will likely result in wafer fracture, at which point the test will be completely qualitative. Second, comparison of results between different research groups can be difficult because measurements such as crack length and how the blade is inserted are often not reported [82]. Furthermore from equations (1.1) and (1.2), it can be seen that there is a strong dependence of γ and G_C on the crack length, such that slight differences in measurements of the crack length can lead to large errors in values of γ and G_C . Moreover, the observed crack length is also dependent on time and humidity, which can make repeatability difficult [83].

1.5.2 Tensile Test

In the tensile test, also known as the pull test, the bonded samples are glued onto attachments, often called pull studs, on both sides of the sample as shown in Figure 1.8. The sample is then fitted onto a tensile strain test machine and the studs are pulled apart. The maximum force, occurring at the point of separation, is recorded. This maximum force divided by the bonded area is taken as the tensile strength.

Figure 1.8: *Schematic illustration of tensile test sample attachment*

Though the tensile test may seem simple to use, there are several factors that if not taken into consideration, will affect the accuracy and the viability of the results [80]. First, the difficulty in specimen attachment is a major alignment problem. Not only do the studs have to be aligned to each other but the application of the glue has to be uniform or else unwanted bending forces may arise and distort the test results. Second, it is important to minimize defects in the samples since the cracks are initiated at the maximum stress point. Uncontrolled defects may occur at sample edges after operations such as dicing and defects can lead to lower than expected failure stress, with significant degrees of scatter in the data set. Finally, the tensile strength also depends on the geometry of the bonded samples, which makes comparing data between different tests difficult.

1.5.3 Chevron Test

The chevron test method can be seen as a natural development of the tensile test, where a load is applied to a specimen with a chevron-shaped notch, i.e. two edges meet at an angle. The test structure is subjected to a gradually increased load applied normal to the bond, as shown in Figure 1.9. A crack is initially formed at the tip of the chevron structure, exhibiting stable growth since the crack width increases as the crack proceeds. When the crack reaches a critical length, its growth becomes unstable which results in an instantaneous fracture of the sample. The

Figure 1.9: *Schematic of chevron test set-up, taken from Bagdahn et al. [84].*

critical load is a measure of the bond strength since the crack length depends only on the specimen geometry and loading condition. Hence, measurement of the fracture load is sufficient for determining the bonded structure's fracture toughness. The challenge is to model the geometry properly.

From the chevron tests, the strain energy release rate G_C can be calculated from the maximum load in the test, $F_{\max}$ using the expressions [84]

$$G_C = \frac{1 - \nu^2}{E} K_{IC}^2 \quad (1.3)$$

and

$$K_{IC} = \frac{F_{\max}}{B\sqrt{W}} Y_{\min} \quad (1.4)$$

where K_{IC} is the critical stress intensity factor, $Y_{\min}$ is the minimum value of the geometry function that corresponds to the crack length at which failure occurs. B , W , E and ν are the width, length, Young's modulus and Poisson's ratio of the specimen, respectively. From equations (1.3) and (1.4), the calculation of the bond strength requires knowledge of the geometry function Y , which is dependent on the thickness of the bonded layers and crack geometry. The geometry function Y can either be experimentally determined [85] or determined using finite-element methods, which can be less convenient in practical environment.

There are three exceptional capabilities that can be associated with the chevron

test method. First, fracture initiation is guided to the bond by the tip of the chevron because of the high stress concentration, hence making the method suitable for measuring high strength bonds. Second, an atomically sharp crack is created at the bond, thus avoiding ambiguity in crack opening angle estimations. Third, the fracture toughness is directly assessed through maximum force measurements. It is not necessary to measure the crack length, thereby reducing the complexity of the measurement equipment. However, it would be laborious to experimentally arrive at and verify the precise specimen geometry as well as determining an expression to take this geometry into account.

1.5.4 Shear Test

Die shear testing is the process of determining the strength of adhesion of a semiconductor die to the package’s die attach substrate (such as the die pad of a lead frame or the cavity of a hermetic package), by subjecting the die to a stress that is parallel to the plane of die attach substrate, resulting in a shearing stress between: 1) the die-die attach material interface; and 2) the die attach material-substrate interface [86]. The general purpose of die shear testing is to assess the overall quality of the die attach process, including the integrity of the materials and the capabilities of the processes used in mounting the die (and other elements, if any) to the package substrate. Mil-Std-883 Method 2019 is the most widely-used industry standard for performing this test.

The force applied to the die during die shear testing must be sufficient to shear the die from its mounting. The direction of the applied force must be perpendicular to the die edge and parallel to the die attach or substrate plane as illustrated in Figure 1.10. After the initial contact has been made and the application of force starts, the relative position of the tool must not change vertically, i.e. it must be prevented from contacting either the die attach material or the substrate.

At atomic scale, the shear force of contacting interface exhibits a dependence of both sliding speed v_c and the true contact area A_c , with the “force law” expressed

Figure 1.10: *Die shear configuration.*

as

$$F_f = \eta v_c A_c, \quad (1.5)$$

and

$$\eta = \frac{\rho_2}{\tau} \quad (1.6)$$

where η is the shear stress per unit velocity, ρ_2 is the mass per unit area of the sliding object, and τ is the characteristic “slip time”, which corresponds to the time for the moving object to fall to $1/e$ of its original value [87]. This relation enables us to determine the true contact area on the interface by measuring its shear strength.

1.5.5 Four Point Bend Test

In 1989, Charalambides *et al.* [88] proposed the four-point bend test (4PBT) for the measurement of interfacial fractural resistance or bond strength. The specimen is a bimaterial beam with a through thickness, central notch in one of the layers, and a pre-crack along the interface, as shown in Figure 1.11 (a). The four loading points provide a constant moment condition in the region between the inner points. At steady state conditions, the crack should propagate at a constant velocity under a constant load, and the strain energy release rate should be constant, as illustrated in Figure 1.11(b). The crack propagation then decelerates near the inner and outer loading points. Further crack growth requires an increase in load [88].

Figure 1.11: *Four Point Delamination Test, (a) Bimaterial notched four-point bending specimen with symmetrical interfacial cracks, taken from Charalambides et al. [88], (b) Schematic of an ideal load-displacement plot.*

Based on beam theory, the strain energy release rate of the specimen in steady state can be given by an analytical expression, simplified from the general form in [88] for the case of identical beams:

$$G_C = \frac{3(1 - \nu^2)}{2E} \left(\frac{Pl}{b} \right)^2 \left(\frac{1}{h_1^3} - \frac{1}{(h_1 + h_2)^2} \right) \left(\frac{1}{F} \right) \quad (1.7)$$

where P is the load at which crack propagation occurs, l is the distance between the inner and outer loading points, b is the width of specimen, and E , ν , h_1 and h_2 are the Young's modulus, the Poisson's ratio, the thickness of the notched wafer and unnotched wafer, respectively. F is the fraction of the specimen width that is bonded.

An advantage of the four-point bend test is that during debonding, the stress relaxation of the film is constrained and does not contribute to the debonding driving force. There is a small component of G_C due to elastic curvature of the wafer containing the film after debonding. However, it has been shown that this is quite negligible [89]. Another factor to be taken into account is the effect of bonding layer thickness on the dissipation of plastic energy. It has been shown that the effects of plastic deformation are higher in thicker copper stacks which surround the bonded interface [90]. These effects greatly enhance the measured interface toughness beyond the true strength of the bonded interface.

For bond strength measurements, cracks that are initiated and propagated due to a purely tensile mechanism, are commonly referred to as mode I failures. In contrast, when the cracks propagate along an interface due to purely shearing mechanisms, it is referred to as mode II failure. Four-point bend tests involve forces of bending moments and hence the delaminations along the interface are essentially mixed mode fractures. A parameter ψ is used to define this mode mixture, given as

$$\psi = \tan^{-1} \left(\frac{K_{II}}{K_I} \right), \quad (1.8)$$

where K_I and K_{II} are the stress intensity factors in mode I and II, respectively. As ψ varies from 0° to 90° , the failure mode changes from a pure mode I to a pure mode II with respect to the direction of crack propagation. The critical strain energy release rate G_C , is known to vary as a function of the parameter ψ and is typically lower in pure mode I [91]. The mode mixture for four-point bend tests also depends on the ratio of the bond layer thickness and the modulus mismatch between the two layers.

The aforementioned methods are among standard testing methods used to characterize the bonding in research and industry. Unfortunately, all these methods are destructive. The cost to conduct such test can be more expensive as the 3D technology becomes mature, especially when it involves destroying device structures. Thus, there is a need for non-destructive methodology to assess the bonding integrity.

1.5.6 Non Destructive Characterization

There has been discussions on the possibility to non-destructively examine the bonding interface. Among those methods are X or γ -ray inspection, resistivity measurement, dye penetrants, and ultrasonic testing which include acoustic microscopy and ultrasonic spectroscopy.

In most industries, ultrasonic techniques is the favorite method of non-destructive inspection. Ultrasound with frequencies above about 20 kHz requires relatively sim-

ple equipment for generation and detection. Hence, it has been used extensively, using piezoelectric transducers with water coupling in an immersion tank, or for direct contact with contact transducers [92]. The technique could identify the presence of voids on the interface, which can be used as the basis to deduce the bond mechanical strength. However, it would not be able to determine the state of chemical bonding at the interface, which could influence the bond strength. Furthermore, requirement of thin coupling layer between transducer and sample/device is inconvenient for testing, which might compromise device - chip performance.

Electrical contact resistance, is sometimes used as an indicator for good bonding. However, the presence of defect in the bonding interface induces only small changes in electrical resistance in conductive material such as Cu. A direct correlation between electrical and mechanical properties of thermocompression bonded Cu has also never been done. Chapter 2 is dedicated to develop a novel non-destructive method for evaluating the adhesion strength of copper bonded interface, along with methodology to correlate electrical and mechanical properties of the bonded interface.

1.6 Electrical Properties of Cu Contact

To implement a 3D architecture for circuit applications, electrical characterizations such as contact resistance measurement of the Cu–Cu bonded interconnects must be made and understood. The electrical contact resistance between surfaces is important in many fields of science and engineering, such as micro-switches in micro-electromechanical systems (MEMS) [93, 94], flip-chip bonding in microelectronics packaging [95, 96], and the head-disk interface of magnetic rigid disks [97]. Electrical contact resistance models have been proposed in the 1960s by Greenwood [98] and Holm [99]. They developed analytical expressions for the constriction resistance due to individual or clusters of circular contact areas. However, when the contact size is smaller than the mean free path of electrons, ballistic transport will have to be considered. A general analytical relation for size-dependent electrical contact

resistance that considers both the diffusive and ballistic components as asymptotic limits has also been proposed [100].

The effects of surface roughness and load on the electrical contact resistance of aluminum have been experimentally studied by Crinon and Evans [101]. On the other hand, Kogut and Komvopoulos [102] carried out numerical analysis on the dependence of electrical contact resistance on load, surface roughness, and apparent area. Jang and Barber [103] developed an electrical contact resistance model that takes into consideration the statistical size and spatial distribution of contact spots. Currently, there are a few reports on the experimental characterization on the impact of process parameters of the fabrication of 3D ICs on the electrical measurements [104].

The contact between two rough surfaces can be modeled as the contact of an equivalent rough surface to a perfectly flat plane [105,106]. From a contact mechanics perspective, the surface asperities are not completely flattened during bonding and only a fraction of the asperities are in contact with the opposite surface. This can be visualized as a distribution of contact spots between the two surfaces. The contact resistance can be assumed to be the equivalent resistance of all the contact spots at the bonded interface. It has been proposed that the prebond surface roughness of the Cu bonding layers and the applied load of the bonding process, which characterize the true contact area [107], are also the main factors affecting the value of the contact resistance of the bond interfaces.

The constriction resistance of an individual asperity between the classical and ballistic electronic conduction regimes can be expressed as [108]

$$R_B = \Gamma(l/a) \left(\frac{\rho}{2a} \right) + \frac{4\rho}{(3\pi a)} \frac{l}{a} \quad (1.9)$$

where ρ is the resistivity of the bonded material, a is the contact radius of a contacting asperity, and l is the electron mean free path, which in our case is that of Cu and has a value of 38.7 nm [108]. l/a is the Knudsen ratio and Γ is a function decreasing from 1 to 0.694 as l/a increases from 0 to ∞ [99,108].

Figure 1.12: Contact resistance reduction under current stressing phenomena extracted from [109]

Figure 1.13: Contact resistance test structure [109]

It has been reported that the contact resistance of Cu-Cu interfaces is reduced under current stressing as shown in 1.12 [109]. Resistance reduction was observed when the current was ramped from 1 mA to 100 mA on a cross structure as shown in Figure 1.13. A commentary paper by Timsit [110] suggests that the true contact area could be small enough that will allow electromigration to occur even at room temperature. Furthermore, elevated temperature around the interface could also enhance this effect.

Leong *et al.* in [75] observed that resistance reduction only started to appear when the current stress level had reached a certain value. Furthermore, Leong *et al.* also reported that this threshold current is higher for smaller initial resistance.

Figure 1.14: Contact resistance measurement results from Leong, which also showed a reduction in contact resistance when being stressed by electrical current [75].

Leong *et al.* observation, unlike earlier reports [109] and [111] that current reduction started from the beginning of current stressing, also only happened at high initial contact resistance as shown in Figure 1.14. Chapter 4 is dedicated to model this phenomena.

1.7 Contact Theory

It is generally accepted that when two nominally smooth surfaces are pressed together, the load will be borne by the contacting surface asperities from both surfaces. The contact area actually covers only certain discrete areas and not the whole nominal contact area, and hence is commonly referred to as the true contact area [112]. The ratio of the true-to-nominal contact area can be a very small value and is the basis of explanation propounded for a variety of phenomena, from friction and wear to adhesion and electrical contact resistance [113]. Hence, the study of deformation behavior of the contacting surface asperities and the accurate modeling of the contact between rough surfaces is important for a detailed understanding of these phenomena.

The contact of rough surfaces has been studied by many researchers and the pioneering contribution to this field was made by Greenwood and Williamson [112], who developed a basic elastic contact model (GW model). In their model, a rough

Figure 1.15: Schematic of multispot contact area. If a rough surface and smooth surface are pressed against each other until the summit mean plane of the rough surface and the mean plane of the smooth surface are separated by an amount of d , summits that have a height $z > d$ will deform.

surface is represented by a population of hemispherical-tipped asperities of identical radius of curvature R with their summit heights following a Gaussian distribution. The GW model assumes the surface asperities follow an elastic deformation behavior as proposed by Hertz [114], the contacts are frictionless and there are no interactions between neighboring asperities. Greenwood and Tripp [115] also showed that the contact of two rough surfaces could be modeled as the contact of an equivalent rough surface to a perfectly flat plane. GW formulated that when large flat surfaces are pressed together, their mean planes become parallel. Thus, if a rough surface and a smooth surface are pressed against each other until the summit mean plane of the rough surface and the mean plane of the smooth surface are separated by an amount d , summits that have a height $z > d$ will deform. In randomly distributed summits, the total number of deformed asperities that form a micro contact is [116]

$$N_t = A_n \eta \int_d^{\infty} f(z) dz \quad (1.10)$$

where A_n is the nominal contacting area, η is the asperities per unit area, and $f(z)$ is the asperity heights distribution function.

Given that if a contacting summit has its height z exceeds d , the summit must deform by an amount $w = z - d$ as shown in Figure 1.15. Hertz's solution gives the

contact area as

$$A_c(w) = \pi R w = \pi R(z - d) = \pi a^2 \quad (1.11)$$

where a is the contact radius and R is the curvature of the tip of the asperity. For multiple asperities equations (1.10) and (1.11) are combined to becomes

$$A_c = \int_d^\infty \eta A_n \pi R(z - d) f(z) dz. \quad (1.12)$$

The amount of load that is supported by a single asperity is given by [116]

$$L_e(w) = \frac{4}{3} E R^{1/2} w^{3/2} = \frac{4}{3} E R^{1/2} (z - d)^{3/2}, \quad (1.13)$$

and for multiple asperities, it then becomes

$$L_{tot} = A_n \eta \int_d^\infty \frac{4}{3} E R^{1/2} (z - d)^{3/2} f(z) dz. \quad (1.14)$$

By solving equation (1.14) for the appropriate d value, the true contact area can then be calculated from equation (1.12).

The GW model has some severe limitations and practicality issues. First, it assumes all surface asperities to have an identical curvature radius R where in reality, one would expect the asperities to have different curvature radius. A more complex way to represents surface roughness have been suggested by Archard in the form of fractal surface, i.e. an asperity consists of yet smaller asperities with even smaller tip curvature radus [117, 118]. Persson, suggested an alternative view to surface roughness and contacts [119]. Instead of a population of asperities, the real surface can be approached as superposition of height variations at multiple spatial wavelengths. This approach is considerably complex and will not be considered in the current thesis. However, the approach would be interesting to be considered in the future to overcome GW models.

Another limitation of GW model is to assumes fully elastic deformation. However, most contacting surfaces under applied load will involve various degrees of plastic deformation of the asperities and without taking into account the plastic deformation component, the true contact area will most likely be underestimated. For instance, Powierza *et al.* [120] performed an experimental verification of the GW model and found that the model was surprisingly accurate at predicting elastic contact phenomena but when the applied load exceeded about half the yield point load, the results predicted by the GW model severely deviated (underestimated) from the experimental results.

In 1933, Abbott and Firestone [121] developed, till today, the most widely used plastic contact model, known as the surface micro-geometry model. This model assumes that the deformation of a rough surface against a rigid smooth flat surface is fully plastic and is equivalent to the truncation of the undeformed rough surface at its intersection with the flat surface. As a result, the true contact area is simply the geometrical intersection of the flat surface with the original undeformed profile of the rough surface, and the contact pressure is the flow pressure. Pullen and Williamson [122] also established a volume conservation model for the fully plastic contact of rough surfaces. However, these two models are only applicable for fully plastic deformations.

To bridge the two extreme approaches of modeling contacts as fully elastic or fully plastic, Chang [123] put forward an elastic-plastic contact model for rough surfaces on the basis of volume conservation of plastically deformed asperities (CEB model). The same principal assumptions as the GW model is applied to the entire deformation range, from fully elastic to fully plastic. However, this model has several shortcomings. The first is the discontinuity in the contact load at the critical point of initial yielding. At this point, the average contact pressure is allowed to jump from the yield point Y to an average stress of $1.6Y$ in the plastic regime, where Y is the yield stress of the material. Another shortcoming is that this model only allows two possible states of deformation for a contacting asperity, either fully elastic or

fully plastic, the transition from elastic to plastic is not modeled.

Zhao *et al.* [124] and Kogut and Etsion [125] have developed models to describe the transition between the fully elastic and fully plastic regimes. Zhao made use of a template function put forth by Francis [126], which satisfies the continuity of the function and its slope at the two transitions, while Kogut and Etsion analyzed the problem with finite-element analysis. Both methods assume full plasticity beyond a certain critical amount of deformation. In all these analyses, the average contact pressure, upon the onset of full plasticity, is taken to be equivalent to a fraction of the hardness H , of the material. Tabor [127] showed that this is true for materials without work hardening characteristics or that have already work hardened, but is not valid for work hardening materials, like most metals.

A contact model that takes into account of work hardening effects had been proposed by Leong *et al.* [75, 107]. Leong *et al.* argued that certain materials suffer work hardening effect. To account for work hardening effect, Leong *et al.* have modified equation(1.12) into

$$A_t = 2\eta A_n \pi R \int_d^{\infty} (z - d) f(z) dz \quad (1.15)$$

and equation (1.14) to

$$L_t = 3(2)^{1+x/2} \eta A_n \pi R^{1-x/2} Y \left(\frac{0.2}{\varepsilon} \right)^x \int_d^{\infty} (z - d)^{1+x/2} f(z) dz \quad (1.16)$$

where Y is the material yield stress, ε is the yield strain and x is the work hardening index.

Apart from the elastic and plastic deformation problem, all of the aforementioned models consider only behavior at a single temperature. As had been known, materials properties change with temperature. Furthermore, plastic deformation is a dynamic process that have time dependent behavior. Hill and Wallach in [128], had considered the time and temperature for their modeling of Cu bonding. How-

Figure 1.16: 3D surface plot from AFM scan [107].

ever, the model oversimplified the surface topography. A contact model that takes into account the temperature and dynamic nature of the bonding will be presented in Chapter 3 of this thesis.

1.8 Roughness Parameter Extraction of Real Surface

To apply the contact theory, one needs to know the surface topography parameters such as the radii of curvature of individual asperity R_i , the standard deviation of summit heights σ_s , and the density of asperities η . Prediction of the true contact area would therefore depend on the accuracy in determining these parameters.

The method for extracting these parameters from atomic force microscopy (AFM) profile measurement had been developed by Leong *et al.* [107]. In that method, profiles are taken from random areas with scan size of $1 \times 1 \mu\text{m}^2$ and scanning interval of approximately 5 nm orthogonally defined as x and y directions. From AFM scan output data, three-dimensional topographical maps that are representations of the surface can be constructed. Each set of points is defined in a Cartesian coordinate system by the three ordinates x , y , z to form a three dimensional surface representation of the surface as shown in Figure 1.16.

A true summit is defined when its z coordinate is larger than at least two consecutive neighboring points in each of the eight directions (two vertical, two horizontal, and four diagonal) to reduce the probability of locating false summits as shown in

Figure 1.17: An identification of asperity summits, if a summit exists at z_{ij} if $z_{ij} > z_{i \pm n, j \pm n}$ for n equals to 1 and 2 (16 total points).

Figure 1.17. The identification of these summit heights provides a distribution of summit heights (parameter σ_s) and the number of summits (parameter η).

The radius of curvature of specific summit is calculated along the x , y and two diagonal axes, which includes all successively lower z -coordinate data points (not just two consecutively two data points). The radius of curvature R_i of an asperity is then represented by the best fit curve calculated using the sum-of-least squares method.

1.9 Objectives

The understanding of the formation mechanism and properties of a Cu bonded interface is paramount for the success of the Cu bonding as the enabling technology for 3D-IC and heterogeneous integration. Specifically, the objective of this thesis are:

- To develop a characterization method to assess the bond integrity in a non-destructive manner. Furthermore, to relate the measurement result from the developed methods to the conventional mechanical method, i.e. correlate the electrical and mechanical properties of bonded Cu interfaces.
- To model the formation of true contact area after bonding. The model should include the dependence of process parameters such as bond temperature, surface roughness and applied loads, on the bond strengths of the Cu-Cu bonds.

- To model bond interface's true contact area enhancement through thermal annealing and direct current stressing.

1.10 Thesis Scope

This thesis consists of five chapters with an appendix for detailing any complex calculation and computing algorithm. Chapter 1 presents the overview of current technology, motivation for the current research and brief review on the essential fundamental knowledge that were used on the research.

In Chapter 2, a new characterization method is proposed. The method utilizes the electrical characteristics of bonded interfaces under alternating current (AC) bias. Instead of relying on the true contact resistance, an extra inductive component would be added externally to amplify the contact's electrical characteristic. The proposed method is tested by creating a test structure that enables direct correlation between the mechanical properties and electrical properties of a metal contact.

Chapter 3 focuses on the modeling of bond integrity of thermocompression process. The effort includes incorporation of surface topographic characteristics, and bonding environment which includes applied load, temperature, and time. The model predicts the bond integrity in terms of true contact area, which is then related to the bond integrity through experiments.

Chapter 4 models the post-bonding bond interface enhancement through thermal annealing and direct current stressing. Earlier published results show that contact resistance of a Cu bonded interface can experience a decrease under electrical current stressing. The model validity would be evaluated by fitting to known experimental results from Chen *et al.* [109]

Chapter 5 summarizes and conclude various aspects of this work. Finally, recommendations for future work is given.

Chapter 2

Development of a Non Destructive Characterization Methodology

2.1 Overview

The ability to assess the bond interface quality non-destructively becomes more important as technology for 3D-IC becomes more mature. Mechanical testing on bonded processed wafers can be very costly, particularly on production wafers which have active devices designed in the chips. Destroying device chips is economically undesirable. Thus, the bond strength needs to be assessed non-destructively.

Measuring the contact resistance and its variation is probably the most common non-destructive method to assess a contact's quality [98,129–133]. However, a direct correlation between the electrical and mechanical properties had never been made. Those two sets of electronic and mechanical test structures are normally fabricated differently and incompatible with each other. For example, an electrical test structure normally consists of chains of contacting interface [131], or a cross structure [104,109]. These structures are not suitable for mechanical characterization due to its small dimension and low bond toughness. On the other hand, a sufficiently large mechanical structure will have a very low contact resistance that becomes insensitive to changes in the mechanical properties.

Dervos had attempted to overcome the electrical measurement sensitivity issue by measuring the electrical energy that is stored in the contact interface under alternating current (AC) bias [132]. This method utilizes the resistive and capacitive effects of the interface [134,135] to quantify the true contact area from its current-voltage characteristic. The measurement gives out a current-voltage (I-V) loop as an indication of contact quality. However, direct correlation of the measured I-V loop to the true contact area is not well defined. Furthermore, the measurement depends on the source frequency, which adds to the complexity of the true contact area determination.

In this chapter, a new characterization methodology based on AC interface characteristic is proposed. As a proof of concept, an experiment is designed to enable direct correlation between the bond shear strength and electrical contact characteristics.

2.2 Multi-spot Electrical Contact Resistance

As a consequence of surface's micro-roughness, contact on nominally flat surface can consist of multiple spots [98] as illustrated in Figure 2.1(a). In this case, any ideally contacted spot may be considered as a temperature independent linear resistor connected in parallel with another, with each of the contacting asperity having an electrical resistance that have been shown in equation (1.9). Equivalent resistance for the entire contacting area is thus

Figure 2.1: *Electrical modeling of a constriction interface, with contact points represented as resistors, and gaps represented as capacitors. (a) Real interface, (b) modeled interface and (c) equivalent electrical circuit.*

$$\frac{1}{R_c} = \sum_{i=1}^{N_t} \frac{1}{R_{ci}} = \sum_{i=1}^{N_t} \frac{1}{\Gamma(l/a_i) \times \left(\frac{\rho}{2a_i} \right) + \frac{4l\rho}{3\pi a_i^2}} \quad (2.1)$$

where ρ is the resistivity of the bonded material, and l is the electron mean free path, which for Cu and has a value of 38.7 nm [108]. l/a is the Knudsen ratio and Γ is a function decreasing from 1 to 0.694 as l/a increases from 0 to ∞ [99, 108], a_i is the radius of each contacting asperity and N_t is the number of contacting asperities.

Individual radius of a contacting asperity can be calculated based on the method discussed in section 1.7. Assuming the contact area for each asperity is circular, the radius of each contacting asperity can be obtained by re-arranging equation (1.11) to become

$$a_i = \sqrt{R(z_i - d)} \quad (2.2)$$

with R is the tip curvature of contacting asperity, z_i is the asperity heights, and d is the mean plane distance of the two contacting surface. The total number of deformed asperities that form a micro contact is given in equation (1.10). Thus, the contact resistance can be related to the bonding condition and surface roughness of the film which affect both a_i and N_t .

Meanwhile, any isolated cavity or non-contacted micro-structure may be treated as a field and temperature independent capacitor [134, 135], as shown in Figure 2.1(c). Based on classical electrostatics, the contact capacitance is given as

$$C_c = \frac{\varepsilon_o(A_n - A_c)}{d} \quad (2.3)$$

where ε_o is the permittivity of vacuum, A_n is the nominal contact area, A_c is the true contact area as defined in equation (1.15), and d is the mean plane distance between the contacting surfaces which is assumed as the mean cavity's gap.

It had been known that there is proportionality between true contact area [87,

136,137] and bond shear strength. Their relation can be represented as

$$F = KA_c, \quad (2.4)$$

with F is the bond shear strength, K is the proportional constant and A_c is the true contact area. Thus, contact resistance from Cu to Cu thermocompression bonded interface should also be inversely proportional to its shear strength, therefore measurement of true contact resistance should be able to predict the bond integrity of Cu to Cu bonding. However, contact resistance measurement becomes less sensitive to the changes in the bond interface at larger true contact area. This limitation is simulated and experimentally proved in sections 2.4 and 2.7 respectively. Thus, the next section proposes a method to assess the bond interface properties with higher sensitivity electrically, even at large true contact area.

2.3 Characterization of Contacts by Resonance Frequency

Due to the good conductivity of Cu, independent measurement of contact resistance R_c and contact capacitance C_c is sometimes difficult. Contact resistance of Cu to Cu thermocompression bonded interface can be too small ($10^{-4} \Omega$ range) to be measured with confidence. However under an applied AC bias, every circuit has resistive, capacitive and inductive properties that give out a unique resonance frequency that can be utilized as contact characterization. Resonance frequency of the interface can be isolated and magnified by introducing an inductor to the electrical measurement circuit as shown in Figure 2.1(c). Figure 2.2 illustrates how the inductive component can be added as part of the measurement circuit.

The external components Z_{ext} consist of a bank of inductors and a resistor in parallel configuration, which is then connected in series to the contacting interface Z_c through a measurement line R_{line} . The total impedance of the circuit as shown in Figure 2.2 is given as,

Figure 2.2: *Proposed non-destructive bond integrity characterization method by resonance frequency measurement. An equivalent circuit for metal contact with added external circuit, which consists of resistor and an inductor.*

$$Z_{tot} = Z_{ext} + Z_c + R_{line} \quad (2.5)$$

where Z_{ext} is the impedance of the external component, Z_c is the impedance of the contacting interface. With ω as the frequency of the AC source, Z_{ext} is given by

$$\frac{1}{Z_{ext}} = \frac{1}{R_{out}} + \frac{1}{R_{in} + j\omega L} \quad (2.6)$$

where R_{in} is the internal resistance of the inductor, $j = \sqrt{-1}$ and R_{out} is the external resistor. Z_c can be expressed as

$$\frac{1}{Z_c} = \frac{1}{R_c} + j\omega C_c. \quad (2.7)$$

By substituting equations (2.6) and (2.7) to (2.5), we have

$$Z_{tot} = \frac{(R_{in}R_{out}^2 + R_{in}^2R_{out} + \omega^2L^2R_{out} + j\omega LR_{out}^2)}{(R_{out} + R_{in})^2 + \omega^2L^2} + \frac{(R_c - j\omega C_cR_c^2)}{1 + \omega^2C_c^2R_c^2} + R_{line} \quad (2.8)$$

At resonance frequency ω_{res} , the circuit's reactance (imaginary part of the impedance)

Figure 2.3: Comparison of $\Gamma(l/a)$ between approximate formula $\Gamma(l/a) \approx \frac{2}{\pi} \int_0^\infty e^{-(l/a)x} \text{sinc } x \, dx$ [100] (dashed line) given and simulated $\Gamma(l/a)$ extracted from [108] (solid line).

goes to zero. Thus, setting the imaginary part of equation (2.5) to zero

$$X = \frac{j\omega_{res}LR_{out}^2}{(R_{out} + R_{in})^2 + \omega_{res}^2L^2} + \frac{(-j\omega_{res}C_cR_c^2)}{1 + \omega_{res}^2C_c^2R_c^2} = 0 \quad (2.9)$$

$$\omega_{res}^2 = \frac{C_cR_c^2(R_{out} + R_{in})^2 - LR_{out}^2}{C_c^2R_c^2LR_{out}^2 - C_cR_c^2L^2}, \quad (2.10)$$

where equation (2.10) is the resonance frequency of the circuit in Figure 2.2 (detail derivation presented in Appendix C.2). From equation (2.10), it can be seen that the resonance frequency of the circuits is independent of R_{line} , which enable an isolated characterization of Cu bonded interface, even in the case of chain resistance, where the line resistance could obscure the contact properties. In resonance frequency method, with the line's impedance excluded, interface resistance can be independently characterized. Furthermore, the measurement sensitivity can be adapted to different measurement sensitivity and range by adjusting the inductor L and external resistor R_{out} . The advantage of contact interface characterization through resonance frequency method is simulated and experimentally proved in section 2.4 and 2.7, respectively.

2.4 Simulation

Value of $\Gamma(l/a)$ in equation 2.1 can be obtained from [108] or mathematical approximation [100]. For the purpose of simulation, $\Gamma(l/a)$ simulated values that were extracted from [108,138] was preferred. Approximation of $\Gamma(l/a) \approx \frac{2}{\pi} \int_0^\infty e^{-(l/a)x} \text{sinc } x \, dx$ [100] suffers larger deviation as l/a increases as shown in Figure 2.3.

Figure 2.4: Calculation results on contact resistance and contact capacitance as a function of true contact area. Represented here are (a) specific contact resistance (contact resistance multiplied by nominal contact area A_n) and (b) specific contact capacitance (contact resistance divided by nominal contact area A_n).

Figure 2.4 (a) and (b) shows the simulated dependence of contact resistance and contact capacitance, as a function of total true contact area, respectively. There is an inverse relation between the true contact area and contact resistance. Based on equation (2.4), the contact resistance of Cu to Cu thermocompression bonded interface should also be inversely proportional to its shear strength. Therefore, knowing the contact resistance should give an indication of the bond integrity of Cu to Cu bonding. However, contact resistance measurements become less sensitive to the changes in the bond interface at larger true contact area, which limit its application at low true contact area.

Meanwhile, Figure 2.4(b) shows that the contact capacitance increases with A_c . This is understandable as contact capacitance that defined by equation (2.3), is proportional to $(A_n - A_c)/d$ and. It can noted from equation (1.15) that an increase in A_c followed by and decrease in $(A_n - A_c)$, and is associated with a decrease in

the main plane distance d . Since d decrease faster than $(A_n - A_c)$, the proportional factor of $(A_n - A_c)/d$ in equation (2.3) increases with A_c , thus contact capacitance increases with A_c . The relationship between d , A_c and $(A_n - A_c)/d$ are illustrated further in Figure D.1 in Appendix D.

Figure 2.5: Simulated Cu contact resonance frequency as a function of true contact area. The measurement sensitivity and range can be adjusted from the component of the external circuits, (a) adjusting the inductor value to $L = 0.1 \text{ H}$, 1 H and 10 , which results in measurement sensitivity of $2.4 \times 10^4 \text{ GHz} / \%A_c$, $7.1 \times 10^3 \text{ GHz} / \%A_c$ and $2.4 \times 10^2 \text{ GHz} / \%A_c$, respectively and (b) adjusting the external resistor value to $R_{out} = 10 \Omega$, 1Ω and 0.1Ω , which results in measurement sensitivity of $6.1 \times 10^4 \text{ GHz} / \%A_c$, $6.1 \times 10^3 \text{ GHz} / \%A_c$ and $6.1 \times 10^2 \text{ GHz} / \%A_c$, respectively.

Figure 2.5 shows the behavior of modeled circuit under AC bias at different frequency and simulated resonance frequency of microscopically rough contact as a function of the fraction of true contact area. In the case of measurements sensitivity, the resonance frequency is also shown to be more sensitive to the change in true contact area as compared to the contact resistance measurement. Theoretically, small changes in true contact area (bond strength) corresponded to large changes in resonance frequency.

The resonance frequency measurement setup can have a sensitivity of $2.4 \times 10^4 \text{ GHz} / \%A_c$, $7.1 \times 10^3 \text{ GHz} / \%A_c$ and $2.4 \times 10^2 \text{ GHz} / \%A_c$ for $L = 0.1 \text{ H}$, 1 H and 10 H , respectively with $R_{in} = 230 \Omega$ and $R_{out} = 0.4 \Omega$ kept constant as shown in Figure 2.5(a). Similarly, measurement sensitivity can also be adjusted by changing the R_{out} such that the setup has a measurement sensitivity of $6.1 \times 10^4 \text{ GHz} / \%A_c$, $6.1 \times 10^3 \text{ GHz} / \%A_c$ and $6.1 \times 10^2 \text{ GHz} / \%A_c$ for $R_{out} = 10 \Omega$, 1Ω and 0.1Ω , respectively as shown in Figure 2.5(b).

This simulation result demonstrated the ability of the proposed method to adapt to different testing conditions. Higher measurement sensitivity can be achieved with lower L and higher R_{out} at the expense of measurement range as the resonance frequency becomes ridiculously high at low L and high R_{out} . On the other hand, a wider measurement range can be obtained with higher L and lower R_{out} at the expenses of measurement sensitivity.

This ability to change the measurement sensitivity is very useful as it helps to overcome the measurement instrument limitation. For example, a lab or a manufacturing site may only have impedance measurement instruments limited to 10 GHz frequency. With $L = 10$ H, $R_{in} = 230$ Ω and $R_{out} = 0.4$ Ω , even 0.1 % A_c will be out of the measurement range. However, by using larger L or lower R_{out} or both, the measurement range can be adjusted such that the measurement range can fall within the instrument's measurement capability. Changing a component of L and R_{out} is a lot cheaper as compared to buying an instrument with a higher frequency range. Using a larger L is more practical as inductance value of a wire coil can be increased theoretically indefinitely by winding more wire in a coil, as compared to lower R_{out} as the resistance value cannot be reduced indefinitely. The resistor used depends on the wire cross section, wire length and the materials properties. Thus, based on equation (2.4), resonance frequency measurement should also be able to give an indication of the bond integrity of Cu to Cu bonding.

2.5 Experiments Design

The experiment is designed to enable three methods of characterization on a single test structure, i.e. electrical contact resistance measurement, AC resonance frequency method, and mechanical shear test. Simple bonding structure that consists of three probing pads for electrical measurement as shown in Figure 2.6(a) was fabricated.

The structure was built by bonding a 2.5 mm $\times$ 2.5 mm size chip on a top of 5 mm $\times$ 5 mm size chip. Insulation lines between the adjacent probing pad A,

Figure 2.6: Chip level bonding test structure that enables both mechanical and electrical characterization of the bonding interface. (a) Pattern on the test structure consists of three probing pads A, B and C that create interface R_1 , R_2 and R_3 , (b) the equivalent electrical circuit for measurement of contact resistance R_1 .

B, and C in Figure 2.6(a) were created by scraping the Cu layer on the bottom chip using a diamond pen. The structure enables four point wire contact resistance measurement, AC resonance frequency measurement as well as mechanical die shear test. R_1 , R_2 and R_3 represent measurable contact resistance between pad A, B or C with the top chip, respectively. Contact resistance R_1 can be determined as a ratio of voltage difference between pad A and B with a current that flowing from pad A to C. Figure 2.6(b) illustrates the equivalent circuits of the measurement set up. With no current flowing across R_2 , V only measures the potential difference across R_1 .

Prior to bonding, surface roughness parameters were taken by atomic force microscopy (AFM), where roughness parameters such as radius of asperity R , asperity density η and asperity height distribution σ were extracted from AFM output data using the method that was developed by Leong *et al.* [75]. Three AFM measurement per sample were taken at random location.

2.6 Measurements

The contact resistance and the resonance frequency of the bonded interface were characterized before subjecting it to the destructive shear test. Contact resistance measurement was carried on a MicromanipulatorTM probe station that was connected to an Agilent 4156C parametric analyzer. Four point contact resistance measurement was done. Contact resistance R_1 was measured by ramping a current between terminal A and C in Figure 2.6(a). At the same time, the voltage difference between terminal A and B was measured. The contact resistance R_1 is calculated from the slope of the measured voltage (I-V).

The sample resonance frequency was measured by an Impedance Analyzer that has 10 Hz - 10 MHz frequency range. Two terminal point probing between A-B and A-C was carried out with an inductor component connected to the sample in series as shown in Figure 2.2. The external component has a total inductance of 0.47 H (consists of ten 47 mH inductors connected in series), which was placed in parallel with 0.4Ω conductor. Several chips bonded so well such that the resonance frequency of the bonded interface were out of the instrument frequency range i.e. higher than 10 MHz. To overcome the instrument limitation and the availability of the large value inductor, the resonance frequency was estimated by fitting the circuit impedance profile up to 10 MHz with the simulation results. The input for simulation, i.e. fraction of true contact area, were adjusted such that the simulation profile could fit the results from measurement.

To assess the mechanical strength, shear testing was carried out on a DAGE 4000 Multi-purpose Bondtester. The bonded samples were put on the stage, in such a way that the bottom chip was being held by a metal stopper, while the top chip was being pushed parallel to the sample surface. The blade traveled with a constant velocity of $50 \mu\text{m/s}$ until fracture was detected, i.e. a sudden drop in applied force. The maximum force required before fracture was then recorded. The shear strength was calculated by dividing the maximum force by the area of the small chip. To avoid friction between the shearing blade and the bottom chip, the tip of the blade

was placed at a distance of $5\text{ }\mu\text{m}$ from the bottom chip's surface.

2.7 Results and Discussion

Figure 2.7(a) shows the measured contact resistance as a function of measured shear strength. The measurement results show an inverse relation between shear strength and the contact resistance, similar to the simulated results shown in Figure 2.4(a). It can be observed as well that the contact resistance flattens as the bond strength increases. This implies that changes in measured resistance cannot be detected even though there are significant changes in the sample shear strength. Two outlier points were also observed, that low contact resistance samples have low shear strength.

Figure 2.7: Measurement of electrical contact properties of chip bonded sample, (a) measured contact resistance and (b) Measured contact resonance frequency as a function of measured shear stress.

Considering the two points represents a significant portion of the entire data set, their presence could be contributed by some other factors that had not been considered in the current thesis. Two possible factors could be interface Cu oxides and high temperature conductive contaminant.

Even though care had been taken to remove Cu oxides prior to bonding through wet cleaning, the chips were still exposed to atmospheric condition briefly before bonding was carried out. In those brief period of time, Cu oxides could form, or any other conductive contaminant could land on the chip's Cu surface. In the case

of Cu oxides, Cu_2O is the most likely candidate due to its conductive property as compared to CuO_2 . Thus, the presence of Cu_2O in the interface would still grant a reasonably low contact resistance. However, since the presence of uncontrolled oxides would be detrimental to bonding quality, the bond interface has low shear strength. In the case of other type of contaminant, it can come from the various source. However, the most likely source would come from the bonder plate that are made from stainless steel. Another source, would be the oven chamber which readily rusted on the exterior, which is also made from steel.

Figure 2.8: Resonance frequency measurement eliminates the effect of sheet resistance effect in determining the contact quality, (a) Oxidized surface of probing pad are indicated by dark color in pad A, and B, and less in C. (b) Changes in sheet resistance shift the impedance measurement up or down, but not the position of the resonance frequency.

On the other hand, Figure 2.7(b) shows the measured contact resonance frequency as a function of measured shear strength. It shows the measured resonance frequency increases with measured shear strength as predicted in Figure 2.5. To demonstrate the independence of the resonance frequency method on line resistance, the probe on pad A was placed on different positions that were oxidized to different degrees as shown in Figure 2.8(a). A low vacuum had caused the exposed Cu to be oxidized, resulting differences in sheet resistance on the probing pad. Figure 2.8(b) shows that changing the position of the probe on the pad did not change the position of the resonance frequency peak. However, as expected, the difference in the line

Figure 2.9: Work flow to estimate the true contact area A_c from contact resistance measurement, resonance frequency measurement and shear test.

resistance changed the absolute magnitude of the circuit's impedance.

Using a combination of equations (2.1), (2.10) and (2.4), true contact area of the samples can be estimated. A look-up table that relates true contact area with contact resistance and resonance frequency can be generated. These look-up table in turn can be used to estimate the true contact area from contact resistance and resonance measurement method as illustrated in Figure 2.9.

Meanwhile, true contact area from shear test can be estimated by dividing the bond shear strength with K . The proper value for K is unknown at this stage. Thus, an initial guess was made that K is set to a the known bulk Cu shear strength. This is reasonable considering the bulk Cu shear strength represents the ultimate shear strength of materials without any interface imperfections. Even though this is true for bulk Cu properties, it might not be true for Cu film case especially bonded ones.

Figure 2.10: Comparison of true contact area calculations from different characterization method. Contact resistance and resonance frequency method produce value fairly close each other, but shear test predict much higher true contact area.

This initial guessed value also further discussed with the empirically determined K in the rest of this section.

Estimation of true contact area from different testing method is presented in Figure 2.10. True contact area estimation from contact resistance measurement and resonance frequency measurement produce values fairly close to each other, but shear test results predict a much larger true contact area. The same trend was obtained between mechanical shear test and resonance frequency measurement.

There are two possible arguments of this discrepancy. First, K is not the bulk Cu shear strength, i.e. K value is much larger [87, 137]. Second, in support of K is the bulk Cu shear strength, i.e. true contact area were calculated with inaccurately assumed surface roughness parameters such that calculated true contact area under predicted the actual true contact area. In addition, there are also various shielding effect from mechanical testing [139].

In support to a larger value of K , the proportional factor was calculated from the slope between shear strength and calculated true contact area A_c obtained from either contact resistance method or resonance frequency method. This produces a value of $K \sim 5 \times 10^{11}$ MPa and $K \sim 9 \times 10^9$ MPa for contact resistance method and resonance frequency method, respectively as shown in Figure 2.11. These values

Figure 2.11: Fitting parameter to correlate shear test measurement to contact resistance and resonance frequency measurement. Constant K obtained from the slope measured shear strength from shear test with respect to estimated true contact area from (a) contact resistance or (b) resonance frequency measurement.

are much larger than typically accepted pure Cu shear strength (172 MPa - ASTM B370). To justify the large value of K from the first principle is beyond the current thesis scope, which led us to discuss from argument in support of K is the bulk Cu shear strength.

One of the supporting arguments of K is the bulk Cu shear strength is the presence of various shielding effects from mechanical testing, i.e. fracture mode, plastic energy dissipation, crack propagation path, geometry of test sample, etc. Measured adhesion strength Γ_i from mechanical characterization, shear test in this case, can be contributed from a number of different processes. Generally, each of these processes can be described as multiplication factor to the work of adhesion, and can be summarized as follows [139]:

$$\Gamma_i = (\xi + \chi + \zeta)\Gamma_o \quad (2.11)$$

where Γ_o is the energy required to separate the interface of interest or to rupture bonds at the interface, ξ is the irreversible contribution of surface creation having

an approximate value between 1 and 10 [140, 141], χ is a roughness-related shielding parameter that scales as the amplitude of the roughness squared and inversely as the wavelength of the roughness [140], and ζ is the plastic energy dissipation characteristic and scales with the square of the yield stress [142]. Electrical contact resistance characterization and resonance frequency method may exclude roughness-related shielding parameter χ and plastic energy dissipation ζ , hence predicting a lower bond strength.

Secondly, the surface parameters characterization by AFM was taken from $1\ \mu\text{m} \times 1\ \mu\text{m}$ spot on the sample, and it was assumed to be representative of the entire surface of the sample. In the current calculation, the curvature radius of all the asperities was assumed to be the same i.e. average radius from AFM scan. In reality, each asperity has a different surface curvature. The asperity tip's curvature radius can range from 10 nm to 100 nm [75]. The average radius of contacting asperities may be different from the average radius from all asperities. Thus, electrical properties from contact resistance measurement and resonance frequency were re-simulated.

Figure 2.12: Simulated effect of asperity tips curvature radius $\bar{R}$ to the estimation of true contact area, (a) from electrical contact resistance and (b) resonance frequency measurement.

Figure 2.12 shows the re-simulated estimation of true contact area from contact resistance and contact resonance frequency with varying average asperity curvature radius ($\bar{R}$). It shows that the true contact area increases with $\bar{R}$. However, there is only a marginal increase in the true contact area estimates with large values of $\bar{R}$.

Figure 2.13: Estimation of true contact area from contact resistance measurement using different value of asperity tip curvature radius. Changing the average asperity curvature radius to the extreme range only approaches shear test prediction by less than one order magnitude.

True contact area estimation from contact resistance measurements at different $\bar{R}$ has less than one order of variation, even for very large $\bar{R}$ as shown in Figure 2.13. This re-simulation suggests that K is being significantly larger than bulk Cu shear strength (172 MPa).

2.8 Summary

A new non-destructive characterization method based on measured resonance frequency has been proposed as an improvement to direct contact resistance measurement. The proposed bond interface characterization method utilizes both resistive and capacitive properties of metal contacts with external inductive component added to generate frequency resonance. The proposed method is able to isolate the bond interface from line resistance for characterization. Furthermore, its measurement range and sensitivity can be easily changed by adjusting the external inductive component. By using the resonance frequency method, only two probes are required instead of four as in contact resistance measurement.

Proof of concept experiments had been conducted, on a test structure that enables characterization of both electrical properties and mechanical properties of the bonded interface. Sample bond strength in theory can be related to measured reso-

nance frequency through estimation of true contact area and a proportional factor K . However to do this, a very large value of K was required. Pro and contra arguments regarding the results was briefly discussed, that first, K is indeed several orders higher than bulk Cu shear strength, and second, inaccuracy of surface roughness parameter used to estimate the true contact area. However, a marginal change in the true contact area when varying radius curvature of asperity tip, shows that a high value of K may be the reason. High value of K also qualitatively justified by the various shielding effect of shear testing. For practical applications K will be considered as fitting parameter.

Further discussion to the model of true contact area based on the surface morphology and bonding condition will be discussed in Chapter 3.

Chapter 3

Modeling of True Contact Area Formation in Thermocompression Bond Process

3.1 Overview

In this chapter, the formation of true contact area through thermocompression bonding is modeled and compared to the experimental results. The objective is to create a tool for predicting the bond integrity given the bonding parameters. A better bond integrity had been observed with application of higher load. Complete contact of the mating surface is prevented by the existence of surface irregularities as elaborated in Chapter 1. Thus, only a small fraction of the nominal area is in contact. Application of load helps to flatten any irregularities on the surface, therefore increasing the true contact area. True contact area is also the common factor relating mechanical and electrical properties of the bonded interface.

Bond integrity can also be improved by bonding at higher temperatures. Metals are softer at higher temperature, which reduces the force required to flatten any surface irregularities, thus improving the contact area. Hence, better bonding is achieved at higher bonding temperature. Bonding duration is another important factor that has not gained much attention as the effect was not significantly observed [70].

3.2 Modeling Approach

Early approach to contact of real surface was developed by Greenwood and Williamson (GW) [112]. The model specifically considers the random nature of surface asperity. The initial GW model considers the contact between a nominally flat but microscopically rough surface pressed on to a perfectly smooth surface. The rough surface is assumed to be covered with asperities that have random height, with each asperity having a curvature radius R and uniformly distributed asperities with known density η . The asperity heights are assumed to follow a Gaussian probability density function (PDF) $f(z)$ expressed as

$$f(z) = \frac{1}{\sigma(2\pi)^{1/2}} \exp\left(-\frac{z^2}{2\sigma^2}\right), \quad (3.1)$$

with σ is the PDF's standard deviation. This assumption can be readily adapted to the case of two rough surfaces, where the two rough surfaces can be described by an equivalent rough surface in contact with a smooth plane using the parameter of [143]

$$\sigma = \sqrt{\sigma_1^2 + \sigma_2^2}, \quad (3.2)$$

where σ_1 and σ_2 are the standard deviations of summit heights for the two contact surfaces.

When two large surfaces are pressed together, their mean planes become parallel. Thus, if a rough surface and a smooth surface are pressed against each other until the summit mean plane of the rough surface and the mean plane of the smooth surface are separated by a distance d , the probability that a randomly selected asperity will be in contact is

$$P(z > d) = \int_d^{\infty} f(z) dz. \quad (3.3)$$

Since the number of asperity per unit area is η , the average expected number of

contacts in any unit area N_t is

$$N_t = \eta A_n \int_d^\infty f(z) dz. \quad (3.4)$$

where A_n is the nominal contact area. Given that an asperity is in contact due to its height z exceeds d , the asperity must deform an amount of $w = z - d$. For a sphere of radius R that is elastically deforming by the amount w , Hertz's solution gives the contact area

$$A_{ci} = \pi a^2 = \pi R w = \pi R(z - d) \quad (3.5)$$

where A_{ci} is the contact area and a is the contact radius. By integrating the equation (3.5) and the probability density of the random variable over the space of possible values, the expected total true contact area can be expressed as

$$\begin{aligned} A_c &= A_{ci} N_t \\ &= \int_d^\infty \pi A_n \eta R(z - d) f(z) dz \end{aligned} \quad (3.6)$$

The corresponding asperity load is [114, 116]

$$L_{i-\text{elastic}} = \frac{4}{3} E' R^{1/2} w^{3/2} = \frac{4}{3} E' R^{1/2} (z - d)^{3/2} \quad (3.7)$$

where E' is the reduced Young's modulus and expressed as [114]

$$E' = \left(\frac{1 - \nu_1^2}{E_1} + \frac{1 - \nu_2^2}{E_2} \right) \quad (3.8)$$

where E_1 , E_2 , ν_1 , ν_2 are Young's modulus and Poisson's ration for the two bodies respectively. By the same argument as equation (3.6), the total load supported by

the asperity can be expressed as

$$\begin{aligned} L_{tot} &= L_i N_t \\ &= \eta A_n \int_d^\infty \frac{4}{3} E' R^{1/2} (z - d)^{3/2} f(z) dz. \end{aligned} \quad (3.9)$$

In plastically dominated asperity deformation, the total load supported by the asperities is also depends on the materials yield stress Y and the work hardening index x and the strain at the onset of yielding ε as shown in equation (1.16) [75, 107]. Leong *et al.* also argued based that on Chang *et al.* [123] volume conservation model, for plastically dominated asperity deformation the asperity's true contact area can be approximated as

$$A_i = \pi a^2 \approx 2\pi R w = 2\pi R (z - d). \quad (3.10)$$

Integrating equation (3.10) for the entire possible values, the true contact area in plastic dominated asperity deformation can be shown to be [107]

$$A_c = 2\eta A_n \pi R \int_d^\infty (z - d) f(z) dz. \quad (3.11)$$

Apart from elastic and plastic deformation, the aforementioned model considers only behavior at a single temperature. As has been known, material properties change with temperature. Furthermore, plastic deformation is a dynamic process that has time dependent behavior. Hence, from this point onward, a model that takes into account the effects of bonding time and temperature will be developed.

The dynamic nature of contact as a function of time is illustrated in Figure 3.1. Under a constant load, asperities that are in contact continuously deforming which can be expressed as decrease in d . From equation (3.4) the number of asperities in contact increases as d decreases, which has the consequence of increasing the true contact area as described in equation (3.11). Thus, d is now replaced by $d(t)$ to

Figure 3.1: *Summits that have height $z > d$ will deform by an amount of $w = z - d$. With the contribution of creep, over time, d will decrease as the asperities give way to plastic flow, resulting in more and more asperities making contacts, increasing the total true contact area.*

shows time dependent of mean plane distance and equation (3.11) modified into

$$A_c = 2\eta A_n \pi R \int_{d(t)}^{\infty} (z - d(t)) f(z) dz. \quad (3.12)$$

Figure 3.2: *The single asperity in contact is modeled as Kelvin-Voigt material that can be represented by pure viscous damper and purely elastic spring connected in parallel.*

The contacting asperity is now considered as having a linear viscoelastic behavior, where the asperity deformation function can be separated into both creep response and load. The single asperity in contact is modeled as Kelvin-Voigt material that can be represented by pure viscous *damper* and purely elastic *spring* connected in parallel as shown in Figure 3.2 [144]. Any deformation on the damper component is assumed to be irreversible.

Under normal loading, the total average stress on the contacting asperity will be the sum of each component expressed as

$$p_{\text{total}} = p_{\text{elastic}} + p_{\text{relax}}, \quad (3.13)$$

where p_{elastic} is equal to the elastic compressive stress. Here, p_{elastic} is simply taken as $L_{i-\text{elastic}}/A_i$, where $L_{i-\text{elastic}}$ and A_i have been defined in equations (3.7) and (3.10), respectively.

Stress relaxation p_{relax} can be expressed as

$$p_{\text{relax}} = - \int E \dot{\epsilon}(p, T) dt, \quad (3.14)$$

which describes the amount of stress that is relaxed by plastic deformation at the particular temperature. $\dot{\epsilon}(p, T)$ is the plastic strain rate of active deformation mechanism(s) and is both pressure and temperature dependent. $\dot{\epsilon}$ is given a negative value, as the deformation rate is decreasing over time. For simplicity, p_{elastic} and p_{relax} will only be written as p_e and p_r , respectively. Similarly L_e and L_r represents the elastic load and relaxation load component. Multiplying equation (3.13) by the asperity true contact area A_i we could obtain the load that being hold by single asperity to obtain

$$\begin{aligned} L_i &= L_e + L_r \\ &= \frac{4}{3} E' R^{1/2} w^{3/2} - A_i \int E \dot{\epsilon}(p, T) dt \\ &= \frac{4}{3} E' R^{1/2} w^{3/2} - 2\pi R w \int E \dot{\epsilon}(p, T) dt \\ &= \frac{4}{3} E' R^{1/2} (z - d(t))^{3/2} - 2\pi R (z - d(t)) \int E \dot{\epsilon}(p, T) dt, \end{aligned} \quad (3.15)$$

where A_i is obtained from equation (3.10) to take into account of volume conservation. Integrating equation (3.15) over the entire possible space value we have

$$L_{\text{tot}} = (4/3) A_n \eta E R^{1/2} \int_{d(t)}^{\infty} (z - d(t))^{3/2} f(z) dz - 2 A_n \eta E \int_{d(t)}^{\infty} \int_0^t \dot{\epsilon} \pi R (z - d(t)) f(z) dt dz, \quad (3.16)$$

where L_{tot} is typically held constant during thermocompression bonding process. Thermocompression process is typically done at a temperature range from 200°C

($\sim 0.3T_m$) to 400°C ($\sim 0.5T_m$). In that range, material deformation is dominated by power law creep [145]. Deformation that is governed by power-law creep can be described by a standard equation given as [145] :

$$\dot{\epsilon} = H_c \frac{D_{\text{eff}} \mu b}{kT} \left(\frac{\sigma}{\mu} \right)^n, \quad (3.17)$$

where H_c is the Dorn constant*, μ is the shear modulus, b is the Burgers vector, and n is the stress exponent and has a value between 3 and 10 [145]. The effective diffusivity, D_{eff} is given by [146]

$$D_{\text{eff}} = D_v \left[1 + a_c \rho \frac{D_c}{D_v} \right] = D_v \left[1 + \frac{10a_c}{b^2} \left(\frac{\sigma}{\mu} \right)^2 \frac{D_c}{D_v} \right], \quad (3.18)$$

where a_c is the dislocation core diameter, ρ is the dislocation density, and D_v and D_c are the lattice and dislocation core diffusivity, respectively. The Dorn constant H_c has been shown to be dependent on stress component. In face-centered cubic metals, the relationship between these qualities has been expressed in [147] by

$$\log_{10} H_c = 2.94 (n - 2.95). \quad (3.19)$$

Grain-boundary diffusion and power-law were considered by Keller *et al.* in [148] as the two possible relaxation mechanism. Gibbs [149] had describes grain-boundary diffusion in thin film:

$$\dot{\epsilon} = A_g \frac{\Omega \sigma}{kT d_g h^2} \delta D_g, \quad (3.20)$$

where A_g is a constant, Ω is the atomic volume, k is the Boltzmann's constant, d_g is the grain size, h is the film thickness, δ is the grain boundary width, and D_g is the grain-boundary diffusivity, and is given as

$$D_g = D_{\text{og}} \exp \left(\frac{-Q_g}{kT} \right), \quad (3.21)$$

* Dorn constant is typically represented as A_c , however in this case H is used to avoid confusion with the true contact area

Table 3.1: *List of physical constants for creep dominated asperity deformation.*

Symbol	Magnitude	Reference
E	128 GPa	
ν	0.34	
A_g	12	[148]
Ω	$1.18 \times 10^{-29} \text{ m}^3$	[145]
δD_{0g}	$5 \times 10^{-15} \text{ m}^3/\text{s}$	[145]
Q_g	104 kJ/mol	[145]
H_c	7.4×10^5	[145]
μ	$4.21 \times 10^4 \text{ MPa}$	[145]
b	$2.56 \times 10^{-10} \text{ m}$	[145]
n	4.8	[145]
$a_c D_{0c}$	$1 \times 10^{-24} \text{ m}^4/\text{s}$	[145]
Q_c	117 kJ/mol	[145]
D_{0v}	$2 \times 10^{-5} \text{ m}^2/\text{s}$	[145]
Q_v	119 kJ/mol	[145]

where D_{0g} is a constant, and Q_g is the activation energy for grain-boundary diffusion.

3.3 Simulation

The two stress relaxation mechanisms are considered and simulated based on equation (3.16). Table 3.1 lists all the constants that are used in the calculation while, details of the algorithm, numerical approximation and coding are available on the Appendix A.1.

Figure 3.3(a) shows the simulation results based on grain boundary diffusion dominated creep stress relaxation. The simulation was conducted by assuming a CMP finish Cu surface which has a surface roughness parameter $\sigma = 3 \text{ nm}$, an average curvature radius asperity $\bar{R} = 50 \text{ nm}$ and an asperity density $\eta = 10^{14} \text{ m}^{-2}$ [75] and average grain size $d_{gb} = 400 \text{ nm}$. The simulation results show that the true contact area has a very strong and unrealistic time dependence. A perfect bond interface (i.e. 100 % true contact area) can be achieved at very short bonding duration. At bonding temperature of 400°C and 200°C , complete bonding can be achieved in $33.9 \mu\text{s}$ and 0.06 respectively, even at a relatively low bonding pressure of 100 kPa . These results does not correlate well with the real case bonding. In general,

Figure 3.3: Simulation results of creep mechanism to true contact area evolution, (a) grain boundary diffusion creep dominated deformation, and (b) power law creep dominated deformation. Power law creep mechanism shows a better agreement with the experiments by Nichting [150].

a temperature above 300°C for 30 min bonding duration is necessary to achieve a reliable bonding quality [73]. These results also do not correlate well with experiment results from [150]. It is clear from this simulation that thermocompression bonding is not governed by grain boundary dominated diffusion creep. One particular reason could be that grain boundary is not the preferred diffusion path in Cu film [151, 152].

Figure 3.3(b) shows the simulation results based on power law creep dominated deformation. The simulation results show a slower evolution of true contact area. A very fast growth happens at the beginning of the bonding and becomes saturated as the bonding duration increases. No significant improvement in the bond integrity with the increase in the bonding duration at low bonding temperature (below 300°C) is observed. On the other hand, simulation at higher bonding temperature (above 300°C), shows that the true contact area growth saturates at a much later time as compared to bonding at low bonding temperature (below 300°C). This implies that bond integrity will benefit from longer bonding duration if the bonding temperature is high enough. Conversely, there may not be much benefit of long bonding duration if the bonding temperature is low.

The simulation results are also consistent with the experimental results shown by Leong *et al.* [75]. Leong observed that at least 3.18×10^{-2} % true contact area is required to obtain 100 % dicing yield. His observation was based on bonding of CMP

finished, 200 mm diameter blanket Cu wafers, 8 kN bonding load (254.8 kPa) for 30 mins (1800 s) at 300°C. Even though the simulations were only conducted up to 1000 s bonding time, rough extrapolation of the simulation results easily suggest that the predicted true contact area is close to $3.18 \times 10^{-2} \%$ for the simulation at 300°C and above. Based on Leong's criteria, it can also be argued that a bonding pressure of 100 kPa and a bonding temperature of 250°C or lower will result in less than 100% dicing yield. Economically, higher yield is always desired. With the current model, the bonding condition required to achieve the maximum bonding yield can be estimated. Hence, economic loss from low bonding yield can be avoided.

Figure 3.4: *Cu bond toughness from pull test method, extracted from experimental result by Nichting in [150].*

The simulation results were also compared against experiment data by Nichting [150] as shown in Figure 3.4. To simplify the comparison, it is assumed that experimentally measurable mechanical strength of the bonded chip can be related to the calculated true contact area by a single constant.

Nichting results also show that the bond integrity improved fast at the early stage of bonding duration. Bond integrity also observed to be less improved with longer bonding duration particularly at low bonding temperature. Overall, simulation when supported by experiment in [150] strongly suggest that the Cu-Cu

Figure 3.5: Measured bond strength from Nichting [150] plotted versus the calculate true contact area, K is the slope of the best-fit line.

thermocompression process is governed by power law creep deformation.

The simulation results predict the true contact area, that can be related to the bond integrity by a single proportional factor K [87] given as

$$F = K \times A_c \quad (3.22)$$

where A_c is the calculated true contact area from equations (3.16) and (3.11) and F is the predicted shear force in shear testing. The true contact area were calculated based on Nichting [150] samples' surface condition and bonding conditions. They are, $40\mu\text{inch}$ - rms ($1.016\mu\text{m}$ - rms), bonding load of 68.9 MPa with bonding temperature and duration range from 200°C - 350°C and 600 sec - 4800 sec, respectively. Other parameters required by the model such as average radius curvature $\bar{R}$, asperity density η and asperity height distributions $f(z)$ (in term of standard deviation σ) were interpolated from Leong's [75]. The proportional factor K is obtained by re-plotting all the experimental data from Nichting *et al.* as a function of the calculated true contact area as shown in Figure 3.5. K then is the slope of the best fit line

between measured bond strength and calculated true contact area. K was found to be 606.7 ± 35.8 MPa, which is relatively close to the shear strength (172 MPa). The current model to experimental fitting had assumed that the proportional factor K is the same between shear test and pull test from Nichting *et al.* [150], which may not be correct. To determine the K , experiments were conducted and explained in the following section.

3.4 Experiments

To verify the model, shear strength of thermocompression bonded Cu samples at different bonding conditions was collected. Two different sizes of ($5 \times 5 \text{ mm}^2$ and $2.5 \times 2.5 \text{ mm}^2$) Si chips with Cu film were bonded face to face with the bigger chip on the bottom facing up. Three pairs of chips were bonded at each bonding cycle at varying conditions. Bonded chips were then subjected to shear testing to measure the bond toughness. The details of sample preparation and bonding process are as follows.

3.4.1 Cu Film Depositions

For the blanket Cu wafers, the first step was to deposit a layer of 200 nm-thick SiO_2 using plasma enhanced chemical vapor deposition (PECVD) at 300°C . This was followed by depositing the Ta barrier (250 Å) and Cu seed layer (150 nm) using physical vapor deposition (PVD) process. Immediately after the PVD process, a Cu layer of 1 μm -thick was grown using electrochemical plating (ECP) process and was annealed in N_2 ambient at 200°C for 30 minutes. Cu chemical mechanical polishing (CMP) was subsequently performed to reduce the Cu thickness to about 400 nm. After the CMP process, the Cu films were typically very smooth with a root-mean-square (rms) roughness of about 0.6 nm, as measured by AFM. After the CMP process, the Cu wafers were diced into sizes of $5 \times 5 \text{ mm}^2$ and $2.5 \times 2.5 \text{ mm}^2$ to perform bonding. Summary of the process flow is given in Figure 3.6.

Figure 3.6: *Cu blanket wafer fabrication process flow*

3.4.2 Pre-bonding Cleaning

Since Cu forms an oxide film under ambient condition [126], removal of the surface oxide prior to bonding is important. Glacial acetic clean was used as a pre-bond cleaning step. Acetic acid was demonstrated to be effective in removing copper oxide and reducing the reoxidation rate of Cu [153]. Both chip went through the same cleaning, that is dipped in the acid for 10 minutes to remove the surface oxide and subsequently blown dry with N₂ air gun. It was observed that oxidation of Cu was reduced when the surfaces were blown-dried instead of rinsing with water, as the latter provides (OH)[−] ions which aid in the oxidation of Cu. Nonetheless, the wafers were exposed to the surrounding ambient for a brief period of time after cleaning and before loading into the bonding chamber. Hence, unless the wafers could be cleaned and bonded without breaking vacuum, Cu reoxidation could not be totally eliminated.

3.4.3 Surface Characterization

Prior to the bonding, the surface roughness of the diced chips was characterized by AFM. AFM surface profile measurements were taken on the pre-bond Cu surfaces with a scan size of 1 x 1 μm^2 . The sampling interval is approximately 4 nm in both the orthogonally defined x and y directions. Such small scan sizes should provide sufficiently high resolutions to reflect the actual surface profiles and obtain maximum accuracy of the surface roughness parameters. Up to six AFM scans per sample were

Figure 3.7: *Typical surface topography after die saw process.*

taken to ensure that these small-area characterizations would be representative of the entire surface.

Scanned data from the AFM measurements were extracted and analyzed using a MATLABTM algorithm developed by Leong *et al.* in [75]. The algorithm generates 3D topographical representations of the surface in the form of a set of points, each of which is defined in a Cartesian coordinate system by the three ordinates x , y and z as shown in Figure 3.7. With the extracted scan data, surface roughness parameters R , σ_s and η can then be estimated and analyzed.

3.4.4 Bonding Process

The samples were bonded face to face with the bigger chip on the bottom facing up. Three pairs of chips were bonded at each bonding cycle. The three pairs were positioned in such a way that allowed the load to be distributed evenly as shown in Figure 3.8(a). That is, the samples were radially distributed with 120° separation to its the nearest neighbors. A customized fixture was fabricated to allow easy placement of the bonding pairs as shown in Figure 3.8(b). The fabricated bonder is equipped with metal alignment plate for more precise placement of the top chip.

Figure 3.8: *Oven bonding set up. (a) Bonding fixture with metal aligner for bottom chip placed inside the fixture's groove, (b) bonder placed inside the oven chamber.*

Figure 3.9: *Oven's temperature and load profile during bonding.*

The oven's chamber was pumped down to approximately 10^{-2} Torr prior to having the temperature applied. The temperature and load profiles are shown in Figure 3.9. The total loads used for the three samples were 400 g (209.1 kPa/sample), 1200 g (627.3 kPa/sample) and 2400 g (1254.4 kPa/sample) for different duration (70 minutes, 240 minutes and 700 minutes), and with a temperature range of 200°C – 400°C .

3.4.5 Testing Procedure For Die Shear Test

To characterize the bond quality, chip shear testing was carried using DAGE 4000 Multi-purpose Bondtester. The bonded samples were put on the stage, in such a way that the bottom chip was being held by a metal stopper, while the top chip was being pushed parallel to the sample surface. The blade travelled with a constant

velocity of 50 $\mu\text{m/s}$ until fracture was detected, i.e. a sudden drop in applied force. The maximum force required before fracture was recorded. To avoid friction between the shearing blade and the bottom chip, the tip of the blade was placed at 5 μm above the bottom chip's surface.

3.5 Results and Discussion

Figure 3.10: Experiment results on chip to chip bonding superimposed with model predictions. The experimental data is represented by solid square, with the error bar represents the standard deviation. The solid lines represent model predictions with stress exponential factor of $n=4.8$ [148] and fitted with a proportional factor of 172 MPa

Figure 3.10 shows the experimental results on chip to chip bonding, superimposed with model prediction. The experimental data mean are represent by solid square, with the error bar represents the standard deviation. Simulation results fitted into the experimental results using a proportional constant of 172 MPa (ASTM B370-09), are represented by the solid lines. The value is the bulk Cu shear strength.

At 70 mins - bonding time (Figure 3.10 a-c), the model predictions are close to the mean value of the measured shear strength for the entire bonding pressure range.

At medium (240 mins) bonding duration (Figure 3.10 d-f), the model predictions are close to the experimental results up to 300°C. At higher temperature, the model starts to deviate and generally under predicts the bonding strength. Furthermore, scattered measurement results obscure any transition point. For longer bonding duration of 700 mins, at lower bonding load, a good correlation between the model and measured values is observed up to 300°C (Figure 3.10 g-h). However, for a high bonding load and long bonding duration (Figure 3.10 i), the model completely under predicts the bond strength.

There are a few possibilities of discrepancy between the model prediction and the experiments results especially at high pressure with long bonding duration, i.e. varying stress exponential factor n , unsuitable K value, and presence of oxide at bonding interface. The oxide argument was ruled out as the presence of oxide on the interface is generally regarded to be detrimental to the bond quality, which the model should over-predicted the bond strength [126].

Figure 3.11: Simulation results with different values of n at high bonding load and longer bonding duration, $n = 9$ is observed to fit best at high bonding stress and longer bonding time.

On the other hand, it has been known that the stress exponential factor in equation (3.17) can vary from $n = 3$ to $n = 10$ at a temperature range from $0.3T_m$ to $0.5T_m$ and at higher applied stress [145]. The simulation was thus further optimized

to consider different values of n . Figure 3.11 shows the model prediction at high bonding load and long bonding duration at varying stress exponent n .

It is observed that at longer bonding time and larger force, $n = 10$ gives better prediction up to 300°C, where beyond that the model becomes unrealistic. Stress exponential factor $n = 9$ is considered to fit the experimental results best, even though it still under-predicts. Changes in the stress exponential factor could be attributed to the shift in the deformation mechanism. Under the same power law regime, dislocation could gain an extra degree of freedom, such as a combination of dislocation climb and dislocation glides [145]. Thus, different n value at different stress levels are possible.

Even though higher n gives a better trend, the absolute values of the model prediction are still lower than the experimental results. The constant K can be empirically determined by fitting model predictions to the experimental values. Fitting was done using the closest n value for each set of experiment. It is found that K values have a range between 42 MPa to 3000 MPa as shown in Figure 3.12. K is observed to be higher at higher bonding pressure. K ranges from 47 MPa to 200 MPa at 209.1 kPa bonding load, from 240 MPa to 320 MPa at 627.2 kPa bonding load and from 1000 MPa to 3000 MPa at bonding load 1254.4 kPa. Relatively close K values within the same bonding load suggest K is a function of bonding pressure.

Wenning and Müser [154] had suggested that $K^\dagger$ is not constant, but varies with pressure. On the other hand, Mo *et al.* [137] argued that an asperity contact A_c consists of yet smaller contacts (A_{real}) which have smaller length scale than the asperity length scale. At high contact force, A_{real} could approach A_c , and that the relationship between asperity contact and shear force is linear, i.e. K is constant. At this moment, there is no way to verify A_{real} and determine the pressure dependence of K . Dependence of K to the bonding pressure is interesting as it may hide a more complex relationship between true contact area and bond shear strength. K could be an interesting topic for further experiments, especially

[†] Wenning and Müser [154] use the term τ for K

Bonding Pressure

Figure 3.12: Empirical determination of K by fitting the measured shear strengths to the calculated true contact area from the model. K is found to be in the range of 42 MPa to 3000 MPa as bonding load increases. (a) At 209.1 kPa bonding load K range from 47 to 200 MPa, (b) at 627.2 kPa bonding load, K ranges from 240 to 320 MPa and (c) at 1254.4 kPa bonding load, K ranges from 1000 to 3000 MPa.

in direct measurement of the true contact area that couple with mechanical and electrical characterizations. However the direct measurement of small value of A_c may require much more sensitive instrumentation and elaborate experiment set up which need to be addressed in future research.

It had also been reported through finite element simulations that there is stress non uniformity on shear test sample, where the edges are shown to experience higher strain than the center of the sample [155]. This stress localization had been reported to depend greatly on the sample geometry, and test condition [155–157]. Currently, it is unclear how significant this factor to the relations between shear load, true contact area, and finally K . Further work is needed to assess the severity of stress localization factor in the future.

Even though the current model only assumes that the true contact area can be

Figure 3.13: Experiment result of four point bending test superimposed with model prediction. Model prediction related to experimental result by the an optimized (least-square) proportional constant $K_{FPB}=1.62 \text{ J/m}^2$, represented by solid line.

related to the mechanical bond strength, similar behavior have also been observed for the case of bond strength characterization by four point bend test. Details of the experiments and analysis are included in the Appendix B.

Direct correlation of four point bend test results to the true contact area is illustrated in Figure 3.13. The measurement results are superimposed with model prediction using proportional constant $K_{FPB} = 1.62 \times 10^4 \text{ J/m}^2$ [‡]. Unlike the results from die shear test, the proportional constant has no obvious physical meaning.

Nevertheless, the current model and experiments on the true contact area formation given the bonding condition, i.e. surface roughness, bonding load, bonding temperature and bonding duration, can provide a practical guidance in bonding process. Alternatively, the model can be seen as an advancement from the previous model by Leong [75], as the current model includes bonding temperature and bonding time as components for prediction, which were not considered in the previous model.

[‡] Subscript FPB is use to indicated that the constant K is for four point bending test

3.6 Bonding Maps

From the point of view of manufacturing, wafer bonding should be performed at a temperature that is reasonably low within a duration as short as possible. One hour bond duration with bond pressure ranging between 200 kPa and 10 MPa [72], at temperature between 200°C and 400°C, is considered to be a reasonable bonding condition.

Figure 3.14: Effects of surface roughness and applied load on the normalized values of true contact to wafer area, for bonding a 200 mm - diameter Si wafers deposited with blanket of 400 nm - thick Cu film at 300°C, extracted from [107].

Leong *et al.* [107] has shown a correlation between the theoretical true contact area and dicing yield of wafers that bonded at 300°C as shown in Figure 3.14. An approximate true contact area of $1 \times 10^{-5} \text{ m}^2$ or above is required for 100% dicing yield for bonding a 8" - diameter Si wafers deposited with blanket of 400 nm - thick Cu film. Meanwhile, $3 \times 10^{-6} \text{ m}^2$ is the threshold for zero dicing yield. Normalized with respect to the wafer area, the boundary condition for 100 % dicing yield and zero threshold dicing yield will be 3.18×10^{-4} and 9.55×10^{-5} , respectively. The normalization was based on the assumption that the bonding is uniform across to the bonding surfaces, which can be considered reasonable for blanket wafers. Leong's also suggest that the results can be generalized for bonding of either 6" or 12" as long as the bond pressure is kept constant.

Thus based on the same criteria, a bonding map that takes into consideration

Figure 3.15: True contact area bonding map of one hour bonding duration for different surface roughness. (a) Linear scale, (b) log scale

of the bond temperature can be constructed. Figure 3.15 shows a bonding map 3.18×10^{-4} and 9.55×10^{-5} fraction of true contact area as a function of bond pressure and temperature for various surface roughness. From the maps, one can estimate a 100% dicing yield will be achieved if the bonding condition falls above the 3.18×10^{-4} curve (100% yield threshold). On the other hand, wafers dicing will have zero yield if the bonding condition falls below 9.55×10^{-5} curve (zero yield threshold).

A bonding condition that falls above the 1% of fraction of true contact area represents a void free interface that can be achieved with post bonding thermal annealing. The source of this criteria will be discussed in Chapter 4. The map assumes a reasonable one hour of bonding duration [68] at bonding pressure ranging from 10 kPa to 10 MPa, a bonding temperature ranging from 200 $^{\circ}\text{C}$ to 400 $^{\circ}\text{C}$, and surface roughness ranging from 1 nm to 5 nm-rms, which is currently achievable by industry standards. The low bonding pressure such as 10 kPa is useful for integration involving low-k materials, which has been known to be mechanically weak [158, 159].

Overall, the maps show little variations with respect varying surface roughness from 1 to 5 nm-rms. The small variation is good for manufacturing as surface roughness is relatively more difficult to control in comparison to other bonding condition. Low variations also give larger tolerance in processing conditions. Furthermore, surface roughness of 1 to 5 nm-rms is easily produce-able in the modern CMP process. Variations in true contact area due to the varying surface roughness is getting lesser as the bond pressure increases. This results implies that the effect of surface roughness to the true contact area can be virtually eliminated with high bonding pressure.

The usage of high bond pressure also enables the bonding process to be done at lower temperature. For example, bonding temperature of 350°C is required to achieve 1% true contact at 2 MPa bond pressure, the same true contact area can be achieved at 200°C with 10 MPa bond pressure. While this result seems to be promising, we are limited by the bonder capability. The current EVG 520 bonder has the capability to supply 10 kN bonding force for 8" wafer size, that is equivalent to 318 kPa bond pressure. Newer system, such as EVG 560 or Suss CB200M could supply up to 60 kN and 90 kN bonding force, respectively, which is equivalent to 1.908 MPa and 2.862 MPa for the EVG 560 and Suss CB200M for 8" wafer, respectively. This capability is far below the required 10 MPa bond pressure. On the other hand, EVG 520 bonder loading capability is sufficient to achieve 100% dicing yield based on Leong's criteria. In terms of manufacturing process, if the wafers are able to withstand the dicing process, it may be able to withstand other post-bond processing too, such as backside wafer thinning.

While the criteria of 100% dicing yield is good enough mechanically, it may not be good enough electrically. 100% dicing yield does not guarantee that the interface is void free. Imperfection in the interface could create contact resistance and contact capacitance that may impact the signal propagation and bonding reliability. Thus, in some cases high bond pressure may still be required. Higher bond pressure with the same machine (EVG 520 bonder) can be achieved by bonding smaller wafers

i.e. 4" or 6", or reducing the Cu nominal area on the wafers, i.e. bonding patterned wafers. However, patterned wafers could suffer from factors such as Cu dishing in the CMP process [107], which may adversely effect the bond integrity, and had not been considered in the construction of the bonding maps.

On the other hand, the maps are still useful for patterned wafers (even with dishing) when use in combination with the non-destructive characterization method as discussed in Chapter 2. The non-destructive method allows for individual identification of weak chip, which is also very useful when the bonding is not uniform across the wafer. By measuring (indirectly) the true contact area, we could determine if the bonded chip will survive the subsequent processes. If the bonding is not strong enough, an appropriate mitigation action can be taken prior to next processing, thus reducing the possibility of chip loss in the subsequent process. One of those action could be in terms of post-bonding bond interface enhancement. The possible post-bonding bond strength enhancement is discussed in detail in Chapter 4.

Electrical properties of the interface also can be used to indicate the mechanical properties of the bond interface as had been discussed in Chapter 2. A theoretical estimate of the contact resistance can be calculated using equation (2.1). Figure 3.16 shows the electrical map of bonded Cu film. The map assumes 1 hour bonding duration at bonding load ranging from 1 kPa to 1 MPa, bonding temperature ranging from 200°C to 400°C, and surface roughness ranging from 1 nm to 5 nm-rms.

The map shows multiple curves in which the specific contact resistance (contact resistance $R_c \times A_n$) will be higher for bonding condition that falls below or on the left of particular line, and lower if falls on the right of the curve. For example, if we take the first curve from the left on Figure 3.16(a), any bonding condition (pair of bonding temperature and pressure) that falls on the line will have a specific contact resistance of $1 \times 10^{-7} \Omega\text{cm}^2$. Meanwhile the specific contact resistance will be higher than $1 \times 10^{-7} \Omega\text{cm}^2$ if the bonding condition falls on the left side of the curve, and lower if the bonding condition falls on the right of the curve. Thus based on the bonding condition, the resulting specific contact resistance can be predicted.

Figure 3.16: *Electrical contact resistance map of bonded Cu film. (a) range from 1 - 10 kPa, (b) 100 kPa - 1 MPa.*

The ability to know the contact resistance based on the bonding condition is important as it enables one to determine whether the device, interconnection or even the system performance target can be met even during the designing stage. For instance, will the contact resistance be small enough such that it will not effect the transmitted signal or will the resistance of the bonded interface consumed too much power or even will there be reliability issues with such contact resistance value.

On the other hand, circuit designers could also utilize the resistive and capacitive effect of the interface as the impedance matching of the active device by choosing the appropriate process condition. For this purpose, the bonding condition is determined from the desired contact resistance. High temperature bonding allows for lower bonding pressure, while lower temperature can be used at higher bonding pressure. High temperature bonding in some case is undesirable, as the process may degrade the active device performance, particularly on devices that use heavily doped junctions. On the other hand, high bonding pressure may not be suitable

for chip that are mechanically weak, such as having low-k materials as inter-metal dielectrics. The maps can be utilized to achieve a compromise between stages of integration i.e. the map allows for more than one combination of bonding condition to achieve the same contact resistance.

3.7 Summary

A model to provide a quantitative estimate of the true contact area achieved in thermocompression bonding was developed. The model predict the bond quality as a function of surface topographic characteristics and bonding condition which includes applied load, temperature, and time. Creep dominated material deformation on the multi-asperities type of contact was utilized to capture the time dependent of the bonding process. Both grain boundary creep and power law creep was considered and simulated. The model that utilizes power law creep dominated deformation was observed to predicts a more realistic results. The model simulation shows a good fit with experimental results on chip to chip bonding.

A proportional constant K that had been introduced in the previous chapter was investigated further in this chapter to correlate the model prediction and experimental result. So far, K has been determined empirically based on least square method and an interesting properties of has been observed i.e. K dependence on the bonding pressure.

Overall, the model has shown to be a sufficient prediction tool for practical application, i.e. short bonding time and low bonding pressure. A true contact area and electrical bonding map have been constructed. The maps allow for the fast estimate of the bonding qualities as well estimations of contact resistance of the bonding interface for a given bonding condition, i.e. surface roughness and applied load, bonding temperature. Conversely, the maps allow the determination of the bonding condition required to achieve a specified contact resistance.

Chapter 4

Modeling of Thermocompression Bonding Improvement Through Thermal Annealing and Direct Current Stressing

4.1 Overview

The high cost of ownership of wafer bonder, means that only few wafers can be bonded at any given time. From the point of view of manufacturing, wafer bonding should be performed at a temperature that is reasonably low within a duration as short as possible. It has been shown that the Cu-Cu bond quality can be enhanced with an anneal step after the application of the load [76]. It has been reported that a longer anneal duration is necessary to achieve a strong bonding [74].

It has also been observed by Chen [109] as well as Leong [75] that contact resistance of bonded Cu interface can decrease under current stressing. As a lower contact resistance implies a better true contact area as shown in Chapter 2, a reduction in contact resistance during current stressing could provide another method for post-bonding bond integrity enhancement.

In this chapter, both bond strength enhancement through annealing and current stressing phenomena will be modeled. To model the phenomena, a concept of contact

growth from the sintering process is applied. The true contact area is assumed to grow during the annealing process due to Cu surface diffusion. Later in the chapter, electron wind force is considered as the driving force for surface diffusion.

4.2 Derivation of True Contact Area Growth During Thermal Annealing

Thermal annealing of Cu bonded wafers is normally done as an isothermal process without application of load. Thus, any increase in the true contact area will be contributed by non-creep driven process. In this case, surface diffusion is considered as the main true contact area growth mechanism. Microstructurally, a contacting asperity when heated or annealed can be approached as a circular body with summit radius curvature of R , contact radius of a and neck radius of u , that is undergo sintering process. The contact area of the asperity could grow by diffusion of atoms from the body to the neck region of the asperity as illustrated in Figure 4.1. Surface diffusion along the contacting asperity surface is assumed to be driven by difference in the local surface chemical potential, generated by a difference in surface curvature of the body and the contacting neck.

Figure 4.1: Cross section schematic of a contacting asperity, with asperity tip's curvature with radius R , asperity contact radius a and the neck curvature with radius u .

Mullins [160] has derived the equation describing the surface flux J_s of atoms along an arbitrary surface

$$J_s = -\frac{D_s \gamma \Omega \nu}{kT} \nabla_s \kappa, \quad (4.1)$$

where D_s is the surface self-diffusion coefficient (assumed isotropic), γ is the surface tension (assumed isotropic), Ω is the atomic volume, ν is the number of diffusing atoms per unit surface area (here $\nu \equiv \Omega^{-\frac{2}{3}}$), k is the Boltzmann's constant, T is the temperature, $\nabla_s \kappa$ is the surface curvature gradient and κ is the surface curvature. Equation (4.1) is valid for all geometries. To apply equation (4.1) to the asperity contact system, a small finitesimal element of the neck's region is considered. The element is assumed to have a radial symmetry with respect to the center of asperity z - axis as illustrated in Figure 4.2.

Figure 4.2: *Magnified view of asperity neck elements*

Flux convergence on this element will drive the outward movement of the surface. We consider flux J_1 , crossing the edge δl_1 at radial distance r_1 and flux J_2 crossing the edge δl_2 at radial distance r_2 . Thus, by conservation of volumes it can be expressed as [161]

$$(J_1 \delta l_1 - J_2 \delta l_2) \delta t \cdot \Omega = \delta s \delta n \delta l, \quad (4.2)$$

where δl is the average chord length of the element, δn is the outward normal distance traveled by the element during the time increment δt , and δs is the incremental arc length measured along a section through the axis of revolution. Since both δl_1 and

δl_2 subtend the same angle, we can rewrite equation (4.2) as

$$(J_1 r_1 - J_2 r_2) \delta \phi \Omega \delta t = \delta s \delta n \delta l$$

or

$$-\delta(J_s r) \delta \phi \Omega \delta t = \delta s \delta n \delta l.$$

Utilizing the relations of

$$\delta \phi = \delta l_1 / r_1 = \delta l_2 / r_2 = \delta l / \bar{r}$$

we obtain

$$\frac{\delta n}{\delta t} = -\frac{\Omega}{\bar{r}} \frac{\delta(J_s r)}{\delta s} \quad (4.3)$$

Substituting equation (4.1) into (4.3), and defining infinitesimal changes we have that*

$$\frac{\partial n}{\partial t} = \frac{B}{r} \frac{\partial}{\partial s} \left(r \frac{\partial \kappa}{\partial s} \right) \quad (4.4)$$

where $B = D_s \gamma \Omega^2 \nu / kT$. Noting that κ is only dependent on s , and δn is having the same direction as the infinitesimal changes in r direction, we have that

$$\frac{\partial n}{\partial t} = \frac{\partial r}{\partial t} = B \frac{\partial^2 \kappa}{\partial s^2} \quad (4.5)$$

Nichols and Mullins has shown that the first and second derivative of κ can be approximated by a division of κ by local radius of curvature [161], in this case the radius curvature of the neck. Thus

$$\frac{\partial \kappa}{\partial s} \simeq \frac{\kappa}{u} \quad (4.6)$$

where u is the radius curvature of the neck. Similarly for the second derivative can

* here, $\delta(J_s r) = r \delta J_s + J_s \delta r$, since $\delta r \rightarrow 0$, the second term becomes zero. Thus, $\delta(J_s r) = r \delta J_s$

be obtained by dividing equation (4.6) by u [161], thus

$$\frac{\partial^2 \kappa}{\partial s} = \frac{\kappa}{u^2} \quad (4.7)$$

Due to the radial symmetry of the surface neck element about z -axis, the neck surface can be simplified into two dimensional problem. Assuming that the surface element can be satisfied by function $r = f(z)$ and assuming the incremental arch length $\delta s \approx \delta z$, surface curvature of the neck can be represented as [162]

$$\kappa = \frac{r''}{(1 - r'^2)^{3/2}}, \quad (4.8)$$

where $r' = dr/dz$ and $r'' = d^2r/dz^2$. Assuming that the first derivation is much smaller than unity, equation (4.8) can be simplified into

$$\kappa \approx \frac{d^2r}{dz^2}. \quad (4.9)$$

For simplicity here we will assumed that the neck curvature is close to element of sphere with radius curvature of u , thus

$$\kappa \approx \frac{1}{u}. \quad (4.10)$$

Substituting equation (4.10) into equation (4.7) and using it for equation (4.5), we have that

$$\frac{\partial r}{\partial t} = B \frac{1}{u^3}. \quad (4.11)$$

Setting $\partial r/\partial t$ as the changes in the contact radius over time da/dt we have that

$$\frac{da}{dt} = \frac{B}{u^3} \quad (4.12)$$

Kuczynski *et al.* [163] had shown geometrically that the neck radius u for a sphere that is in contact into a plane is given by [161]

$$u = \frac{a^2}{4R}, \quad (4.13)$$

where R is the asperity tip curvature radius. Substituting equation (4.13) into equation (4.12), we have

$$\frac{da}{dt} = \frac{64R^3B}{a^6}. \quad (4.14)$$

Re-arranging the common factor and integrating

$$\begin{aligned} \int a^6 da &= \int 64R^3B dt \\ \frac{1}{7}a^7 &= 64R^3Bt + C, \end{aligned} \quad (4.15)$$

where C is the integration constant. Setting the initial boundary condition of $a(t = 0) = \sqrt{2wR}$, where $w = (z - d)$ is the instantaneous asperity deformation during initial thermocompression bonding [107], thus we have,

$$a^7 = 448BR^3t + (2(z - d)R)^{7/2}. \quad (4.16)$$

The true contact area of a nominal flat surface has been given by [107]

$$A_c = \eta\pi A_n \int_d^\infty a(z, d, R)^2 f(z) dz, \quad (4.17)$$

where d is the mean plane distance of the two contacting surface, and $f(z)$ is the asperity height distribution function. Substituting equation (4.16) for a into (4.17), we have

$$A_c = \eta\pi A_n R \int_d^\infty \left(448 \frac{Bt}{\sqrt{R}} + [2(z - d)]^{7/2} \right)^{2/7} f(z) dz, \quad (4.18)$$

where $B = D_s \gamma \Omega^2 \nu / kT$. Equation (4.18) basically gives the true contact area evolution during thermal annealing. A quick glance, there is positive growth of true

contact area during thermal annealing, which is expected as the bond enhancement process. The next section, we will simulate the true contact growth during annealing process.

4.3 Simulation on True Contact Area Growth by Surface Diffusion

A simulation on the true contact area growth due to surface diffusion was carried out by assuming a surface roughness of 2 nm-rms with $\eta = 10^{14} \text{ m}^{-2}$, $\sigma_s = 2 \text{ nm}$ and $R = 50 \text{ nm}$, obtained from Leong *et al.* [75]. The d values were predetermined to exclude the complexity of the thermocompression bonding condition. Generally, smaller d corresponds to a combination of larger force, longer bonding duration, or higher bonding temperature during thermocompression bonding. As the model simulates the true contact growth during annealing process after thermocompression bonding, there is no applied force. With no applied force, d can be assumed to be constant, and simulation can be done with only equation (4.18). All the diffusion data used in the simulations were extracted from [128, 145] and summarized in Table 4.1. Source codes (MATLAB/OCTAVE) uses in this simulation are included in Appendix A.2.

Table 4.1: List of physical constants for surface diffusion contribution to the true contact area evolution, as extracted from [128, 145]

Parameter	Symbol	Units	Value for copper
Atomic volume	Ω	nm^3	1.18×10^{-2}
Density	ρ	kg m^{-2}	8.96×10^3
Surface energy	γ	J m^{-2}	1.75
<i>Diffusion</i>			
Surface pre-exponential	D_{os}	$\text{m}^2 \text{s}^{-1}$	7×10^{-6}
Surface activation energy	Q_s	kJ mol^{-1}	79.1
Number of diffusing atom per unit area	$\nu = \Omega^{-\frac{2}{3}} [161]$	nm^{-2}	$(1.18 \times 10^{-2})^{-\frac{2}{3}}$

Figure 4.3 shows the simulation results of Cu surface diffusion contribution to the growth of true contact area. It can be observed that its contribution to the true contact area depends greatly on the initial true true contact area, i.e. before

Figure 4.3: Simulation on the evolution interface true contact area from the contribution of Cu surface diffusion. (a) low initial true contact area ($\sim 4.3 \times 10^{-4}$ %), (b) medium initial true contact area ($\sim 1.9 \times 10^{-1}$ %), (c) high initial true contact area (~ 1.0 %).

annealing. It also has a strong temperature dependence. Initial true contact area is influenced by the bonding force, bonding duration, and the bonding temperature. Significant improvement in the contact area can be observed in all the simulation results at high temperature. For low ($\sim 4.3 \times 10^{-4}$ %) and medium ($\sim 1.9 \times 10^{-1}$ %) initial true contact area as shown in Figure 4.3(a) and Figure 4.3(b) respectively, more than an order increase in true contact area can be achieved with annealing at temperature of 300°C or higher for half an hour. Complete bonding, i.e. void free interface, would be achieved for bonding interface that has high initial true contact area (~ 1.0 %) as shown in Figure 4.3(c). All of the simulations assumed the Cu surfaces are oxide free at all time. In reality, the oxide free condition may only be possible under ultra-high vacuum annealing (10^{-10} Torr [164]), as any presence of oxide on the surface has been reported to retard surface diffusion [165, 166], and thus preventing the formation of void free interface even with annealing.

4.4 Experiments on True Contact Area Growth by Surface Diffusion

To verify the model, thermocompression bonded Cu samples were annealed at different duration. Two different size of ($5 \times 5 \text{ mm}^2$ and $2.5 \times 2.5 \text{ mm}^2$) Si chips with Cu film were bonded face to face with the bigger chip on the bottom facing up with similar bonding process as illustrated in Chapter 3. Bonded chips were then subjected to shear testing to measure the bond toughness. Detail of sample preparation and bonding process are describe in section 3.4. The surface roughness parameters was found to be $\bar{R} = 50 \text{ nm}$, $\sigma_s = 3.6 \text{ nm}$ and $\eta = 3.4 \times 10^{14} \text{ m}^{-2}$.

Three pairs of chips were bonded at each bonding cycle. To exclude the effects of initial bonding condition, all samples were bonded at the same condition, i.e. 10^{-2} Torr vacuum followed by 20 minutes incremental heating to 300°C , holding at that temperature for 10 minutes and finally cooled down to room temperature within 20 minutes. A bond pressure of 99.3 kPa was applied during thermocompression bonding. To study the true contact area growth during annealing, samples were annealed for different duration with the same annealing temperature. 1 hour and 4 hours annealing was done at 300°C with room temperature anneal (zero hour) as the measurement benchmark. Effect of annealing after bonding on the bond quality was quantified by shear testing using DAGE 4000 Multi-purpose Bondtester, as described in sub-section 3.4.5.

Using equations (3.16) and (3.12), the initial true contact area A_c was estimated to be $\sim 0.0308 \%$ with a mean plane $d \sim 11.23 \text{ nm}$. From there, the true contact growth during annealing can be calculated using equation (4.18).

Chapter 2 has shown that the calculated true contact area can be related to the mechanical properties by a proportional factor K such that [87, 137]

$$F = K A_c \quad (4.19)$$

with F is the measured shear strength of the samples. Figure 4.4 shows the plot

Figure 4.4: Plot of measured shear strengths versus the calculated true contact area. The plot is use to find the proportional factor K that can relates the true contact area and measured shear strength.

of measured shear strength as a function of calculated true contact area. The proportional factor was determined from the slope between the shear strength and calculated true contact area and was found to be $K = 11.92$ MPa. This value is an order smaller than the bulk Cu shear strength (172 MPa). There are two arguments that can explain the small value of K , that are the effect of interface oxide to the retardation of surface diffusion and pressure dependence of K as had been observed in Chapter 3.

Smaller value of K has the implication that the true contact area growth is slower than the model has predicted. The model assumes an oxide free interface. In reality, oxide free condition may only be possible under ultra high vacuum annealing (10^{-10} Torr [164]), as at lower vacuum level, oxide can still form on the Cu surface and retard the act of surface diffusion [165, 166], thus preventing the formation of void free interface.

Figure 4.5 shows the effect of post-bond annealing effect superimposed with the model prediction $K = 172$ MPa (typical bulk Cu shear strength) and best fit $K = 11.92$ MPa. With $K=172$ MPa, the model over predicted the bond strength at longer bonding time. Cu oxide induced diffusion retardation at longer bonding duration could be the main reason for their low bonding strength [167–169]. Further

Figure 4.5: *Experiment result on the effect of thermal annealing superimposed with model prediction. The solid line and dashed line represents model prediction fitted with proportional factor of $K = 11.92$ MPa and $K = 172$ MPa respectively.*

study on the Cu oxide induce diffusion retardation would be out of the current thesis scope.

On the other hand, considering the pressure dependence of K as discussed in Chapter 3, $K=11.92$ is a reasonable value for bonding pressure of 99.3 kPa as K has the range from 42 to 3000 MPa for bonding pressure of 200 kPa to 1200 kPa, and generally is smaller for lower bond pressure. Nevertheless, post-bond improvement by thermal annealing has been shown and modeled.

4.5 Derivation of Electromigration Induced Contact Resistance Reduction During Current Stressing

Since 1969, electromigration has been considered as the interconnect enemy [170, 171]. Electromigration remains a dominant reliability concern for the modern IC, due to the aggressive decrease in interconnect dimensions and the comparably aggressive increase in current densities required during operation. On the contrary, recent observations by Chen [109] as well as Leong [75] that contact resistance of bonded Cu interface can decrease under current stressing, which suggests another method for post thermocompression bond enhancement. As discussed and shown in

Figure 4.6: *Contacting asperity diagram under current stressing. Electron flow indicated by the thick arrow.*

Chapter 2, a lower contact resistance also corresponds to better bond strength. Thus, direct current stressing to the contact interface can enhance the bond properties. This subsequent section will derive the mathematical model for contact resistance reduction under direct current stressing.

4.5.1 Derivation for single contact

Unlike the surface diffusion mechanism that was considered earlier, consider now the main driving force for atomic migration in electromigration is electron wind passing through the constriction on the contacting asperity, as shown in Figure 4.6. General electromigration's atomic flux on the interconnect line is given by [165, 172]

$$J = -\frac{DC}{kT} Z^* e E \quad (4.20)$$

where D is the diffusivity, C is the atomic density, k is the Boltzmann's constant, T is the temperature, Z^* is the effective charge, e is the electron charge and E is the electric field. Considering only electromigration induced surface diffusion, C in the equation (4.20) can be substituted by the surface density ν (here $\nu \equiv \Omega^{-\frac{2}{3}}$) [128]. Thus, equation (4.20) becomes

$$J_s = -\frac{D\nu}{kT}Z^*eE. \quad (4.21)$$

Following the similar approach as discussed in section 4.2, we can consider a small finite element of the neck shown in Figure 4.2. Atomic flux due to electron wind force convergence on this element ($J_{e1} - J_{e2}$) will drive the outward movement of the surface.

Substituting equation (4.21) into equation (4.3) and assuming infinitesimal changes, we have

$$\frac{\partial n}{\partial t} = \frac{\Omega}{\bar{r}} \frac{\partial}{\partial z} \left(\bar{r} \frac{D\nu}{kT} Z^* e E \right). \quad (4.22)$$

Note that, due to the rotational symmetry, E is only dependent on z . Furthermore, since we are assuming D , ν and Z^* are isotropic, we can have

$$\frac{\partial n}{\partial t} = \frac{D\Omega\nu}{kT} Z^* e \frac{\partial E}{\partial z} \quad (4.23)$$

and E can also be expressed as

$$E = \rho j, \quad (4.24)$$

where ρ is the materials resistivity, and j is the electron current density. Outward movement on the neck region corresponds to changes in the radius of contact, therefore

$$\frac{\partial a}{\partial t} \approx \frac{\partial n}{\partial t}, \quad (4.25)$$

where a is the contact radius of the asperity. Thus, equation (4.23) becomes

$$\frac{\partial a}{\partial t} = \frac{D\Omega\nu Z^* e \rho}{kT} \frac{\partial j}{\partial z}. \quad (4.26)$$

Considering the rotational symmetry as given in Figure 4.6, j can be expressed as:

$$j = \frac{-I}{\pi(R \sin \theta)^2}, \quad (4.27)$$

where I is the current flowing through a single contacting asperity, and θ is the angle between R and vertical axis z as defined in Figure 4.6. A negative sign is used to indicate that the direction of the flux. Electron flux is considered instead of the traditional current direction. Substituting equation (4.27) to equation (4.24), we have

$$\frac{\partial a}{\partial t} = \frac{D\Omega\nu Z^* e \rho}{kT} \frac{\partial}{\partial z} \left(\frac{-I}{\pi(R \sin \theta)^2} \right). \quad (4.28)$$

Since we can express $z = R \cos \theta$ and $\partial z = -R \sin \theta \partial \theta$, thus

$$\begin{aligned} \frac{\partial a}{\partial t} &= \frac{-D\Omega\nu Z^* e \rho I}{kT \pi R^2} \frac{\partial}{\partial z} \left(\frac{1}{(\sin \theta)^2} \right) \\ &= -\frac{2\Omega\nu D Z^* e}{kT} \frac{\rho I}{\pi R^3 \sin \theta} \left(\frac{\cos \theta}{\sin^3 \theta} \right) \\ &= \frac{-D\Omega\nu Z^* e \rho I}{kT \pi R^2} \frac{\partial}{-R \sin \theta \partial \theta} \left(\frac{1}{(\sin \theta)^2} \right) \\ &= \frac{D\Omega\nu Z^* e \rho I}{kT \pi R^3} \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\frac{1}{(\sin \theta)^2} \right) \\ &= \frac{D\Omega\nu Z^* e \rho I}{kT \pi R^3} \frac{1}{\sin \theta} \frac{-2 \cos \theta}{\sin^3 \theta} \\ &= -\frac{2D\Omega\nu Z^* e \rho I}{kT \pi R^3} \frac{\cos \theta}{\sin^4 \theta}. \end{aligned} \quad (4.29)$$

We can also express $a = R \sin \theta$ and $\partial x = R \cos \theta \partial \theta$, thus equation (4.29) becomes

$$\begin{aligned} \frac{R \cos \theta \partial \theta}{\partial t} &= -\frac{2D\Omega\nu Z^* e \rho I}{kT \pi R^3} \frac{\cos \theta}{\sin^4 \theta} \\ \frac{\partial \theta}{\partial t} &= -\frac{2D\Omega\nu Z^* e \rho I}{kT \pi R^3} \frac{1}{\sin^4 \theta} \\ \sin^4 \theta \partial \theta &= -\frac{2\Omega\nu D Z^* e}{kT} \frac{\rho I}{\pi R^4} \partial t \end{aligned} \quad (4.30)$$

Defining $B_2 = \frac{2\Omega\nu DZ^*\rho e}{\pi kTR^4}$, we have

$$\int \sin^4 \theta \partial \theta = \int -B_2 I \partial t. \quad (4.31)$$

Integrating the left hand side of equation (4.31) by parts[†], considering that $a \ll R$ and with small angle approximation, i.e. $\sin \theta \approx \tan \theta = a/R$ and $\cos \theta \approx 1$, we have

$$\begin{aligned} \int \sin^4 \theta \, d\theta &= -\frac{1}{4} \sin^3 \theta \cos \theta + \frac{3}{8} \theta - \frac{3}{16} \sin 2\theta + C \\ \int \sin^4 \theta \, d\theta &\approx -\frac{1}{4} \theta^3 + \frac{3}{8} \theta - \frac{3}{8} \theta + C = -\frac{1}{4} \theta^3 \end{aligned} \quad (4.32)$$

$$= -\frac{1}{4} \frac{a^3}{R^3} + C \quad (4.33)$$

Combining equation (4.33) and equation (4.31), we have

$$-\frac{a^3}{4R^3} = -B_2 I t + C. \quad (4.34)$$

With boundary condition $a = a_o$ at $t = 0$, thus $C = -\frac{a_o^3}{4R^3}$. The complete formulation for the true contact area increment can be given as

$$a(t) = (a_o^3 + 4R^3 B_2 I t)^{1/3} = \left(a_o^3 + \frac{8\Omega\nu D}{kT} Z^* e \frac{\rho I}{\pi R} t \right)^{1/3} \quad (4.35)$$

Equation (4.31) basically gives the radius of the contacting asperity evolution under constant current stressing. Given the asperity tip curvature radius, the evolution of the true contact area can be calculated.

4.5.2 Case of current ramp in single contact

In the case of a ramped current as presented in Leong [75] and Chen [109], a minor modification to equation (4.31) is required. Assuming a linear current increment is applied to the contact area as $I = ct$, where c is the current increment rate, hence

[†] Using integral table from [162]

$$\int \sin^2 x \, dx = \frac{1}{2}x - \frac{1}{4} \sin 2x + C \text{ and } \int \cos^2 x \, dx = \frac{1}{2}x + \frac{1}{4} \sin 2x + C$$

the right hand side of equation(4.31) becomes

$$\int -B_2 I \partial t = \int -B_2 c t \partial t = -\frac{B_2 c t^2}{2} + C. \quad (4.36)$$

By substituting right hand side of equation (4.34) with (4.36), thus gives

$$a = \left(a_o^3 + \frac{4\Omega\nu D}{kT} Z^* e \frac{\rho c}{\pi R} t^2 \right)^{1/3}. \quad (4.37)$$

Given the contact radius, the contact resistance can be calculated by substituting a into the constriction resistance formula given as [138]

$$R_c = \Gamma(l/a) \left(\frac{\rho}{2a} \right) + \frac{4\rho}{(3\pi a)} \frac{l}{a} \quad (4.38)$$

where l/a is Knudsen ratio, l is the electron mean free path, a is the contact radius, $\Gamma(l/a)$ is a function decreasing from 1 to 0.694 as l/a increase from 0 to ∞ . Approximate function of $\Gamma(l/a)$ is given in [100] as[‡] :

$$\Gamma(K) \approx \frac{2}{\pi} \int_0^\infty e^{-(l/a)x} \text{sinc } x \, dx \quad (4.39)$$

with $\text{sinc } x = \frac{\sin x}{x}$ [§] is the unnormalized sinc[¶] function.

4.5.3 Multiple contact

In the case of multiple contacts, Kirchhoff's current law [173] requires that the total current passing through the contact is the summation of current that passes through each asperity, and can be given as

$$I_{tot} = \sum_{i=1}^{N_t} I_i, \quad (4.40)$$

[‡] the original formula was $\Gamma(K) \approx \frac{2}{\pi} \int_0^\infty e^{-2(\lambda/D)x} \text{sinc } x \, dx$, with λ used as the electron mean free path instead of l

[§] http://en.wikipedia.org/wiki/Sinc_function

[¶] unnormalized sinc also known as zeroth order of Bassel function

where I_{tot} is the external applied current, I_i is the current on each contacting asperity and N_t is the number of contacting asperity. It can be assumed that the current density is uniform for the entire contacting asperity such that current density j can be expressed as

$$j = \frac{I_{tot}}{A_c} = \frac{I_{tot}}{\sum_{i=1}^{N_t} \pi a_i^2},$$

where A_c is the true contact area. This assumption is reasonable as small contact will have high contact resistance which lead to smaller current. On the other hand, bigger contact will have lower resistance which lead to higher current through it. Thus, the current that passes through each contacting asperity can be given as

$$I_i = \frac{I_{tot} \pi a_i^2}{\sum_{i=1}^{N_t} \pi a_i^2} = \frac{I_{tot} a_i^2}{\sum_{i=1}^{N_t} a_i^2}. \quad (4.41)$$

As a result, the contact radius of each contacting asperity under constant current bias and linearly increasing current can be expressed as

$$a_i = \left(a_o^3 + \frac{8\Omega\nu D}{kT} Z^* e \frac{\rho t}{\pi R} \times \frac{I_{tot} a_i^2}{\sum_{i=1}^{N_t} a_i^2} \right)^{1/3} \quad (4.42)$$

and

$$a_i = \left(a_o^3 + \frac{4\Omega\nu D}{kT} Z^* e \frac{\rho t^2}{\pi R} \times \frac{c_{tot} a_i^2}{\sum_{i=1}^{N_t} a_i^2} \right)^{1/3}, \quad (4.43)$$

respectively.

Multispot contact can be viewed as a configuration of multiple spots in parallel arrangement [132]. Thus, the total contact resistance can be given by

$$\frac{1}{R_c} = \sum_{i=1}^{N_t} \frac{1}{R_{ci}} = \sum_{i=1}^{N_t} \frac{1}{\Gamma(l/a_i) \times \left(\frac{\rho}{2a_i} \right) + \frac{4l\rho}{3\pi a_i^2}}, \quad (4.44)$$

where a_i is given in equation (4.42) and equation (4.43) for constant and ramped current stressing, respectively.

Table 4.2: Lists of physical constants for simulation of contact resistance reduction under current stressing

Parameter	Symbol	Units	Value for copper	References
Atomic volume	Ω	nm^3	1.18×10^{-2}	[145]
<i>Diffusion</i>				
Surface pre-exponential	D_{os}	$\text{m}^2 \text{s}^{-1}$	10^7	[174, 175]
Surface activation energy	E_A	kJ mol^{-1}	56 (0.58 eV)	[174, 175]
resistivity	ρ	Ωm	1.7×10^{-8}	[108]
Electron mean free path	l	nm	38.7	[108]
	Z^*		1	

4.5.4 Simulation

A simulation on the true contact area growth due to electromigration was carried out by assuming a surface roughness of 2 nm-rms with $\eta = 10^{12} \text{ m}^{-2}$, $\sigma_s = 2 \text{ nm}$ and $R = 50 \text{ nm}$, as obtained from Leong *et al.* [75]. The simulation assumes a $100 \times 100 \mu\text{m}^2$ nominal contact area A_n that was being stressed with a ramped current rate $c = 0.1 \text{ A/s}$ ($j = 10^5 \text{ A/m}^2\text{s}$). The initial contact resistance was predetermined from the value of d , which also excludes the complexity of the thermocompression bonding condition. Generally, smaller d corresponds to either of combination of larger force, longer bonding duration, or higher bonding temperature during thermocompression bonding, thus determining the initial contact resistance.

All the diffusion data used in the simulations were extracted from various source and summarized in Table 4.2. Source codes (MATLAB/OCTAVE) used in this simulation are included in Appendix A.3. $\Gamma(l/a)$ values were extracted from [108] since the calculation $\Gamma(K) \approx \frac{2}{\pi} \int_0^\infty e^{-(l/a)x} \text{sinc } x \text{ dx}$ [100] shows large deviation as l/a increases as has been shown in Figure 2.3.

Simulations on the model show that the resistance decrease is dependent on the initial contact resistance. The contact resistance starts to drop significantly as it reaches certain critical current as shown in Figure 4.7. The critical current has an inverse trend with the initial resistance value as observed in [107]. In this case, the critical current decreases as the initial resistance increases. Beyond the critical current, the resistance decreases exponentially. The critical current is consistent with the observation reported in [75].

The presence of a critical current can be viewed from electromigration mechanism. The main driving force for electromigration is electron wind force. Electron

Figure 4.7: *Simulation result of contact resistance reduction model as a result of current stressing.*

wind force is associated with the current density as shown by equation (4.24). At low current density, there is less force to drive atomic migration. As the current is increased, so does the current density, and at a certain current level, there is enough force to drive atomic migration. In the current model, it has been shown that the current density at the neck regions (neck had been defined in 4.1), can be sufficiently high to cause electromigration, which eventually leads to the increase in the contact radius and reduction in contact resistance.

In addition, the current density depends on the size of the contact area normal to the current flows. The smaller the contact radius, the less current required to reach the critical current density for atomic migration. Since smaller contact radius also associated with higher contact resistance, it makes perfect sense that the critical current decreases with initial contact resistance. Furthermore, Leong had estimated the critical current density (applied current divided by estimated true contact area)

which resistance reduction start to occurs are relatively constant at 10^8 A/cm² [176].

Figure 4.8: *Simulation results of contact resistance reduction , this time incorporating contact heating effect. No significant increase in contact resistance observed.*

Figure 4.8 shows the simulation results incorporating the contact heating to increase in the contact resistance [110]. It shows no significant increase of contact resistance. Hence initial increased in contact resistance prior to contact resistance drop as observed by Leong [75,176] cannot be explained by the effect of contact heating during current stressing.

4.6 Model and Experiment Comparison

Figures 4.9 show the model prediction and measured contact resistances of bonded interconnects extracted from [109] when the stress current was ramped gradually from 1 to 100 mA at a rate of 1 mA/s. It was observed that the contact resistance decreases and converges to a constant value at high stress current, which is well

Figure 4.9: Comparison between experiment observation of contact resistance reduction during current stressing (square) extracted from Chen et al. [109] and model prediction by the same surface and bonding parameter (solid line). (a) 7 μm bonding lines, (b) 10 μm bonding lines.

described by the model.

Chen *et al.* [109] reported that the contact resistance reduction happens on the bonding structure that has surface roughness of 1.15 nm - rms. Surface roughness parameter such as asperity tip curvature radius R , asperity density η and the asperity height distribution σ_s were taken from Leong statistical data [75] for the same rms-roughness. The model was found to fit well with a pre-exponential diffusivity of $D_o = 85 \text{ m}^2/\text{s}$, giving the room temperature (27°C) diffusivity of $1.58 \times 10^{-8} \text{ m}^2/\text{s}$ and activation energy $E_A = 0.58 \text{ eV}$. This pre-exponential factor is five order lower than what was reported in [163]. This difference is mainly attributed to the difference in driving force for surface diffusion, i.e. surface curvature in [163] versus electron wind force in the current model. Nevertheless, the current model has justified theoretically the electromigration-induced reduction in the initial contact resistance of bonded interconnects. The model also provides a mechanism for post-bonding bond property improvement for 3D-ICs.

4.7 Summary

The effects of surface diffusion to the evolution of true contact area have been modeled. Simulation based on the model shows that contribution to the true contact area depends greatly on the initial true contact area, i.e before annealing. It also has a strong temperature dependence. Significant improvement in the contact area due to the surface diffusion mechanism is observed in all simulations at high temperature (300°C or higher). A void free interface can be achieved for bonding interface from the act of surface diffusion alone, provided that the Cu interface is maintained oxide free. In reality, oxides free condition may only be possible under ultra high vacuum annealing (10^{-10} Torr [164]), as at lower vacuum level, oxide can still be present on the Cu surface and retard the act of surface diffusion [165, 166], thus preventing the formation of void free interface.

Electromigration assisted contact resistance reduction based on the phenomenon observed in [75, 109] has been modeled. The model shows the resistance starts to drop exponentially as it reaches a certain critical current level. The critical current dependence on the initial resistance value as observed by Leong [75] has been captured by the model as well. This mechanism may provide another avenue in improving the contact resistance after bonding.

Chapter 5

Conclusion

In this chapter, the various aspects of this work are summarized and discussed, key conclusions are made, and recommendations for future work are given. First, the thesis is summarized and general comments about the integration of the various parts of the work made. Then, the key conclusions that can be drawn from this work are identified and recommendations for future work itemized.

5.1 Summary and Conclusion

Chapter 1 has given an overview of current technology, motivation for the current research as well as a brief review on the essential fundamental knowledge that were used in the research.

In Chapter 2, the importance of the ability to assess the bonding interface quality non-destructively was discussed. The argument is that mechanical testing on bonded process wafers can be very costly, particularly due to multilayer devices that had been integrated in the chips. Thus, the quality of the bond strength needs to be assess non-destructively. Characterization method to bridge between mechanical and electrical properties of the bond interface was constructed. In which, the methodology has enable the non-destructive determination of Cu bond strength. Electrical-based characterization was chosen as it is a fast and relatively simple method. Modeling and measurement of electrical contact resistance has shown a

diminishing sensitivity as the bond strength increases.

To overcome this limitation, bond quality characterization by resonance frequency was proposed. Unlike any other measurement, the proposed method includes a construction of an external circuit modifier which consists of inductors and resistors, in such a way that allows for generation of AC signal resonance frequency. The resulting resonance frequency was then used as an indicator for the quality of the bonded interface in terms of true contact area A_c .

Resonance frequency is able to characterize the bond properties with only two probes, unlike measurement of contact resistance which requires four probes. The proposed method is also able to eliminate the effect of cabling resistance and sheet resistance. The proposed method is able to locally characterize the bonding interface independently.

The external circuit also provides the flexibility to adapt the measurement method into different measurement range and sensitivity. This range modification is important as it allow one to overcome the limitation of the available characterization instrument. Particularly in in-line manufacturing process, upgrading of characterization instrument may require significant capital investment and possible operational disruption.

As a proof of concept, an experiment was designed to enable a direct correlation between mechanical and electrical properties of the bond interface. One of the challenge was to design a test structure that enables three characterization methods, i.e. mechanical shear test, contact resistance measurement, and resonance frequency measurement. To overcome the fabrication limitation, particularly the cost of lithography, Chapter 2 gives the detailed construction of a simple yet functional test structure that satisfies the three requirements. Furthermore, the external modifier circuits had been shown can be built cheaply using discreet electronics component that can easily found in the market such as passive resistor, inductor and capacitor.

The experimental results have established the correlation between the electrical

properties and mechanical properties through the true contact area. The mechanical bond strength and true contact area has been shown to be related by a single proportional factor K . However, relation between the true contact area and bond interface electrical properties, i.e. contact resistance and resonance frequency, was shown to be more complex. Details of their relation had been described and discussed in Chapter 2. Meanwhile, the formation of true contact area and empirical determination of K was studied further in Chapter 3.

In Chapter 3 the formation of true contact area as a function of the bonding condition, i.e. surface morphology, bond pressure, bond temperature, and bond duration was modeled. The surface micro-roughness has led to the true contact area to be only a small fractions of the nominal contact area. To account for the surface roughness, the two contacting surfaces were assumed to consist of multiple asperities that have random heights. The asperity height can be approached by a Gaussian distribution function, with standard deviation σ , asperity radius curvature R , and number of asperity per unit area η . The true contact area is assumed to be contributed by asperities that are tall enough to make contact with the other surface. The parameters of the surface roughness were obtained from analyzing surface profiles from AFM measurements by utilizing algorithm given by Leong [75]. During thermocompression bonding, asperities were assumed to be deforming continuously. The deformation rate depends on the bonding temperature, applied pressure and material's properties. Time dependent deformation was captured by utilizing creep dominated deformation.

The model based on power-law creep was found to have the best correlation between the simulation and experimental results. Simulation on the model shows a reasonable agreement with real case bonding experiments reported by others [107, 150, 177]. Simulation on the model also shows that the bond integrity will not benefit much from longer bonding duration if the bonding temperature is too low, i.e. less than 300°C. On the other hand, bond interface integrity could significantly benefit from a longer bonding duration for high bonding temperature, i.e. above 300°C.

Experiments were conducted as the proof of concept, as well as the empirical determination of the proportional factor K . Shear tests were used to determine the mechanical strength of bonded chip at different bonding conditions. The proportional factor K was obtained from the best fit slope between the calculated true contact area and measured shear strength. It was found that K has dependence on the bonding pressure. The bonding pressure dependence on K may imply a more complex relation between the true contact area and the bond shear strength.

These complexities were reflected in the huge variation of across different studies. First, in Chapter 2, the value of K could reach 9×10^9 MPa, on the mechanical-electrical test structures. In Chapter 3, on a simple bonding test structure, K has a value range from 42-3000 MPa, which increases with bonding pressure from 200 - 1200 kPa. Finally in Chapter 4, on the modeling and experiment of thermal annealing to bond integrity, it was found to be as low as 12 MPa.

Efforts had been made to rationalize those discrepancies for each case. Arguments from various shielding effects of mechanical testing to the possible variations of surface roughness parameter had yet yielded a satisfactory explanation for the case of huge K value such as that found in Chapter 2. Apparent pressure dependence of K was found in Chapter 3 had been both supported and contradicted by the literature, with both arguments coming from atomic scale simulations. To prove the actual value of K is beyond the scope of the current thesis. Finally, a low K in Chapter 4 is expected, as it is still in line with the range of K values obtained in Chapter 3, which of 12 MPa for 99.3 kPa bonding pressure is an extrapolation of 42-3000 MPa for 200-1200 kPa bonding pressure.

Mechanical strength determination by four point bending test was also observed to have similar proportionality between the measured mechanical strength and calculated true contact area. This consistency from the two mechanical characterization method could mean that the model can be generalized to different type of mechanical characterization.

To apply the model into a practical application, a bonding map was constructed

that gives the true contact area as a function of surface roughness, bonding pressure and bonding temperature for one bond duration. The ability of the map to predict the true contact area from any bonding condition, and coupled with the criteria to obtain 100% dicing yield from Leong, i.e. 3.18×10^{-2} % (from the nominal contact area) [75], could be a powerful tool for manufacturing process. In the map, fraction of true contact area $A_c = 3.18 \times 10^{-2}$ threshold has been represented by series of curves, each for different surface roughness. Any bonding condition that lies on the right and above the curve will give 100 % dicing yield, and less than 100 % if it falls on the left or below the curve. The ability to predict the dicing yield based on the bonding condition could significantly reduce the manufacturing cost from a bad yield.

While a bonding condition that can give 100% dicing yield may be sufficient for further mechanical processing, it may not be good enough in terms of electrical performance. Thus, a curve that represents ~ 1 % true contact area from thermocompression bonding, and can be improved to achieved 100 % true contact area by thermal annealing, was added. The source of that criteria has been discussed in detail in Chapter 4.

Chapter 4 discussed two types of post bonding bond interface enhancement, i.e. through thermal annealing and direct current stressing. An analytical model was constructed to describe the effect of the thermal annealing after the thermocompression bonding. The model utilizes surface diffusion contribution to the true contact area growth based on sintering concept of contacting spherical bodies. Simulation on the model has shown that the true contact area growth has a time and temperature dependence. It was also observed that it is highly dependence on the initial true contact area, i.e. true contact area as the result of thermocompression bonding. The simulation on the model predicted that with $\sim 1\%$ initial true contact area, a void free interface can be achieved when annealed above 300°C .

The post bonding bond interface improvement by direct current stressing was based on observed contact resistance reduction of Cu bonded interface under direct

current stressing [75, 109]. The contact area growth was modeled as a surface diffusion on the surface of contacting asperities that are driven by the electron wind force. The model predicts the resistance starts to decrease exponentially as it reaches a certain critical current level. The model has well captured the critical current dependence on the initial resistance value, as observed by Leong [75, 176]. Improvement in the true contact area can be indicated by the decrease in contact resistance. This could also mean that direct current stressing can be used to improve the mechanical integrity.

Bond integrity improvement by direct current stressing has several advantages. For instance, direct current stressing can be done at room temperature. Room temperature improvement is particularly interesting as it could reduce the reliability issues due to the thermal mismatch, and thermal stress build up as it happens in thermal annealing. Bond improvement could also be done on the localized area. This is particularly useful when the bond quality across the wafer is not uniform. The chip that has weaker bond that unlikely to survive further processing can be identified by non-destructive methodology as described in Chapter 2. The weaker chip can then be selectively stressed with direct current to improve the bonding prior to further processing. Finally, there is also the possibility that bond improvement happens during the device operation, which means the device performance is just getting better as it is being used.

In conclusion, this thesis has made substantial contributions in the modeling of Cu-Cu bonding for 3D ICs and direct bonding. The main conclusions of this work are:

- Contact capacitance and contact resistance are two main contact interface characteristics that can be used to characterize the bond strength non-destructively. Combining contact capacitance and contact resistance, and amplifying it with an external circuit that consists of an inductor could provide more sensitive non-destructive bonding interface characterization methodology. Furthermore, it could also eliminate the stray resistance effect from line

resistance and probing contact resistance.

- Current stressing could enhance (or reduce) the Cu-Cu bonded interface contact resistance. The main mechanism is contributed by electromigration on the surface of contacting asperity. The identification of the mechanism and developed model could provide an alternative method for Cu-Cu bonding improvement. While thermal annealing provides general enhancement of the bonding interface, bond interface enhancement by current stressing could be done locally and happened during the device operations. Furthermore, current stressing could be done at room temperature, which is particular advantage for temperature sensitive application and specific bonding.
- A more general model for thermocompression bonding has been built as compared to previous work. The dynamic nature of the bonding has been captured. Results from die shear test can be related to the model by a single proportional constant, which is obtained empirically. The work has enabled a constructions of a true contact area and electrical bonding maps for the fast estimate of the bonding quality given bonding duration, surface roughness, bonding pressure and bonding temperature.

5.2 Recommendation for Future Works

The work that was performed in this thesis has addressed several key issues in copper wafer bonding technology for 3D ICs. While this work has led to significant advances, it has also highlighted several topics that require further work. These are itemized below:

- The contact model in this thesis has been based by Greenwood and Williamson (G&W) with particular limitation to represent the surface as a series of asperities with different heights but uniform radius of curvature. An alternative view of a real surface have been proposed by recent works such as modeling surface roughness as a superposition of height variations at multiple spatial

wavelengths [119]. It would be interesting to consider those models in the future, as it may be able to overcome G&W based models.

- The true contact area model developed in Chapter 2 has mainly focused on single creep dominated deformation to model Cu deformation for the entire bonding condition. However, it has been reported that there is a possible transition from power law creep to exponential creep, especially at high bonding temperature and high stress [178]. It would be interesting to modify the model to incorporate such transition.
- Introduction of a constant K in Chapter 2 has enabled correlation between contact electrical properties with die shear test results. However, its actual physical meaning of the constant has not been fully explored and explained. Non-empirical determination of K needs to be addressed in the future. Furthermore, whether K is really a constant needs to be verified as the current experiments indicate a pressure dependence of K .
- Electrical quality improvement of Cu interface has been experimentally and theoretically shown by applying a current stress. It would be interesting to verify that if the current stress could also improve the mechanical properties.
- The current work has focused on the die shear test due to its simple and fast sample preparation (with some work on four point bend test) for mechanical characterization. However, its simplicity had come at a price. It has been observed that die shear test produce highly scattered data. The possibility of stress localization on the shear test samples which depends greatly on the exact loading and specimen geometry [155–157] had not been considered. The significance of the stress localization to current stress geometry is unknown. Thus, the simple relations between shear load, true contact area, and K , probably needs to be evaluated by considering the severity of stress localization factor in the future
- It may be necessary and interesting to verify the models with other mechanical

test methodology such as chevron test. Chevron test system has been known to yield lower data scatter, thus combining chevron test with electrical test structure could be very a interesting topic.

- The current work also only focus on Cu-Cu bonding. However, the model that was developed is not limited to Cu. Substitution with other material system is possible given the physical constants known. It would be interesting as well to apply the current model of thermocompression bonding model in Chapter 3, post-bonding bond-enhancement model in Chapter 4 and non-destructive characterization method in Chapter 2 into other materials system such as Au-Au bonding.

Bibliography

- [1] R. Chanchani, "3D integration technologies - an overview," in *Materials for Advanced Packaging*, pp. 1–50, 2009.
- [2] K. Banerjee, A. Mehrotra, K. Saraswat, and S. Souri, "Multiple si layer ICs: motivation, performance analysis, and design implications," in *7th Conference on Design Automation (DAC'00)*, 2000.
- [3] B. Davari, R. Dennard, and G. Shahidi, "CMOS scaling for high performance and low power-the next ten years," *Proceedings of the IEEE*, vol. 83, no. 4, pp. 595–606, 1995.
- [4] G. Sai-Halasz, "Performance trends in high-end processors," *Proceedings of the IEEE*, vol. 83, no. 1, pp. 20–36, 1995.
- [5] K. Saraswat and F. Mohammadi, "Effect of scaling of interconnections on the time delay of VLSI circuits," *Solid-State Circuits, IEEE Journal of*, vol. 17, no. 2, pp. 275–280, 1982.
- [6] M. Bohr, "Interconnect scaling-the real limiter to high performance ULSI," pp. 241–244, *Electron Devices Meeting, 1995.*, International, 1995.
- [7] J. Meindl, "Low power microelectronics: retrospect and prospect," *Proceedings of the IEEE*, vol. 83, no. 4, pp. 619–635, 1995.
- [8] M. Bohr and Y. El-Mansy, "Technology for advanced high-performance microprocessors," *Electron Devices, IEEE Transactions on*, vol. 45, no. 3, pp. 620–625, 1998.
- [9] C. Barrett, "Microprocessor evolution and technology impact," pp. 7–10, *VLSI Technology, 1993. Digest of Technical Papers. 1993 Symposium on*, 1993.
- [10] "A perspective on asynchronous microprocessor." <http://www.hal.rcast.u-tokyo.ac.jp/research/titac/perspect/perspect-j.html>.
- [11] K. Saraswat, K. Banerjee, A. Joshi, P. Kalavade, P. Kapur, and S. Souri, "3-D ICs: motivation, performance analysis, and technology," *Solid-State Circuits Conference, 2000. ESS-CIRC'00. Proceedings of the 26th European*, pp. 406–414, 2000.
- [12] J. Colinge, E. Demoulin, and M. Lobet, "Stacked transistors CMOS (ST-MOS), an NMOS technology modified to CMOS," *Electron Devices, IEEE Transactions on*, vol. 29, no. 4, pp. 585–589, 1982.
- [13] G. Goeloe, E. Maby, D. Silversmith, R. Mountain, and D. Antoniadis, "Vertical single-gate CMOS inverters on laser-processed multilayer substrates," *1981 International Electron Devices Meeting*, vol. 27, 1981.
- [14] S. Kawamura, N. Sasaki, T. Iwai, M. Nakano, and M. Takagi, "Three-dimensional CMOS IC's fabricated by using beam recrystallization," *Electron Device Letters, IEEE*, vol. 4, no. 10, pp. 366–368, 1983.
- [15] S. Akiyama, Y. Terui, and S. Ogawa, "Method of manufacturing a multilayer semiconductor device," Jan. 1986.
- [16] M. Nakano, "3-D SOI/CMOS," *1984 International Electron Devices Meeting*, vol. 30, 1984.
- [17] Y. Akasaka and T. Nishimura, "Concept and basic technologies for 3-D IC structure," *1986 International Electron Devices Meeting*, vol. 32, 1986.

- [18] S. Tatsuno, "Japan's push into creative semiconductor research: 3-dimension IC's," *Solid State Technol*, pp. 29–30, 1987.
- [19] M. Geis, D. Flanders, D. Antoniadis, and H. Smith, "Crystalline silicon on insulators by graphoepitaxy," *1979 International Electron Devices Meeting*, vol. 25, 1979.
- [20] T. Nishimura, Y. Inoue, K. Sugahara, S. Kusunoki, T. Kumamoto, S. Nakagawa, M. Nakaya, Y. Horiba, and Y. Akasaka, "Three dimensional IC for high performance image signal processor," in *Electron Devices Meeting, 1987 International*, vol. 33, pp. 111–114, 1987.
- [21] A. Wang and K. Saraswat, "A strategy for modeling of variations due to grain size in polycrystalline thin-film transistors," *Electron Devices, IEEE Transactions on*, vol. 47, no. 5, pp. 1035–1043, 2000.
- [22] V. Subramanian, M. Toita, N. Ibrahim, S. Souri, and K. Saraswat, "Low-leakage germanium-seeded laterally-crystallized single-grain 100-nm TFTs for vertical integration applications," *Electron Device Letters, IEEE*, vol. 20, no. 7, pp. 341–343, 1999.
- [23] M. Crowder, P. Carey, P. Smith, R. Sposili, H. Cho, and J. Im, "Low-temperature single-crystal Si TFTs fabricated on Si films processed via sequential lateral solidification," *Electron Device Letters, IEEE*, vol. 19, no. 8, pp. 306–308, 1998.
- [24] A. Kohno, T. Sameshima, N. Sano, M. Sekiya, and M. Hara, "High performance poly-Si TFTs fabricated using pulsed laser annealing and remote plasma CVD with low temperature processing," *Electron Devices, IEEE Transactions on*, vol. 42, no. 2, pp. 251–257, 1995.
- [25] S. Pae, T. Su, J. Denton, and G. Neudeck, "Multiple layers of silicon-on-insulator islands fabrication by selective epitaxial growth," *Electron Device Letters, IEEE*, vol. 20, no. 5, pp. 194–196, 1999.
- [26] S. Jung, H. Lim, and K. Kim, "CVD selective epitaxial lateral overgrowth technique for 3D stacked SRAM cell on SOI-like silicon films," *Electrochemical and Solid-State Letters*, vol. 12, pp. H392–H394, Oct. 2009.
- [27] H. Lin, C. Chang, T. F. Lei, J. Cheng, H. Tseng, and L. Chen, "Characterization of polycrystalline silicon thin film transistors fabricated by Ultrahigh-Vacuum chemical vapor deposition and chemical mechanical polishing," *Japanese Journal of Applied Physics*, vol. 36, pp. 4278–4282, 1997.
- [28] T. Noguchi, "Appearance of single-crystalline properties in fine-patterned Si thin film transistors (TFTs) by solid phase crystallization (SPC)," *Jpn. J. Appl. Phys.*, vol. 32, no. 11A Part 2, pp. 1584–1587, 1993.
- [29] T. Little, H. Koike, K. Takahara, T. Nakazawa, and H. Ohshima, "A 9.5 inch, 1.3 megapixel low temperature poly-Si TFT-LCD fabricated by SPC of very thin films and an ECR-CVD gate insulator," *Display Research Conference, 1991., Conference Record of the 1991 International*, pp. 219–222, 1991.
- [30] N. Yamauchi and R. Reif, "Polycrystalline silicon thin films processed with silicon ion implantation and subsequent solid-phase crystallization: Theory, experiments, and thin-film transistor applications," *Journal of Applied Physics*, vol. 75, no. 7 American Institute of Physics, pp. 3235–3257, 1994.
- [31] D. Kouvatsos, A. Voutsas, and M. Hatalis, "Polycrystalline silicon thin film transistors fabricated in various solid phase crystallized films deposited on glass substrates," *Journal of Electronic Materials*, vol. 28, no. 1, pp. 19–25, 1999.
- [32] V. Subramanian and K. Saraswat, "High-performance germanium-seeded laterally crystallized TFTs for vertical device integration," *Electron Devices, IEEE Transactions on*, vol. 45, no. 9, pp. 1934–1939, 1998.
- [33] J. Tsai, "Effects of Ge on material and electrical properties of polycrystalline Si. sub. 1-x Ge. sub. x for Thin-Film transistors," *J. Electrochem. Soc.*, vol. 142, no. 9, 1995.
- [34] S. Lee and S. Joo, "Low temperature poly-Si thin-film transistor fabrication by metal-induced lateral crystallization," *Electron Device Letters, IEEE*, vol. 17, no. 4, pp. 160–162, 1996.

- [35] S. Y. Yoon, S. K. Kim, J. Y. Oh, Y. J. Choi, W. S. Shon, C. O. Kim, and J. Jang, "A high performance polycrystalline silicon thin film transistor using a metal induced crystallization with a ni solution," in *Microprocesses and Nanotechnology Conference, 1998 International*, pp. 331–332, 1998.
- [36] J. Nakata and K. Kajiyama, "Novel low-temperature recrystallization of amorphous silicon by high-energy ion beam," *Applied Physics Letters*, vol. 40, pp. 686–688, Apr. 1982.
- [37] Y. W. Choi, J. N. Lee, T. W. Jang, and B. T. Ahn, "Thin-film transistors fabricated with poly-Si films crystallized at low temperature by microwave annealing," *Electron Device Letters, IEEE*, vol. 20, no. 1, pp. 2–4, 1999.
- [38] A. Heya, A. Masuda, and H. Matsumura, "Low-temperature crystallization of amorphous silicon using atomic hydrogen generated by catalytic reaction on heated tungsten," *Applied Physics Letters*, vol. 74, pp. 2143–2145, Apr. 1999.
- [39] A. R. Joshi and K. C. Saraswat, "Sub-micron thin film transistors with metal induced lateral crystallization," *Ulsi Process Integration*, p. 361, 1999.
- [40] K. W. Guarini, A. Topol, V. Chan, K. Bernstein, L. Shi, R. Joshi, W. E. Haensch, and M. Jeong, "3D IC technology: Capabilities and applications," in *Conference on 3D Architecture for Semiconductors and Packaging (sponsored by Research Triangle Institute)*, Burlingame, CA, 2004.
- [41] M. Bonkhara, "3D stacked LSI interconnection by Cu-Vias & 3D system integration," in *Conference on 3D Architecture for Semiconductors and Packaging (sponsored by Research Triangle Institute)*, Burlingame, CA, 2004.
- [42] A. Topol, J. D. C. L. Tulipe, L. Shi, D. Frank, K. Bernstein, S. Steen, A. Kumar, G. Singco, A. Young, K. Guarini, and M. Jeong, "Three-dimensional integrated circuits," *IBM Journal of Research and Development*, vol. 50, no. 4/5, p. 491, 2006.
- [43] A. Krupp *et al.*, "3D integration with ICV-Solid technology," in *Conference on 3D Architecture for Semiconductors and Packaging (sponsored by Research Triangle Institute)*, Tempe, AZ, 2005.
- [44] W. Weber, "Three-dimensional integration of silicon chips for automotive applications," in *MATERIALS RESEARCH SOCIETY SYMPOSIUM PROCEEDINGS*, vol. 970, p. 103, 2007.
- [45] S. Lee and R. Hon, "Multi-Stacked flip chips with copper plated through silicon vias and Re-Distribution for 3-D System-in-Package integration," in *MATERIALS RESEARCH SOCIETY SYMPOSIUM PROCEEDINGS*, vol. 970, p. 179, 2007.
- [46] R. Hon, S. Lee, S. Zhang, and C. Wong, "Multistack flip chip 3D packaging with copper plated through-silicon vertical interconnection," in *Electronic Packaging Technology Conference, 2005. EPTC 2005. Proceedings of 7th*, vol. 2, p. 6 pp., 2005.
- [47] "http://www.yole.fr/pagesAn/products/pdf/3DIC_TSV_2009_reports_flyer.pdf."
- [48] J. B. Lasky, "Wafer bonding for silicon-on-insulator technologies," *Applied Physics Letters*, vol. 48, pp. 78–80, Jan. 1986.
- [49] M. Shimbo, K. Furukawa, K. Fukuda, and K. Tanzawa, "Silicon-to-silicon direct bonding method," *Journal of Applied Physics*, vol. 60, pp. 2987–2989, Oct. 1986.
- [50] S. Bengtsson, "Semiconductor wafer bonding: a review of interfacial properties and applications," *Journal of Electronic Materials*, vol. 21, no. 8, pp. 841–862, 1992.
- [51] C. S. Tan, A. Fan, K. N. Chen, and R. Reif, "Low-temperature thermal oxide to plasma-enhanced chemical vapor deposition oxide wafer bonding for thin-film transfer application," *Applied Physics Letters*, vol. 82, pp. 2649–2651, Apr. 2003.
- [52] K. T. Turner and S. M. Spearing, "Modeling of direct wafer bonding: Effect of wafer bow and etch patterns," *Journal of Applied Physics*, vol. 92, p. 7658, 2002.

- [53] R. E. Belford and S. Sood, "Surface activation using remote plasma for hydrophilic bonding at elevated temperature," *Electrochemical and Solid-State Letters*, vol. 10, pp. H145–H148, May 2007.
- [54] C. Gui, M. Elwenspoek, N. Tas, and J. G. E. Gardeniers, "The effect of surface roughness on direct wafer bonding," *Journal of Applied Physics*, vol. 85, p. 7448, 1999.
- [55] S. Bengtsson and P. Amirfeiz, "Room temperature wafer bonding of silicon, oxidized silicon, and crystalline quartz," *Journal of Electronic Materials*, vol. 29, pp. 909–915, July 2000.
- [56] G. Wallis and D. I. Pomerantz, "Field assisted Glass-Metal sealing," *Journal of Applied Physics*, vol. 40, no. 10, pp. 3946–3949, 1969.
- [57] S. Mack, H. Baumann, and U. Gosele, "Gas tightness of cavities sealed by silicon wafer bonding," in *Micro Electro Mechanical Systems, 1997. MEMS '97, Proceedings, IEEE., Tenth Annual International Workshop on*, pp. 488–493, Micro Electro Mechanical Systems, 1997. MEMS '97, Proceedings, IEEE., Tenth Annual International Workshop on, 1997.
- [58] M. Schmidt, "Wafer-to-wafer bonding for microstructure formation," *Proceedings of the IEEE*, vol. 86, no. 8, pp. 1575–1585, 1998.
- [59] S. Cho and F. Erdmann, "An on-chip hermetic packaging technology for micromechanical devices," in *Solid-State Sensor and Actuator Workshop*, p. 229, 1998.
- [60] F. Niklaus, G. Stemme, J. Q. Lu, and R. J. Gutmann, "Adhesive wafer bonding," *Journal of Applied Physics*, vol. 99, pp. 031101–28, Feb. 2006.
- [61] F. Niklaus, P. Enoksson, P. Griss, E. Kalvesten, and G. Stemme, "Low-temperature wafer-level transfer bonding," *Journal of Microelectromechanical Systems*, vol. 10, no. 4, pp. 525–531, 2001.
- [62] J. Lu, A. Jindal, Y. Kwon, J. McMahon, M. Rasco, R. Augur, T. Cale, and R. Gutmann, "Evaluation procedures for wafer bonding and thinning of interconnect test structures for 3D ICs," in *IEEE International Interconnect Technology Conference*, (Burlingame, CA, USA), pp. 74–6, IEEE, June 2003.
- [63] H. Tilmans, D. van de Peer, and E. Beyne, "The indent reflow sealing (IRS) technique—a method for the fabrication of sealed cavities for MEMS devices," *Microelectromechanical Systems, Journal of*, vol. 9, no. 2, pp. 206–217, 2000.
- [64] C. Wang and C. Lee, "An eutectic bonding technology at a temperature below the eutectic point," in *Electronic Components and Technology Conference, 1992. Proceedings., 42nd*, pp. 502–507, Electronic Components and Technology Conference, 1992. Proceedings., 42nd, 1992.
- [65] C. Hoge and S. Thomas, "Some considerations of the Gold-Silicon die bond based on surface chemical analysis," in *Reliability Physics Symposium, 1980. 18th Annual*, pp. 301–311, Reliability Physics Symposium, 1980. 18th Annual, 1980.
- [66] J. S. Dunn, "The low temperature oxidation of copper," *Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character*, vol. 111, pp. 210–219, May 1926. ArticleType: primary_article / Full publication date: May 1, 1926 / Copyright © 1926 The Royal Society.
- [67] R. Tadepalli, *Characterization of bonded copper interconnects for three-dimensional integrated circuits*. PhD thesis, Massachusetts Institute of Technology, 2002.
- [68] K. Chen, A. Fan, C. Tan, and R. Reif, "Bonding parameters of blanket copper wafer bonding," *Journal of Electronic Materials*, vol. 35, pp. 230–234, Feb. 2006.
- [69] M. Waelti, N. Schneeberger, O. Paul, and H. Baltes, "Low temperature packaging of CMOS infrared microsystems by Si-Al-Au bonding," in *Proceedings of the 4th International Symposium on Semiconductor Wafer Bonding*, pp. 147–154, 1997.
- [70] C. H. Tsau, *Fabrication and characterization of wafer-level gold thermocompression bonding*. PhD thesis, Massachusetts Institute of Technology, 2003. Ph.D.

- [71] A. Fan, A. Rahman, and R. Reif, "Copper wafer bonding," *Electrochemical and Solid-State Letters*, vol. 2, no. 10, Electrochemical Society, pp. 534–536, 1999.
- [72] T. Suga, "Cu-Cu room temperature bonding-current status of surface activated bonding (SAB)," *ECS Trans*, vol. 6, pp. 155–163, 2006.
- [73] K. Chen, C. Tan, A. Fan, and R. Reif, "Copper bonded layers analysis and effects of copper surface conditions on bonding quality for three-dimensional integration," *Journal of Electronic Materials*, vol. 34, pp. 1464–1467, Dec. 2005.
- [74] K. Holloway, P. M. Fryer, J. Cabral, J. M. E. Harper, P. J. Bailey, and K. H. Kelleher, "Tantalum as a diffusion barrier between copper and silicon: Failure mechanism and effect of nitrogen additions," *Journal of Applied Physics*, vol. 71, pp. 5433–5444, June 1992.
- [75] H. L. Leong, *Quantitative analysis of the mechanical and electrical properties of Cu-Cu bonds for three-dimensional integrated circuits (3D ICs)*. PhD thesis, Singapore MIT Alliance, Nanyang Technological University, 2007.
- [76] K. Chen, A. Fan, and R. Reif, "Interfacial morphologies and possible mechanisms of copper wafer bonding," *Journal of Materials Science*, vol. 37, pp. 3441–6, Aug. 2002. Copyright 2002, IEE.
- [77] A. Shigetou, T. Itoh, K. Sawada, and T. Suga, "Bumpless interconnect of 6- μ m-Pitch Cu electrodes at room temperature," *Advanced Packaging, IEEE Transactions on*, vol. 31, no. 3, pp. 473–478, 2008.
- [78] T. H. Kim, M. M. R. Howlader, T. Itoh, and T. Suga, "Room temperature Cu-Cu direct bonding using surface activated bonding method," *Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films*, vol. 21, pp. 449–453, Mar. 2003.
- [79] X. F. Ang, F. Y. Li, W. L. Tan, Z. Chen, C. C. Wong, and J. Wei, "Self-assembled monolayers for reduced temperature direct metal thermocompression bonding," *Applied Physics Letters*, vol. 91, no. 6, pp. 061913–3, 2007.
- [80] O. Vallin, K. Jonsson, and U. Lindberg, "Adhesion quantification methods for wafer bonding," *Materials Science and Engineering: R: Reports*, vol. 50, pp. 109–165, Dec. 2005.
- [81] W. Maszara, G. Goetz, A. Caviglia, and J. McKitterick, "Bonding of silicon wafers for silicon-on-insulator," *Journal of Applied Physics*, vol. 64, no. 10, American Institute of Physics, pp. 4943–4950, 1988.
- [82] D. Pasquariello and K. Hjort, "Mesa-Spacers: enabling nondestructive measurement of surface energy in room temperature wafer bonding," *Journal of The Electrochemical Society*, vol. 147, pp. 2343–2346, June 2000.
- [83] T. Martini, J. Steinkirchner, and U. Gosele, "The crack opening method in silicon wafer bonding," *Journal of The Electrochemical Society*, vol. 144, pp. 354–357, Jan. 1997.
- [84] J. Bagdahn and M. Petzold, "Fatigue of directly wafer-bonded silicon under static and cyclic loading," *Microsystem Technologies*, vol. 7, pp. 175–182, Nov. 2001.
- [85] D. S. Hurd, R. Caretta, and W. W. Gerberich, "An experimental fracture mechanics study of a strong interface: The silicon/glass anodic bond," *Journal of Materials Research*, vol. 10, no. 2, pp. 387–400, 1995.
- [86] "Die shear testing - Mil-Std-883 method 2019." <http://www.siliconfareast.com/die-shear-test.htm>.
- [87] J. Krim, "Atomic-Scale origins of friction," *Langmuir*, vol. 12, pp. 4564–4566, Jan. 1996.
- [88] P. Charalambides, J. Lund, A. Evans, and R. McMeeking, "Test specimen for determining the fracture resistance of bimaterial interfaces," *Journal of Applied Mechanics, Transactions ASME*, vol. 56, no. 1, pp. 77–82, 1989.
- [89] R. H. Dauskardt, M. Lane, Q. Ma, and N. Krishna, "Adhesion and debonding of multi-layer thin film structures," *Engineering Fracture Mechanics*, vol. 61, pp. 141–162, Aug. 1998.

- [90] M. Lane, R. H. Dauskardt, A. Vainchtein, and H. Gao, "Plasticity contributions to interface adhesion in thin-film interconnect structures," *Journal of Materials Research*, vol. 15, no. 12, pp. 2758–2769, 2000.
- [91] S. Howard, A. Phillipps, and T. Clyne, "The interpretation of data from the Four-Point bend delamination test to measure interfacial fracture toughness," in *Conference on Fatigue and Fracture of Inorganic Composites*, (Cambridge; UK), pp. pp. 103–112., 1992.
- [92] J. D. Achenbach, "Quantitative nondestructive evaluation," *International Journal of Solids and Structures*, vol. 37, pp. 13–27, Jan. 2000.
- [93] D. Hyman and M. Mehregany, "Contact physics of gold microcontacts for MEMS switches," *Components and Packaging Technologies, IEEE Transactions on*, vol. 22, no. 3, pp. 357–364, 1999.
- [94] H. Lee, C. Leung, J. Shi, S. Chang, S. Lorincz, and L. Nedelescu, "Integrated microrelays: concept and initial results," *Microelectromechanical Systems, Journal of*, vol. 11, no. 2, pp. 147–153, 2002.
- [95] K. Oh and C. Ahn, "A new flip-chip bonding technique using micromachined conductive polymer bumps," *Advanced Packaging, IEEE Transactions on*, vol. 22, no. 4, pp. 586–591, 1999.
- [96] F. G. Shi, M. Abdullah, S. Chungpaiboonpatana, K. Okuyama, C. Davidson, and J. M. Adams, "Electrical conduction of anisotropic conductive adhesives: effect of size distribution of conducting filler particles," *Materials Science in Semiconductor Processing*, vol. 2, pp. 263–269, Oct. 1999.
- [97] S. Wang and K. Komvopoulos, "Static friction and initiation of slip at magnetic Head-Disk interfaces," *Journal of Tribology*, vol. 122, pp. 246–256, Jan. 2000.
- [98] J. Greenwood, "Constriction resistance and the real area of contact," *British Journal of Applied Physics*, vol. 17, no. 12, p. 1621, 1966.
- [99] R. Holm and E. Holm, *Electric contacts: theory and applications*. Springer Berlin, Heidelberg, New York, 2000.
- [100] A. Mikrajuddin, F. G. Shi, H. K. Kim, and K. Okuyama, "Size-dependent electrical constriction resistance for contacts of arbitrary size: from sharvin to holm limits," *Materials Science in Semiconductor Processing*, vol. 2, pp. 321–327, Dec. 1999.
- [101] E. Crinon and J. T. Evans, "The effect of surface roughness, oxide film thickness and interfacial sliding on the electrical contact resistance of aluminium," *Materials Science and Engineering A*, vol. 242, pp. 121–128, Feb. 1998.
- [102] L. Kogut and K. Komvopoulos, "Electrical contact resistance theory for conductive rough surfaces," *Journal of Applied Physics*, vol. 94, no. 5, pp. 3153–3162, 2003.
- [103] Y. H. Jang and J. R. Barber, "Effect of contact statistics on electrical contact resistance," *Journal of Applied Physics*, vol. 94, pp. 7215–7221, Dec. 2003.
- [104] H. L. Leong, C. L. Gan, R. I. Made, C. V. Thompson, K. L. Pey, and H. Y. Li, "Experimental characterization and modeling of the contact resistance of Cu–Cu bonded interconnects," *Journal of Applied Physics*, vol. 105, pp. 033514–6, Feb. 2009.
- [105] K. Willner, "Elasto-plastic contact of rough surfaces," *Trans. Engineering Sci*, pp. pp 13–22, 1997.
- [106] K. L. Johnson, *Contact mechanics*. Cambridge Univ Pr, 1987.
- [107] H. Leong, C. Gan, C. Thompson, K. Pey, and H. Li, "Application of contact theory to metal-metal bonding of silicon wafers," *Journal of Applied Physics*, vol. 102, no. 10, p. 103510, 2007.
- [108] R. S. Timsit, "Electrical conduction through small contact spots," *Components and Packaging Technologies, IEEE Transactions on*, vol. 29, no. 4, pp. 727–734, 2006.

- [109] K. Chen, C. Tan, A. Fan, and R. Reif, "Abnormal contact resistance reduction of bonded copper interconnects in three-dimensional integration during current stressing," *Applied Physics Letters*, vol. 86, pp. 11903–1, Jan. 2005. Copyright 2005, IEE.
- [110] R. S. Timsit, "Comment on "Abnormal contact resistance reduction of bonded copper interconnects in three-dimensional integration during current stressing" [Appl. phys. lett. [bold 86], 011903 (2005)]," *Applied Physics Letters*, vol. 88, pp. 066101–2, Feb. 2006.
- [111] R. S. Timsit, "Evidence of room-temperature sintering in aluminum contacts in vacuum and in oxygen," *Applied Physics Letters*, vol. 35, no. 5, pp. 400–402, 1979.
- [112] J. A. Greenwood and J. B. P. Williamson, "Contact of nominally flat surfaces," *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences*, vol. 295, pp. 300–319, Dec. 1966. ArticleType: primary_article / Full publication date: Dec. 6, 1966 / Copyright © 1966 The Royal Society.
- [113] F. P. Bowden and D. Tabor, *The friction and lubrication of solids*. Oxford University Press, USA, 2001.
- [114] H. Hertz and J. Angew, *Translated and reprinted in English in "Hertz's Miscellaneous Paper"*. Macmillan & Co., London, 1986.
- [115] J. A. Greenwood and J. H. Tripp, "The contact of two nominally flat rough surfaces," *Proc. Instn. Mech. Engrs*, vol. 185, pp. 625–633, 1971.
- [116] J. I. McCool, "Comparison of models for the contact of rough surfaces," *Wear*, vol. 107, pp. 37–60, Jan. 1986.
- [117] J. F. Archard, "Contact and rubbing of flat surfaces," *Journal of Applied Physics*, vol. 24, no. 8, pp. 981–988, 1953.
- [118] J. F. Archard, "Elastic deformation and the laws of friction," *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences (1934-1990)*, vol. 243, pp. 190–205, Dec. 1957.
- [119] B. N. J. Persson, "Elastoplastic contact between randomly rough surfaces," *Physical Review Letters*, vol. 87, no. 11, p. 116101, 2001.
- [120] Z. Powierza, T. Klimczak, and A. Polijanniuk, "On the experimental verification of the Greenwood-Williamson model for the contact of rough surfaces," *Wear*, vol. 154, no. 115, 1992.
- [121] E. Abbott and F. Firestone, "Specifying surface quality," *Mech. Eng.*, vol. 55, no. 569, 1933.
- [122] J. Pullen and J. Williamson, "On the plastic contact of rough surfaces," *Proc. Of Roy. Soc. London Series A*, vol. 327, no. 159, 1972.
- [123] W. R. Chang, I. Etsion, and D. B. Bogy, "An elastic-plastic model for the contact of rough surfaces," *Journal of tribology*, vol. 109, no. 2, pp. 257–263, 1987.
- [124] Y. Zhao, D. Maietta, and L. Chang, "An asperity microcontact model incorporating the transition from elastic deformation to fully plastic flow," *J. Tribology*, vol. 122, no. 86, 2000.
- [125] L. Kogut and I. Etsion, "Elastic-Plastic contact analysis of a sphere and a rigid flat," *Journal of Applied Mechanics*, vol. 69, no. 5, pp. 657–662, 2002.
- [126] H. Francis, "Phenomenological analysis of plastic spherical indentation," *ASME J. Eng. Mater. Tech*, vol. 98, no. 272, 1976.
- [127] D. Tabor, *The Hardness of Metals*. Clarendon Press, Oxford, 1951.
- [128] A. Hill and E. Wallach, "Modelling solid-state diffusion bonding," *Acta Metallurgica*, vol. 37, no. 9, pp. 2425–2437, 1989.
- [129] L. Kogut and K. Komvopoulos, "Analytical current-voltage relationships for electron tunneling across rough interfaces," *Journal of Applied Physics*, vol. 97, no. 7, pp. 073701–5, 2005.

- [130] A. Lumbantobing, L. Kogut, and K. Komvopoulos, "Electrical contact resistance as a diagnostic tool for MEMS contact interfaces," *Microelectromechanical Systems, Journal of*, vol. 13, no. 6, pp. 977–987, 2004.
- [131] A. Kamto, Y. Liu, L. Schaper, and S. Burkett, "Reliability study of through-silicon via (TSV) copper filled interconnects," *Thin Solid Films*, vol. In Press, Accepted Manuscript.
- [132] C. Dervos and J. Michaelides, "The effect of contact capacitance on current-voltage characteristics of stationary metal contacts," in *Electrical Contacts, 1997., Proceedings of the Forty-Third IEEE Holm Conference on*, pp. 152–164, 1997.
- [133] R. Malucci, "Multispot model of contacts based on surface features," in *Electrical Contacts, 1990., Proceedings of the Thirty-Sixth IEEE Holm Conference on ... and the Fifteenth International Conference on Electrical Contacts*, pp. 625–634, 1990.
- [134] A. Hebard, S. Ajuria, and R. Eick, "Interface contribution to the capacitance of thin-film Al-Al₂O₃-Al trilayer structures," *Appl. Phys. Lett.*, vol. 51, no. 17, pp. 1349–1351, 1987.
- [135] K. T. McCarthy, S. B. Arnason, and A. F. Hebard, "Frequency-dependent interface capacitance of Al-Al₂O₃-Al tunnel junctions," *Applied Physics Letters*, vol. 74, pp. 302–304, Jan. 1999.
- [136] I. Szlufarska, M. Chandross, and R. W. Carpick, "Recent advances in single-asperity nanotribology," *Journal of Physics D: Applied Physics*, vol. 41, no. 12, p. 123001, 2008.
- [137] Y. Mo, K. T. Turner, and I. Szlufarska, "Friction laws at the nanoscale," *Nature*, vol. 457, pp. 1116–1119, Feb. 2009.
- [138] G. Wexler, "The size effect and the non-local boltzmann transport equation in orifice and disk geometry," *Proceedings of the Physical Society*, vol. 89, no. 4, pp. 927–941, 1966.
- [139] M. Lane, "Interface fracture," *Annual Review of Materials Research*, vol. 33, no. 1, pp. 29–54, 2003.
- [140] A. Evans and J. Hutchinson, "Effects of non-planarity on the mixed mode fracture resistance of bimaterial interfaces," *Acta Metallurgica*, vol. 37, pp. 909–916, Mar. 1989.
- [141] R. M. Cannon, "MECHANICAL PROPERTIES OF MGO AND AL₂O₃," *Advances in Ceramics*, vol. 10, p. 818, 1984.
- [142] A. Evans, M. Rhle, B. Dalgleish, and P. Charalambides, "The fracture energy of bimaterial interfaces," *Metallurgical and Materials Transactions A*, vol. 21, no. 9, pp. 2419–2429, 1990.
- [143] M. O'Callaghan and M. Cameron, "Static contact under load between nominally flat surfaces in which deformation is purely elastic," *Wear*, vol. 36, pp. 79–97, Jan. 1976.
- [144] M. A. Meyers and K. K. Chawla, *Mechanical behavior of materials*. Prentice Hall New York, 1998.
- [145] H. J. Frost and M. F. Ashby, *Deformation-Mechanism Maps: The Plasticity and Creep of Metals and Ceramics*. Pergamon Press, 1982.
- [146] R. Keller, S. Baker, and E. Arzt, "Quantitative analysis of strengthening mechanisms in thin Cu films: Effects of film thickness, grain size and passivation," *Journal of Materials Research*, vol. 13, no. 5, p. 1307, 1998.
- [147] A. Brown and M. Ashby, "On the power-law creep equation," *Scripta Metallurgica*, vol. 14, pp. 1297–1302, Dec. 1980.
- [148] R. Keller, S. Baker, and E. Arzt, "Stress-temperature behavior of unpassivated thin copper films," *Acta Materialia*, vol. 47, pp. 415–426, Jan. 1999.
- [149] G. B. Gibbs, "Diffusion creep of a thin foil," *Philosophical Magazine*, vol. 13, no. 123, pp. 589–593, 1966.
- [150] R. Nhting, D. Olson, and G. Edwards, "Low-temperature solid-state bonding of copper," *Journal of Materials Engineering and Performance*, vol. 1, pp. 35–44, Feb. 1992.

- [151] D. Weiss, H. Gao, and E. Arzt, "Constrained diffusional creep in UHV-produced copper thin films," *Acta Materialia*, vol. 49, pp. 2395–2403, Aug. 2001.
- [152] C. Hu, R. Rosenberg, and K. Y. Lee, "Electromigration path in cu thin-film lines," *Applied Physics Letters*, vol. 74, no. 20, p. 2945, 1999.
- [153] K. Chavez and D. Hess, "A novel method of etching copper oxide using acetic acid," *J. Electrochem. Soc.*, vol. 148(11), G640, 2001.
- [154] L. Wenning and M. H. MÅEser, "Friction laws for elastic nanoscale contacts," *Europhysics Letters (EPL)*, vol. 54, no. 5, pp. 693–699, 2001.
- [155] P. A. Cundall, "Numerical experiments on localization in frictional materials," *Archive of Applied Mechanics*, vol. 59, pp. 148–159, Mar. 1989.
- [156] J. Poirier, "Shear localization and shear instability in materials in the ductile field," *Journal of Structural Geology*, vol. 2, no. 1-2, pp. 135–142, 1980.
- [157] H. Chai, "Observation of deformation and damage at the tip of cracks in adhesive bonds loaded in shear and assessment of a criterion for fracture," *International Journal of Fracture*, vol. 60, pp. 311–326, Apr. 1993.
- [158] A. A. Volinsky, J. B. Vella, and W. W. Gerberich, "Fracture toughness, adhesion and mechanical properties of low-K dielectric thin films measured by nanoindentation," *Thin Solid Films*, vol. 429, pp. 201–210, Apr. 2003.
- [159] J. Vella, I. Adhihetty, K. Junker, and A. Volinsky, "Mechanical properties and fracture toughness of organo-silicate glass (OSG) low-k dielectric thin films for microelectronic applications," *International Journal of Fracture*, vol. 120, pp. 487–499, Jan. 2003.
- [160] W. W. Mullins, "Theory of thermal grooving," *Journal of Applied Physics*, vol. 28, pp. 333–339, Mar. 1957.
- [161] F. A. Nichols and W. W. Mullins, "Morphological changes of a surface of revolution due to Capillarity-Induced surface diffusion," *Journal of Applied Physics*, vol. 36, pp. 1826–1835, June 1965.
- [162] E. Kreyszig, *Advanced Engineering Mathematics*. Wiley, 1962.
- [163] G. C. Kuczynski, "Self diffusion in sintering metal powders," *Trans. AIME*, vol. 185, p. 169, 1949.
- [164] T. Suga, "Feasibility of surface activated bonding for ultra-fine pitch interconnection-a new concept of bump-less direct bonding for system level packaging," in *Electronic Components and Technology Conference, 2000. 2000 Proceedings. 50th*, pp. 702–705, 2000.
- [165] C. S. Hau-Riege, "An introduction to cu electromigration," *Microelectronics Reliability*, vol. 44, pp. 195–205, Feb. 2004.
- [166] K. Yin, L. Chang, F. Chen, J. Kai, C. Chiang, G. Chuang, P. Ding, B. Chin, H. Zhang, and F. Chen, "Oxidation of ta diffusion barrier layer for cu metallization in thermal annealing," *Thin Solid Films*, vol. 388, pp. 27–33, June 2001.
- [167] C. Hu, L. Gignac, R. Rosenberg, E. Liniger, J. Rubino, C. Sambucetti, A. Domenicucci, X. Chen, and A. K. Stamper, "Reduced electromigration of cu wires by surface coating," *Applied Physics Letters*, vol. 81, no. 10, pp. 1782–1784, 2002.
- [168] S. L. Lehoczky, "Retardation of dislocation generation and motion in Thin-Layered metal laminates," *Physical Review Letters*, vol. 41, p. 1814, Dec. 1978. Copyright (C) 2009 The American Physical Society; Please report any problems to prola@aps.org.
- [169] Y. Z. Hu, R. Sharangpani, and S. Tay, "In situ rapid thermal oxidation and reduction of copper thin films and their applications in ultralarge scale integration," *Journal of The Electrochemical Society*, vol. 148, pp. G669–G675, Dec. 2001.
- [170] I. A. Blech, "Electromigration in thin aluminum films on titanium nitride," *Journal of Applied Physics*, vol. 47, pp. 1203–1208, Apr. 1976.

- [171] J. Black, "Electromigration-A brief survey and some recent results," *Electron Devices, IEEE Transactions on*, vol. 16, no. 4, pp. 338–347, 1969.
- [172] I. A. Blech and C. Herring, "Stress generation by electromigration," *Applied Physics Letters*, vol. 29, no. 3, pp. 131–133, 1976.
- [173] C. R. Paul and C. R. Paul, *Fundamentals of Electric Circuit Analysis*. John Wiley & Sons, 2001.
- [174] F. Nichols, "Theory of sintering of wires by surface diffusion," *Acta Metallurgica*, vol. 16, pp. 103–113, Jan. 1968.
- [175] G. C. Kuczynski, "Measurement of Self-Diffusion of silver without radioactive tracers," *Journal of Applied Physics*, vol. 21, pp. 632–635, July 1950.
- [176] H. L. Leong, C. L. Gan, C. V. Thompson, K. L. Pey, and H. Y. Li, "Electromigration-induced bond improvement for three-dimensional integrated circuits," *Applied Physics Letters*, vol. 94, no. 8, p. 081901, 2009.
- [177] C. Tsau, S. Spearing, and M. Schmidt, "Characterization of wafer-level thermocompression bonds," *Microelectromechanical Systems, Journal of*, vol. 13, no. 6, pp. 963–971, 2004.
- [178] S. Raj and T. Langdon, "Creep behavior of copper at intermediate temperatures—III. a comparison with theory," *Acta Metallurgica et Materialia*, vol. 39, pp. 1823–1832, Aug. 1991.
- [179] R. Tadepalli, K. T. Turner, and C. V. Thompson, "Mixed-mode interface toughness of wafer-level Cu-Cu bonds using asymmetric chevron test," *Journal of the Mechanics and Physics of Solids*, vol. 56, pp. 707–718, Mar. 2008.
- [180] R. Tadepalli and K. Turner, "A chevron specimen for the measurement of mixed-mode interface toughness of wafer bonds," *Engineering Fracture Mechanics*, vol. 75, pp. 1310–1319, Apr. 2008.
- [181] F. Bartels, J. Morris, G. Dalke, and W. Gust, "Intermetallic phase formation in thin solid-liquid diffusion couples," *Journal of Electronic Materials*, vol. 23, no. 8, pp. 787–790, 1994.
- [182] H. Baker and H. Okamoto, "ASM handbook. vol. 3. alloy phase diagrams," *ASM International, Materials Park, Ohio 44073-0002, USA, 1992. 501*, 1992.
- [183] F. Shieu, C. Chen, J. Sheen, and Z. Chang, "Intermetallic phase formation and shear strength of a Au-In microjoint," *Thin Solid Films*, vol. 346, no. 1-2, pp. 125–129, 1999.
- [184] R. Chuang and C. Lee, "High-temperature non-eutectic indium-tin joints fabricated by a fluxless process," *Thin Solid Films*, vol. 414, no. 2, pp. 175–179, 2002.
- [185] R. Chuang and C. Lee, "Silver-indium joints produced at low temperature for high temperature devices," *IEEE Transactions on Components and Packaging Technologies*, vol. 25, no. 31521-3331, pp. 453–458, 2002.
- [186] R. Made, C. L. Gan, C. Lee, L. Yan, A. Yu, and S. W. Yoon, "Effect of bonding pressure on the bond strengths of low temperature Ag-In bonds," in *Physical and Failure Analysis of Integrated Circuits, 2008. IPFA 2008. 15th International Symposium on the*, pp. 1–5, 2008.
- [187] J. Lin, L. Huang, G. Jang, and S. Lee, "Solid-liquid interdiffusion bonding between in-coated silver thick films," *Thin Solid Films*, vol. 410, no. 1-2, pp. 212–221, 2002.
- [188] R. Roy and S. Sen, "The kinetics of formation of intermetallics in Ag/In thin film couples," *Thin Solid Films*, vol. 197, pp. 303–318, Mar. 1991.
- [189] V. Simic and Z. Marinkovic, "Room temperature interactions in ag-metals thin film couples," *Thin Solid Films*, vol. 61, no. 2, pp. 149–160, 1979.
- [190] T. Chuang, Y. Huang, and L. Tsau, "AgIn₂/Ag₂In transformations in an In-49Sn/Ag soldered joint under thermal aging," *Journal of Electronic Materials*, vol. 30, no. 8, 2001.
- [191] L. Karpenkopf, N. Frage, A. Ripp, N. Froumin, and M. Dariel, "Sealing technique for wafer-level integrated cavity using In-Ag multilayers," in *Reliability, Packaging, Testing, and Characterization of MEMS/MOEMS IV*, vol. 5716, (Bellingham, WA), SPIE, 2005.

- [192] R. I. Made, C. L. Gan, C. Lee, L. L. Yan, A. Yu, S. W. Yoon, J. H. Lau, A. L. Hartzell, and R. Ramesham, "Study of Ag-In solder as low temperature wafer bonding intermediate layer," in *Reliability, Packaging, Testing, and Characterization of MEMS/MOEMS VII*, vol. 6884, (San Jose, CA, USA), pp. 68840H-9, SPIE, Feb. 2008.
- [193] D. Porter and K. Easterling, *Phase Transformations in Metals and Alloys*. London UK: Chapman & Hall, 1992.

Appendix A

Source Code

A.1 Power Law dominated creep simulation source code

Below are the MATLABTM scripts and supporting files that were used to simulate the thermocompression bonding model in Chapter 3. The model is used to calculate the true contact area as a function of surface roughness (represent as η , R , and σ_s), bonding duration, temperature, and applied load. The script is called `pwcreep_dcalc_v3.m`, and it also required a lookup table in the form of file `F15.txt` and `F10.txt` which give out integral value $\int_d^\infty (z-d)^{3/2} f(z) dz$ and $\int_d^\infty (z-d) f(z) dz$ normalized to the standard deviation σ_s , respectively. The two supporting files need to be placed on the same working directory as `pwcreep_dcalc_v3.m`. The calculation results dumped into a file `A_temp.txt` in a subdirectory “out” in format of duration and fraction of bonded area for the first column and second column, respectively.

A.1.1 Code listing for `pwcreep_dcalc_v3.m`

```
pressure = 1e5; %pascal
A_nom = 1e-8; %m2
E = 128e9; %pascal
poisson_ratio = 0.34;
boltzman = 1.3806503e-23; %SI unit
E_young = E/(1-poisson_ratio);
radi = 50e-9;
sigma = 3e-9;
```

```

eta = 1e14;
n = 4.8; %from keller
miu = 4.21e10;
Ac_dorn = 10^(2.94*(n-2.95));

Qv = 197*1000 /6.02e23;
Dv0 = 2e-5;

Qc = 117 * 1000 /6.02e23;
acDc0 = 1e-24;

T=350;

Dv = Dv0 * exp(-Qv /(boltzman * (T+273)));
acDc = acDc0 * exp(-Qc/(boltzman * (T+273)));
rho_dislocation = 0.4794e14 + 4.0826e14 * exp(-T/(113.7));%dislocation
density
D_eff = Dv + acDc * rho_dislocation;
burger = 2.56e-10;
B = Ac_dorn * D_eff * miu * burger / (boltzman * (T+273) * miu^n);

L_old = A_nom * pressure
F_15 = pressure / ((4/3) * E_young * radi^0.5 * sigma^1.5 * eta);
F15 = textread('F15.txt', '', 'delimiter', ' ', 'emptyvalue', NaN);
d_ovr_sigma = interp1(F15(:,2), F15(:,1), F_15);

F10 = textread('F10.txt', '', 'delimiter', ' ', 'emptyvalue', NaN);
F_1 = interp1(F10(:,1), F10(:,2), d_ovr_sigma);

A_frac = eta * radi * sigma * F_1;

t=0;

fid = fopen ('out\A_temp.txt', 'w');
fprintf(fid, '%e %e \n', t, A_frac);
fclose(fid);

bond_duration = 1000;

%short time
delta = 0.000001;

if bond_duration > 1000*delta
    t_stop = 1000*delta;
else
    t_stop = bond_duration
end

for t=delta:delta:t_stop

    L_relax = B*E_young*(pressure/A_frac)^n * A_nom * A_frac * delta;

    L_old = L_old + L_relax;

    F_15 = L_old / ((4/3) * E_young * radi^0.5 * sigma^1.5 * eta *
        A_nom);

```

```

    d_ovr_sigma = interp1(F15(:,2),F15(:,1), F_15);
    F_1 = interp1(F10(:,1),F10(:,2), d_ovr_sigma);
    A_frac = eta * radi * sigma * F_1;

    fid = fopen ('out\A_temp.txt','a');
    fprintf(fid, '%e %e \n',t+delta,A_frac);
    fclose(fid);

end

t_resume = t + delta

%Medium Time
delta = 0.0001;

if bond_duration > 1000*delta
    t_stop = 1000*delta;
else
    t_stop = bond_duration;
end

for t=t_resume:delta:t_stop

    L_relax = B*E_young*(pressure/A_frac)^n * A_nom * A_frac * delta;

    L_old = L_old + L_relax;

    F_15 = L_old / ((4/3) * E_young * radi^0.5 * sigma^1.5 * eta *
        A_nom);
    d_ovr_sigma = interp1(F15(:,2),F15(:,1), F_15);
    F_1 = interp1(F10(:,1),F10(:,2), d_ovr_sigma);
    A_frac = eta * radi * sigma * F_1;

    fid = fopen ('out\A_temp.txt','a');
    fprintf(fid, '%e %e \n',t+delta,A_frac);
    fclose(fid);

end

t_resume = t+ delta
%long time
delta = 0.01;

if bond_duration > 1000*delta
    t_stop = 1000*delta;
else
    t_stop = bond_duration;
end

for t=t_resume:delta:t_stop

    L_relax = B*E_young*(pressure/A_frac)^n * A_nom * A_frac * delta;

    L_old = L_old + L_relax;

```

```

    F_15 = L_old / ((4/3) * E_young * radi^0.5 * sigma^1.5 * eta *
        A_nom);
    d_ovr_sigma = interp1(F15(:,2),F15(:,1), F_15);
    F_1 = interp1(F10(:,1),F10(:,2), d_ovr_sigma);
    A_frac = eta * radi * sigma * F_1;

    fid = fopen ('out\A_temp.txt','a');
    fprintf(fid, '%e %e \n',t+delta,A_frac);
    fclose(fid);

end

t_resume = t+ delta
%long long time
delta = 1;

if bond_duration > 1000*delta
    t_stop = 1000*delta;
else
    t_stop = bond_duration;
end

for t=t_resume:delta:t_stop

    L_relax = B*E_young*(pressure/A_frac)^n * A_nom * A_frac * delta;

    L_old = L_old + L_relax;

    F_15 = L_old / ((4/3) * E_young * radi^0.5 * sigma^1.5 * eta *
        A_nom);
    d_ovr_sigma = interp1(F15(:,2),F15(:,1), F_15);
    F_1 = interp1(F10(:,1),F10(:,2), d_ovr_sigma);
    A_frac = eta * radi * sigma * F_1;

    fid = fopen ('out\A_temp.txt','a');
    fprintf(fid, '%e %e \n',t+delta,A_frac);
    fclose(fid);

end

t_resume = t+ delta
%long long long time
delta = 10;

if bond_duration > 1000*delta
    t_stop = 1000*delta;
else
    t_stop = bond_duration;
end

for t=t_resume:delta:t_stop

    L_relax = B*E_young*(pressure/A_frac)^n * A_nom * A_frac * delta;

    L_old = L_old + L_relax;

```

```

F_15 = L_old / ((4/3) * E_young * radi^0.5 * sigma^1.5 * eta *
    A_nom);
d_ovr_sigma = interp1(F15(:,2),F15(:,1), F_15);
F_1 = interp1(F10(:,1),F10(:,2), d_ovr_sigma);
A_frac = eta * radi * sigma * F_1;

fid = fopen ('out\A_temp.txt','a');
fprintf(fid, '%e %e \n',t+delta,A_frac);
fclose(fid);

end

% X = textread('out\A_temp.txt', '', 'delimiter', ' ', 'emptyvalue', NaN);
% plot(X(:,1),X(:,2))

```

A.1.2 Code listing to generate F15.txt

```

%this code to calculate integral F1.5

a = 0 ; % set lower limit of integration,
% also value for x
x_top = 20 ; % top value for x
b = 20; % set upper limit for the integration,
% b=10 gives pretty close value with
% the table on Abramowitz
n = 1.5; % integral power

fid = fopen('out\F15.txt','w');

for x=a:0.1:x_top
    x

    f = @(t) (1/(2*pi)^0.5)*(t-x)^n*exp(-t^2/2);
    dA=0;
    delta = 0.001;
    for t = x:delta:b
        dA = dA + (f(t)+ f(t+delta))* delta/2;
    end
    dA
    fprintf(fid,'%f %e \n', x,dA);

end

fclose(fid)

```

A.1.3 Code listing to generate F10.txt

```

%this code to calculate integral F1.0

a = 0 ; % set lower limit of integration,
% also value for x
x_top = 20 ; % top value for x

```

```

b = 20; % set upper limit for the integration,
        % b=10 gives pretty close value with
        % the table on Abramowitz
n = 1.0; % integral power

fid = fopen('out\F10.txt','w');

for x=a:0.1:x_top
    x

    f = @(t) (1/(2*pi)^0.5)*(t-x)^n*exp(-t^2/2);
    dA=0;
    delta = 0.001;
    for t = x:delta:b
        dA = dA + (f(t)+ f(t+delta))* delta/2;
    end
    dA
    fprintf(fid,'%f %e \n', x,dA);

end

fclose(fid)

```

A.1.4 Example of F10.txt

```

0.000000 3.989422e-001
1.000000 8.331545e-002
2.000000 8.490698e-003
3.000000 3.821539e-004
4.000000 7.145247e-006
5.000000 5.346153e-008

```

A.2 Surface Diffusion contribution to True Contact Area

Below is the MATLABTM code used to execute a simulation on the effect of surface diffusion on true contact area as developed in Chapter 4. The script are called `contact_growth.m`. The calculation results dumped as a textfile in a subdirectory “out” in format of time (in secon) and fraction of bonded area for the first column and second column, respectively.

A.2.1 Code Listing For `contact_growth.m`

```

%this code time dependent surface diffusion on rough surface contact

Do_s = 7e-6;
Ea = 79.1e3/6.02e23; % change from J/mol to J
surface_energy = 1.75; % J/m2
omega = 1.18e-29; % in meter cubic
v = omega^(-2/3); % based on nichols 1965
boltz = 1.3806504e-23; % in J/K, 8.617343 in eV/K
Tempe = 0; % in degree C

D_s = Do_s*exp(-Ea/(boltz*(Tempe+273)));

```

```

B = D_s * surface_energy * omega^2 * v / (boltz * (Tempe+273));
radi = 50e-9;
sigma = 2e-9;
eta = 1e14;
d_ovr_sigma = 4 ;           % set lower limit of integration, also value for x
x_top = 10 ;                 % top value for x, suppose to be infinity,
                             % but 10 gives close enough
                             % approximation with abramowitch

dF_g = 0;

fid = fopen([ 'out\F_g-' num2str(Tempe) 'DegC-roughness3.txt'], 'w' );
for duration = 0:100:10000
    f = @(x) ((224*B*duration)/(sigma^3.5 * radi^0.5) + ...
        ( 2*x - d_ovr_sigma )^3.5 )^(2/7) * (1/(2*pi)^0.5)*exp(-x^2/2);
    dF_g = 0;
    for x=d_ovr_sigma:0.001:x_top
        dF_g = dF_g + (f(x)+ f(x+0.01))* 0.001/2;
    end
    A_frac = eta*pi*radi*sigma*dF_g; %F_g is the complex integral, defined above
    fprintf(fid,'%f %e \n' , duration ,A_frac);
end

fclose(fid);

```

A.3 Electromigration

Below are the MATLABTM scripts and supporting files that used to simulate contact resistance reduction during current stressing Chapter 4. The model is used to calculate the true contact area increament as a function of surface roughness (represent as η , R , and σ_s), bonding duration, temperature, and applied current.

The model consists of two .m files and .dat files:

- Emcontact.m - scripts that take all the necessary constant for the simulation and approximation of multiple asperity contact growth as given by equation (4.43) and then proceed to calculate the evolution of the contact resistance value as given by equation (4.44).
- Emcontact_ramp_current.m - is a modification from Emcontact.m script to simulate contacting interface under increasing current stressing.
- wexler_script.m - scripts that calculate the $\Gamma(l/x)$ value in equation (4.38).
- F_0.m - contains function to automate the calculation of $N_{ti} = \int_d^\infty f(z) dz$.
- F00.dat - a two column file tha acts as a look-up table for integral $\int_d^\infty f(z) dz$.
- wexler.dat - a two column lookup table for value of $\Gamma(K)$ as given in [108].

A.3.1 Code Listing for Emcontact.m

```
meanfreepath = 38.7e-9;
radi = 50e-9;
sigma = 2e-9;
eta = 1e12;
rho = 1.7e-8;
An = 1e-8; %meter-square
Ea = 0.58; % Nichols 1968
k_boltz = 8.617342301e-5; % in eV per kelvin
T = 300; %temperature
D_o = 1e7%7e-6;
Diff = D_o*exp(-Ea/(k_boltz*T));
Zeff = 1;
elec = 1.6021764623e-19; %electron charge
omega = 1.18e-29;
d=3e-9;

stress_time = 1e3; %stressing time in secon
W = textread('wexler.dat', '', 'delimiter', ' ', 'emptyvalue', NaN);
I_curr = 1; % Ampere

%Determine Z1 to Z10

%setting asperity group
z1 = d + sigma/1000;
z2 = d + sigma/10;
z3 = d + 2*sigma/10;
z4 = d + 3*sigma/10;
z5 = d + 4*sigma/10;
z6 = d + 5*sigma/10;
z7 = d + 6*sigma/10;
z8 = d + 7*sigma/10;
z9 = d + 8*sigma/10;
z10 = d + 9*sigma/10;

%counting numbers of asperity group
n_z1 = An * eta * ( F_0(z1, sigma) - F_0(z2, sigma) );
n_z2 = An * eta * ( F_0(z2, sigma) - F_0(z3, sigma) );
n_z3 = An * eta * ( F_0(z3, sigma) - F_0(z4, sigma) );
n_z4 = An * eta * ( F_0(z4, sigma) - F_0(z5, sigma) );
n_z5 = An * eta * ( F_0(z5, sigma) - F_0(z6, sigma) );
n_z6 = An * eta * ( F_0(z6, sigma) - F_0(z7, sigma) );
n_z7 = An * eta * ( F_0(z7, sigma) - F_0(z8, sigma) );
n_z8 = An * eta * ( F_0(z8, sigma) - F_0(z9, sigma) );
n_z9 = An * eta * ( F_0(z9, sigma) - F_0(z10, sigma) );
n_z10 = An * eta * ( F_0(z10, sigma) - F_0(z10 + sigma/10, sigma) );

%initial radius of each asperity group
x_z1 =sqrt(radi*(z1-d));
x_z2 =sqrt(radi*(z2-d));
x_z3 =sqrt(radi*(z3-d));
x_z4 =sqrt(radi*(z4-d));
x_z5 =sqrt(radi*(z5-d));
x_z6 =sqrt(radi*(z6-d));
x_z7 =sqrt(radi*(z7-d));
x_z8 =sqrt(radi*(z8-d));
x_z9 =sqrt(radi*(z9-d));
x_z10 =sqrt(radi*(z10-d));

%contact area of each asperity group
A_z1 = An*n_z1*pi*x_z1^2;
A_z2 = An*n_z2*pi*x_z2^2;
A_z3 = An*n_z3*pi*x_z3^2;
A_z4 = An*n_z4*pi*x_z4^2;
A_z5 = An*n_z5*pi*x_z5^2;
A_z6 = An*n_z6*pi*x_z6^2;
A_z7 = An*n_z7*pi*x_z7^2;
A_z8 = An*n_z8*pi*x_z8^2;
A_z9 = An*n_z9*pi*x_z9^2;
A_z10 = An*n_z10*pi*x_z10^2;
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%Total Contact area
Atot = A_z1+A_z2+A_z3+A_z4+A_z5+A_z6+A_z7+A_z8+A_z9+A_z10;

%Current Density
%J=I_curr/Atot;

%Contact resistance for each individual asperity group

Kudson = (meanfreepath / x_z1); wexler_scrip ;

R_z1 = wexler * rho / (2*x_z1) + 4*meanfreepath*rho/(3*pi*x_z1^2);
Kudson = (meanfreepath / x_z2); wexler_scrip ;

R_z2 = wexler * rho / (2*x_z2) + 4*meanfreepath*rho/(3*pi*x_z2^2);
Kudson = (meanfreepath / x_z3); wexler_scrip ;

R_z3 = wexler * rho / (2*x_z3) + 4*meanfreepath*rho/(3*pi*x_z3^2);
Kudson = (meanfreepath / x_z4); wexler_scrip ;

R_z4 = wexler * rho / (2*x_z4) + 4*meanfreepath*rho/(3*pi*x_z4^2);
Kudson = (meanfreepath / x_z5); wexler_scrip ;

R_z5 = wexler * rho / (2*x_z5) + 4*meanfreepath*rho/(3*pi*x_z5^2);
Kudson = (meanfreepath / x_z6); wexler_scrip ;

R_z6 = wexler * rho / (2*x_z6) + 4*meanfreepath*rho/(3*pi*x_z6^2);
Kudson = (meanfreepath / x_z7); wexler_scrip ;

R_z7 = wexler * rho / (2*x_z7) + 4*meanfreepath*rho/(3*pi*x_z7^2);
Kudson = (meanfreepath / x_z8); wexler_scrip ;

R_z8 = wexler * rho / (2*x_z8) + 4*meanfreepath*rho/(3*pi*x_z8^2);
Kudson = (meanfreepath / x_z9); wexler_scrip ;

R_z9 = wexler * rho / (2*x_z9) + 4*meanfreepath*rho/(3*pi*x_z9^2);
Kudson = (meanfreepath / x_z10); wexler_scrip ;

R_z10 = wexler * rho / (2*x_z10) + 4*meanfreepath*rho/(3*pi*x_z10^2);

Conduc_tot = n_z1/R_z1 + n_z2/R_z2 + n_z3/R_z3 + n_z4/R_z4 + n_z5/R_z5 ...
+ n_z6/R_z6 + n_z7/R_z7 + n_z8/R_z8 + n_z9/R_z9 + n_z10/R_z10;

Contact_res = 1/Conduc_tot;

t=0;
fid = fopen('out/em-contact-v2.txt', 'w');
fprintf(fid,'%e %e %e \n', t, Contact_res*An, Atot/An );

%time, specific resistance, fraction of true contact,
fclose(fid);

hold on;
plot(t,Contact_res*An, 'or');
drawnow;

%Update Contact radius===== start of
%loop here
delta_time = 1;
for k = 0:delta_time:stress_time

    t = t + delta_time;
    x_z1 = ( x_z1^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...

        * rho * I_curr * delta_time * x_z1^2 * pi / ...

        (k_boltz * T * pi * radi * Atot) )^(1/3);
    x_z2 = ( x_z2^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...

        * rho * I_curr * delta_time * x_z2^2 * pi / ...

        (k_boltz * T * pi * radi * Atot) )^(1/3);
    x_z3 = ( x_z3^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...

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* rho * I_curr * delta_time * x_z3^2 * pi / ...

(k_boltz * T * pi * radi * Atot) ^ (1/3);
x_z4 = ( x_z4^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...

* rho * I_curr * delta_time * x_z4^2 * pi / ...

(k_boltz * T * pi * radi * Atot) ^ (1/3);
x_z5 = ( x_z5^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...

* rho * I_curr * delta_time * x_z5^2 * pi / ...

(k_boltz * T * pi * radi * Atot) ^ (1/3);
x_z6 = ( x_z6^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...

* rho * I_curr * delta_time * x_z6^2 * pi / ...

(k_boltz * T * pi * radi * Atot) ^ (1/3);
x_z7 = ( x_z7^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...

* rho * I_curr * delta_time * x_z7^2 * pi / ...

(k_boltz * T * pi * radi * Atot) ^ (1/3);
x_z8 = ( x_z8^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...

* rho * I_curr * delta_time * x_z8^2 * pi / ...

(k_boltz * T * pi * radi * Atot) ^ (1/3);
x_z9 = ( x_z9^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...

* rho * I_curr * delta_time * x_z9^2 * pi / ...

(k_boltz * T * pi * radi * Atot) ^ (1/3);
x_z10 = ( x_z10^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...

* rho * I_curr * delta_time * x_z10^2 * pi / ...

(k_boltz * T * pi * radi * Atot) ^ (1/3);

%Update contact resistance
Kudson = (meanfreepath / x_z1); wexler_scrip ;

R_z1 = wexler * rho / (2*x_z1) + 4*meanfreepath*rho/(3*pi*x_z1^2);
Kudson = (meanfreepath / x_z2); wexler_scrip ;

R_z2 = wexler * rho / (2*x_z2) + 4*meanfreepath*rho/(3*pi*x_z2^2);
Kudson = (meanfreepath / x_z3); wexler_scrip ;

R_z3 = wexler * rho / (2*x_z3) + 4*meanfreepath*rho/(3*pi*x_z3^2);
Kudson = (meanfreepath / x_z4); wexler_scrip ;

R_z4 = wexler * rho / (2*x_z4) + 4*meanfreepath*rho/(3*pi*x_z4^2);
Kudson = (meanfreepath / x_z5); wexler_scrip ;

R_z5 = wexler * rho / (2*x_z5) + 4*meanfreepath*rho/(3*pi*x_z5^2);
Kudson = (meanfreepath / x_z6); wexler_scrip ;

R_z6 = wexler * rho / (2*x_z6) + 4*meanfreepath*rho/(3*pi*x_z6^2);
Kudson = (meanfreepath / x_z7); wexler_scrip ;

R_z7 = wexler * rho / (2*x_z7) + 4*meanfreepath*rho/(3*pi*x_z7^2);
Kudson = (meanfreepath / x_z8); wexler_scrip ;

R_z8 = wexler * rho / (2*x_z8) + 4*meanfreepath*rho/(3*pi*x_z8^2);
Kudson = (meanfreepath / x_z9); wexler_scrip ;

R_z9 = wexler * rho / (2*x_z9) + 4*meanfreepath*rho/(3*pi*x_z9^2);
Kudson = (meanfreepath / x_z10); wexler_scrip ;

R_z10 = wexler * rho / (2*x_z10) + 4*meanfreepath*rho/(3*pi*x_z10^2);

Conduc_tot = n_z1/R_z1 + n_z2/R_z2 + n_z3/R_z3 + n_z4/R_z4 + n_z5/R_z5 ...

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        + n_z6/R_z6 + n_z7/R_z7 + n_z8/R_z8 + n_z9/R_z9 + + n_z10/R_z10;

Contact_res = 1/Conduc_tot;

t=t+delta_time
fid = fopen('out/em-contact-v2.txt', 'a');
fprintf(fid,'%e %e %e \n', t, Contact_res*An, Atot/An );
%time, specific resistance, fraction of true contact,
fclose(fid);

hold on;
plot(t,Contact_res*An, 'or');
drawnow;

%Update Area

Atot = An*n_z1*pi*x_z1^2 + ...
        An*n_z2*pi*x_z2^2 + ...
        An*n_z3*pi*x_z3^2 + ...
        An*n_z4*pi*x_z4^2 + ...
        An*n_z5*pi*x_z5^2 + ...
        An*n_z6*pi*x_z6^2 + ...
        An*n_z7*pi*x_z7^2 + ...
        An*n_z8*pi*x_z8^2 + ...
        An*n_z9*pi*x_z9^2 + ...
        An*n_z10*pi*x_z10^2;

end
%=====end of loop

```

A.3.2 Code Listing for Emcontact_ramp_current.m

```

meanfreepath = 38.7e-9;
radi = 50e-9;
sigma = 2e-9;
eta = 1e12;
rho = 1.7e-8;
An = 1e-8; %meter-square
Ea = 0.58; % Nichols 1968
k_boltz = 8.617342301e-5; % in eV per kelvin
T = 300; %temperature
D_o = 1e7%7e-6;
Diff = D_o*exp(-Ea/(k_boltz*T));
Zeff = 1;
elec = 1.6021764623e-19; %electron charge
omega = 1.18e-29;
d=3e-9;

stress_time = 1e3; %stressing time in secon
W = textread('wexler.dat', '', 'delimiter',' ','emptyvalue',NaN);
I_curr = 1; % Ampere

%Determine Z1 to Z10

%setting asperity group
z1 = d + sigma/1000;
z2 = d + sigma/10;
z3 = d + 2*sigma/10;
z4 = d + 3*sigma/10;
z5 = d + 4*sigma/10;
z6 = d + 5*sigma/10;
z7 = d + 6*sigma/10;
z8 = d + 7*sigma/10;
z9 = d + 8*sigma/10;
z10 = d + 9*sigma/10;

%counting numbers of asperity group

```

```

n_z1 = An * eta * ( F_0(z1, sigma) - F_0(z2, sigma) );
n_z2 = An * eta * ( F_0(z2, sigma) - F_0(z3, sigma) );
n_z3 = An * eta * ( F_0(z3, sigma) - F_0(z4, sigma) );
n_z4 = An * eta * ( F_0(z4, sigma) - F_0(z5, sigma) );
n_z5 = An * eta * ( F_0(z5, sigma) - F_0(z6, sigma) );
n_z6 = An * eta * ( F_0(z6, sigma) - F_0(z7, sigma) );
n_z7 = An * eta * ( F_0(z7, sigma) - F_0(z8, sigma) );
n_z8 = An * eta * ( F_0(z8, sigma) - F_0(z9, sigma) );
n_z9 = An * eta * ( F_0(z9, sigma) - F_0(z10, sigma) );
n_z10 = An * eta * ( F_0(z10, sigma) - F_0(z10 + sigma/10, sigma) );

%initial radius of each asperity group
x_z1 =sqrt(radi*(z1-d));
x_z2 =sqrt(radi*(z2-d));
x_z3 =sqrt(radi*(z3-d));
x_z4 =sqrt(radi*(z4-d));
x_z5 =sqrt(radi*(z5-d));
x_z6 =sqrt(radi*(z6-d));
x_z7 =sqrt(radi*(z7-d));
x_z8 =sqrt(radi*(z8-d));
x_z9 =sqrt(radi*(z9-d));
x_z10 =sqrt(radi*(z10-d));

%contact area of each asperity group
A_z1 = An*n_z1*pi*x_z1^2;
A_z2 = An*n_z2*pi*x_z2^2;
A_z3 = An*n_z3*pi*x_z3^2;
A_z4 = An*n_z4*pi*x_z4^2;
A_z5 = An*n_z5*pi*x_z5^2;
A_z6 = An*n_z6*pi*x_z6^2;
A_z7 = An*n_z7*pi*x_z7^2;
A_z8 = An*n_z8*pi*x_z8^2;
A_z9 = An*n_z9*pi*x_z9^2;
A_z10 = An*n_z10*pi*x_z10^2;

%Total Contact area
Atot = A_z1+A_z2+A_z3+A_z4+A_z5+A_z6+A_z7+A_z8+A_z9+A_z10;

%Current Density
%J=I_curr/Atot;

%Contact resistance for each individual asperity group

Kudson = (meanfreepath / x_z1); wexler_scrip ;
R_z1 = wexler * rho / (2*x_z1) + 4*meanfreepath*rho/(3*pi*x_z1^2);
Kudson = (meanfreepath / x_z2); wexler_scrip ;
R_z2 = wexler * rho / (2*x_z2) + 4*meanfreepath*rho/(3*pi*x_z2^2);
Kudson = (meanfreepath / x_z3); wexler_scrip ;
R_z3 = wexler * rho / (2*x_z3) + 4*meanfreepath*rho/(3*pi*x_z3^2);
Kudson = (meanfreepath / x_z4); wexler_scrip ;
R_z4 = wexler * rho / (2*x_z4) + 4*meanfreepath*rho/(3*pi*x_z4^2);
Kudson = (meanfreepath / x_z5); wexler_scrip ;
R_z5 = wexler * rho / (2*x_z5) + 4*meanfreepath*rho/(3*pi*x_z5^2);
Kudson = (meanfreepath / x_z6); wexler_scrip ;
R_z6 = wexler * rho / (2*x_z6) + 4*meanfreepath*rho/(3*pi*x_z6^2);
Kudson = (meanfreepath / x_z7); wexler_scrip ;
R_z7 = wexler * rho / (2*x_z7) + 4*meanfreepath*rho/(3*pi*x_z7^2);
Kudson = (meanfreepath / x_z8); wexler_scrip ;
R_z8 = wexler * rho / (2*x_z8) + 4*meanfreepath*rho/(3*pi*x_z8^2);
Kudson = (meanfreepath / x_z9); wexler_scrip ;
R_z9 = wexler * rho / (2*x_z9) + 4*meanfreepath*rho/(3*pi*x_z9^2);
Kudson = (meanfreepath / x_z10); wexler_scrip ;
R_z10 = wexler * rho / (2*x_z10) + 4*meanfreepath*rho/(3*pi*x_z10^2);

Conduc_tot = n_z1/R_z1 + n_z2/R_z2 + n_z3/R_z3 + n_z4/R_z4 + n_z5/R_z5 ...
+ n_z6/R_z6 + n_z7/R_z7 + n_z8/R_z8 + n_z9/R_z9 + n_z10/R_z10;

Contact_res = 1/Conduc_tot;

t=0;
fid = fopen('out/em-contact-v2.txt', 'w');
fprintf(fid,'%e %e %e \n', t, Contact_res*An, Atot/An );
%time, specific resistance, fraction of true contact,

```

```

fclose(fid);

hold on;
plot(t,Contact_res*An, 'or');
drawnow;

%Update Contact radius===== start of
%loop here
delta_time = 1;
for k = 0:delta_time:stress_time

    t= t + delta_time;
    x_z1 = ( x_z1^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...
        * rho * I_curr * delta_time * x_z1^2 * pi / ...
        (k_boltz * T * pi * radi * Atot) )^(1/3);
    x_z2 = ( x_z2^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...
        * rho * I_curr * delta_time * x_z2^2 * pi / ...
        (k_boltz * T * pi * radi * Atot) )^(1/3);
    x_z3 = ( x_z3^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...
        * rho * I_curr * delta_time * x_z3^2 * pi / ...
        (k_boltz * T * pi * radi * Atot) )^(1/3);
    x_z4 = ( x_z4^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...
        * rho * I_curr * delta_time * x_z4^2 * pi / ...
        (k_boltz * T * pi * radi * Atot) )^(1/3);
    x_z5 = ( x_z5^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...
        * rho * I_curr * delta_time * x_z5^2 * pi / ...
        (k_boltz * T * pi * radi * Atot) )^(1/3);
    x_z6 = ( x_z6^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...
        * rho * I_curr * delta_time * x_z6^2 * pi / ...
        (k_boltz * T * pi * radi * Atot) )^(1/3);
    x_z7 = ( x_z7^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...
        * rho * I_curr * delta_time * x_z7^2 * pi / ...
        (k_boltz * T * pi * radi * Atot) )^(1/3);
    x_z8 = ( x_z8^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...
        * rho * I_curr * delta_time * x_z8^2 * pi / ...
        (k_boltz * T * pi * radi * Atot) )^(1/3);
    x_z9 = ( x_z9^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...
        * rho * I_curr * delta_time * x_z9^2 * pi / ...
        (k_boltz * T * pi * radi * Atot) )^(1/3);
    x_z10 = ( x_z10^3 + 8 * omega^(1/3)*Diff * Zeff * elec ...
        * rho * I_curr * delta_time * x_z10^2 * pi / ...
        (k_boltz * T * pi * radi * Atot) )^(1/3);

    %Update contact resistance

    Kudson = (meanfreepath / x_z1); wexler_scrip ;
    R_z1 = wexler * rho / (2*x_z1) + 4*meanfreepath*rho/(3*pi*x_z1^2);
    Kudson = (meanfreepath / x_z2); wexler_scrip ;
    R_z2 = wexler * rho / (2*x_z2) + 4*meanfreepath*rho/(3*pi*x_z2^2);
    Kudson = (meanfreepath / x_z3); wexler_scrip ;
    R_z3 = wexler * rho / (2*x_z3) + 4*meanfreepath*rho/(3*pi*x_z3^2);
    Kudson = (meanfreepath / x_z4); wexler_scrip ;
    R_z4 = wexler * rho / (2*x_z4) + 4*meanfreepath*rho/(3*pi*x_z4^2);
    Kudson = (meanfreepath / x_z5); wexler_scrip ;
    R_z5 = wexler * rho / (2*x_z5) + 4*meanfreepath*rho/(3*pi*x_z5^2);
    Kudson = (meanfreepath / x_z6); wexler_scrip ;
    R_z6 = wexler * rho / (2*x_z6) + 4*meanfreepath*rho/(3*pi*x_z6^2);
    Kudson = (meanfreepath / x_z7); wexler_scrip ;
    R_z7 = wexler * rho / (2*x_z7) + 4*meanfreepath*rho/(3*pi*x_z7^2);
    Kudson = (meanfreepath / x_z8); wexler_scrip ;
    R_z8 = wexler * rho / (2*x_z8) + 4*meanfreepath*rho/(3*pi*x_z8^2);
    Kudson = (meanfreepath / x_z9); wexler_scrip ;
    R_z9 = wexler * rho / (2*x_z9) + 4*meanfreepath*rho/(3*pi*x_z9^2);
    Kudson = (meanfreepath / x_z10); wexler_scrip ;
    R_z10 = wexler * rho / (2*x_z10) + 4*meanfreepath*rho/(3*pi*x_z10^2);

    Conduc_tot = n_z1/R_z1 + n_z2/R_z2 + n_z3/R_z3 + n_z4/R_z4 + n_z5/R_z5 ...
        + n_z6/R_z6 + n_z7/R_z7 + n_z8/R_z8 + n_z9/R_z9 + n_z10/R_z10;

    Contact_res = 1/Conduc_tot;

    t=t+delta_time
    fid = fopen('out/em-contact-v2.txt', 'a');

```

```

fprintf(fid,'%e %e %e \n', t, Contact_res*An, Atot/An );
%time, specific resistance, fraction of true contact,
fclose(fid);

hold on;
plot(t,Contact_res*An, 'or');
drawnow;

%Update Area

Atot = An*n_z1*pi*x_z1^2 + ...
      An*n_z2*pi*x_z2^2 + ...
      An*n_z3*pi*x_z3^2 + ...
      An*n_z4*pi*x_z4^2 + ...
      An*n_z5*pi*x_z5^2 + ...
      An*n_z6*pi*x_z6^2 + ...
      An*n_z7*pi*x_z7^2 + ...
      An*n_z8*pi*x_z8^2 + ...
      An*n_z9*pi*x_z9^2 + ...
      An*n_z10*pi*x_z10^2;

end
%=====end of loop

```

A.3.2.1 Code Listing for wexler_script.m

```

wexler = interp1(W(:,1),W(:,2),Kudson);
if Kudson < 0.016
    wexler = 1
end

if Kudson > 3
    wexler = 0.694;
end

```

A.3.2.2 Code Listing for F_0.m

```

function nZ = F_0(z , sigma)
    d_ovr_sigma = z/sigma;
    F = textread('F00.dat', ' ','delimiter',' ','emptyvalue',NaN);
    nZ = interp1(F(:,1),F(:,2),d_ovr_sigma);

```

A.3.2.3 Code Listing To Generate F00.dat

```

%this code to calculate integral F0.0

a = 0 ; % set lower limit of integration, also value for x
x_top = 20 ; % top value for x
b = 20; % set upper limit for the integration, b=10 gives pretty close value with
        % the table on Abramowitz
n = 0; % integral power

fid = fopen('out\F00.dat','w');

for x=a:0.1:x_top
    x

    f = @(t) (1/(2*pi)^0.5)*(t-x)^n*exp(-t^2/2);
    dA=0;

```

```

    delta = 0.001;
    for t = x:delta:b
        dA = dA + (f(t)+ f(t+delta))* delta/2;
    end
    dA
    fprintf(fid,'%f %e \n', x,dA);

end

fclose(fid)

```

A.3.2.4 Table for Wexler.dat

```

0.01544 0.9868
0.04347 0.9672
0.05119 0.9572
0.05839 0.9522
0.0955 0.9276
0.11076 0.91761
0.12846 0.908
0.15129 0.898
0.1784 0.88301
0.20323 0.8684
0.2357 0.85341
0.32733 0.82381
0.38599 0.8092
0.43972 0.79421
0.50997 0.7846
0.60059 0.7746
0.70822 0.75999
0.84803 0.745
1.01675 0.73501
1.17769 0.7254
1.36586 0.7104
1.6355 0.70541
1.99119 0.70079
2.38734 0.6958
2.85864 0.6958
3.53863 0.6908

```


Appendix B

Four Point Bending Test

B.1 Bonding Process

The four point bending test experiments was conducted by bonding 8" - blanket Cu wafers with CMP surface finish. The Cu depositions and surface roughness characterization was following the same methodology as discussed in Chapter 3. Wafer bonding conducted on commercial bonder EVG 520 as shown in figure B.1a. Since the alignment for blanket-blanket wafer bonding is not critical, wafer alignment was performed manually with respect to the wafer notch [75]. After alignment, the wafers were clamped together in a bond chuck, but separated by three 30 μm -thick metal flaps. The aligned wafers were then transferred to an bond chamber, which was subjected to three pump-purge cycles in order to reduce the ambient oxygen amount.

(a)

(b)

Figure B.1: (a) EVG 520 wafer bonder, (b) Setup of the DISCO DAD651 automated dice saw

The chamber was pumped down to approximately 5×10^{-4} Torr followed by pre-programmed piston load. Bonding of identical wafers was carried out under a force of 2.5 kN at 250 °C, 300 °C, 350 °C and 400 °C in a vacuum condition of 1 mTorr, for 30 minutes. Bonded wafers were then annealed in N₂ ambient at their respective bonding temperatures for 30 minutes. The bonded wafers were diced into rectangular strips using DISCO DAD651 automated dice saw as shown in Figure B.1b. Wafers bonded at 250 °C, 300 °C and 350 °C were diced into dimensions of 30.31 mm $\times$ 5.85 mm. The total thickness of the bonded wafers was 1.46 mm. Figure B.2 shows the fabricated test samples. A notch was diced on every test sample prior to dicing by cutting into the top wafer, as close as possible to the bonded interface, without cutting into the bottom wafer. The test samples which remained after dicing were labeled numerically before the actual test was carried out.

Figure B.2: *Four point bend test structure*

B.2 Testing Procedure

Testing was carried out on an actuator-controlled test equipment with four-point bend test fixtures as shown in Figure B.3. The outer and inner loading points can be set to a maximum separation of 35 mm and 27 mm respectively. For this experiments, the outer and inner loading points were spaced at 25 mm and 17 mm apart respectively. The loading points are supported by steel pins of approximately 2 mm in diameter, rested on V-grove supports. As the test progressing, the system measures the amount of displacement and corresponding load simultaneously, to a maximum of 180 N. The system can be connected to any computer with installed data acquisition software DTSTM which records the displacement and load data.

Figure B.3: *Four Point Bend Tester*

Sometimes miss alignment in the four-point test fixture occurs when the loadings are not symmetrical about the notch on the sample, resulting in uneven loadings on both ends of the sample [91]. Uneven loading may cause crack initiation and propagation on one side, that is on the side where the loading is stronger. As results, there will be erroneous fracture toughness values. On the test fixture, there is an alignment mark as shown in Figure B.3. This alignment marker help ensure symmetrical application of load on both ends of the sample. Hence, any errors on the measured fracture toughness due to misalignment would be minimized. The test samples were stressed at a constant displacement rate of $0.5 \mu\text{m/s}$. The dimensions of the specimen such as thickness and width were measured with a digital micrometer. Physical dimensions of the sample and the critical load for delamination obtained from the test were substituted into equation (1.7) to calculate values for G_C .

B.3 Results and Discussion

Theoretically, the critical load for delamination P is obtained when the crack propagates at a constant velocity under a constant load as illustrated in the ideal case in Figure 1.11. The ideal load-displacement characteristic was usually not observed in this work. In most test, non-ideal behaviors as shown in Figure B.4a were observed and only few samples exhibit the ideal load displacement behavior as shown in Figure B.4c. For non-ideal case, the average of several load values is taken as the load P in equation (1.7). On another occasion, some of the samples showed a load

Figure B.4: Variation in load-displacement observed in the experiments

peak followed by a load minimum, upon which elastic loading resumed, as shown in Figure B.4b. The load peak probably corresponds to the load required to initiate the crack and the actual load for crack propagation could be lower. Hence, in these cases, the average between the load peak and load minimum was being used to calculate G_C . There were also samples exhibiting a continuous series of load peaks and load minimums and the calculations of G_C for these samples were based on the approximated average load, as shown in Figure B.4a.

There were cases that the samples exhibit only elastic loading behavior as shown in Figure B.4d. They represent failure of the specimen by crack propagation through the substrate. No G_C can be determined from such failure, as the crack propagated into the bulk Si substrate instead of delaminating at the bonded interface. Over-notching of the test samples and pre-existing delamination could possibly account for the failure. There are also samples which displayed several constant load regions, as shown in Figure B.4e. The first constant load was observed due to the delamination of one side of the sample while the second constant load region could correspond to the delamination of the other side. To avoid overestimated of bond strength, in our analysis, the first constant load region was taken as the delamination load in the calculation of G_C . General trend is observed that bonding strength increases as

Figure B.5: Four point bending measurement results

bonding temperature increased.

An interesting dicing yield results were observed due to the usage of reclaimed-wafer that are thinner than prime wafer. It was observed that there is a correlation between substrate thickness and the dicing yield were observed. Dicing yield refer to the number of chip survive the dicing process. Table B.1 shows dicing yield dependent on substrate thickness. The effect of the substrates thickness to the dicing yield can be utilized to improve the bonded wafers ability to survive the post bonding processing.

Table B.1: Substrate thickness dependent dicing yield

Condition	Wafer thickness (mm)		Thk Ratio	Dicing Yield (%)
	1	2		
2.5 kN 275°C	0.5675	0.598	0.949	13.19
2.5 kN 275°C	0.622	0.7255	0.857	80.55
2 kN 300°C	0.5985	0.7254	0.825	94.44
2 kN 300°C	0.7	0.7	1	66

The phenomenon can be explained in term of failure mode mixity of mode I (K_I) and mode II (K_{II}). Mode mixity commonly expressed in term of phase angle ψ as shown in equation (1.8). Tadepally and Turner [179] had reported that mode mixity depends on the substrate thickness ratio, where in turn mode mixity could effect

the measured bond toughness as shown in Figure B.6 [179].

Figure B.6: Bond toughness as function of mode mixity [179].

In our case, during wafer die saw process, the wafers are subjected to compressive as well as shear stress. Higher thickness ratio will increase phase angle of mode mixity, thus increase the bond toughness of the die. Higher bond toughness of the die will increase the chances to survive the dicing process. This observation can be easily explained in term of mode mixity of the fractured sample. During dicing process, wafer exposed to normal and tangential stress (shear) by the dicing blade. Tadepalli *et al.* [180] in thinner wafer will have lower shear stress component, will have higher bond toughness. Therefore thinner wafer have higher chances to survive die saw process.

Figure B.7: Experiment result of four point bending test superimposed with model prediction. Model prediction related to experimental result by the an optimized (least-square) proportional constant $K=1.62 \times 10^4$ J/m², represented by solid line.

Figure B.8: Proportional factor optimization (a) For chip-to-chip die shear test, (b) four-point-bend test on wafer level bonding.

Figure B.7 shows the experimental result on four point bending test superimposed with model prediction that have been developed in Chapter 3. Simulation result were first fitted by the closest proportional constant as determined by least-square method as shown in B.8b. Unlike the die shear test, there was no physical constant that can be used as starting reference for the proportional constant. A single optimized proportional constant fits to the experimental results well. However, the meaning of the large proportional constant need to be investigated further.

B.4 Summary

Bond strength characterization using four point bending test have been conducted. The experiment investigates the effect of bonding temperature to the bond integrity. The experiments is also intended to investigate the possibility of generalizing the thermcompression bonding model that have been developed in Chapter 3, i.e. die shear testing method into four point bending test. The result shows that the model prediction of true contact area A_c can be related to the measured energy release rate G_c with a single proportional factor K , which indicates that the model also applicable for the case of four point bending test.

The experiments also observed that bonding of thinner wafer has higher chance to survive die saw process. This phenomena is explainable in term of failure mode mixity of bonded wafer, that a thinner wafer will have lower shear stress component,

will have higher bond toughness. This results provide another method to improve the bonded wafers ability to withstand mechanical processing.

Appendix C

Integration and Derivation

In this part, several integration definitions that are used in the thesis are presented. Also detailed steps for integration is presented.

C.1 Integration of $\int \sin^4 \theta \partial \theta$

Integration of $\int \sin^4 \theta \partial \theta$ can be done by parts.

$$\int \sin^4 \theta \, d\theta = - \int \sin^3 \theta \, d(\cos \theta)$$

with substitution of $\sin \theta \, d\theta = -d(\cos \theta)$. Integrating by parts

$$\int U \, dV = UV - \int V \, dU$$

We define

$$U = \sin^3 \theta \longrightarrow dU = 3 \sin^2 \theta \cos \theta \, d\theta$$

$$dV = d(\cos \theta) \longrightarrow V = \cos \theta$$

thus

$$\begin{aligned}
\int \sin^4 \theta \, d\theta &= - \int \sin^3 \theta \, d(\cos \theta) \\
&= - \sin^3 \theta \cos \theta + \int \cos \theta \times 3 \sin^2 \theta \cos \theta \, d\theta \\
&= - \sin^3 \theta \cos \theta + \int 3 \cos^2 \theta \sin^2 \theta \, d\theta \\
&= - \sin^3 \theta \cos \theta + \int 3 (1 - \sin^2 \theta) \sin^2 \theta \, d\theta \\
&= - \sin^3 \theta \cos \theta + \int 3 \sin^2 \theta \, d\theta - \int 3 \sin^4 \theta \, d\theta
\end{aligned}$$

gathering the $\sin^4 \theta$ term

$$\begin{aligned}
\int \sin^4 \theta \, d\theta &= - \sin^3 \theta \cos \theta + \int 3 \sin^2 \theta \, d\theta - \int 3 \sin^4 \theta \, d\theta \\
4 \int \sin^4 \theta \, d\theta &= - \sin^3 \theta \cos \theta + 3 \int \sin^2 \theta \, d\theta
\end{aligned}$$

from [162] we have that

$$\int \sin^2 x \, dx = \frac{1}{2}x - \frac{1}{4} \sin 2x + C$$

thus

$$\begin{aligned}
4 \int \sin^4 \theta \, d\theta &= - \sin^3 \theta \cos \theta + 3 \int \sin^2 \theta \, d\theta \\
&= - \sin^3 \theta \cos \theta + 3 \left(\frac{1}{2}\theta - \frac{1}{4} \sin 2\theta + C \right) \\
&= - \sin^3 \theta \cos \theta + \frac{3}{2}\theta - \frac{3}{4} \sin 2\theta + C \\
\int \sin^4 \theta \, d\theta &= -\frac{1}{4} \sin^3 \theta \cos \theta + \frac{3}{8}\theta - \frac{3}{16} \sin 2\theta + C
\end{aligned}$$

C.2 Resonance Frequency Derivation

$$Z_{tot} = Z_{ext} + Z_c + R_{line} \tag{C.1}$$

where Z_{ext} is the impedance of the external component. With ω is the frequency of the AC source, Z_{ext} is given by

$$\frac{1}{Z_{ext}} = \frac{1}{R_{out}} + \frac{1}{R_{in} + j\omega L} \quad (C.2)$$

where $j = \sqrt{-1}$ and Z_c is the contact interface impedance and can be expressed as

$$\frac{1}{Z_c} = \frac{1}{R_c} + j\omega C_c \quad (C.3)$$

substituting equation (C.2) and equation (C.3) to equation (C.1) we have

$$Z_{tot} = \frac{R_{out}(R_{in} + j\omega L)}{R_{out} + R_{in} + j\omega L} + \frac{R_c}{1 + j\omega C_c R_c} + R_{line} \quad (C.4)$$

$$Z_{tot} = \frac{R_{out}(R_{in} + j\omega L) \times (R_{out} + R_{in} - j\omega L)}{(R_{out} + R_{in} + j\omega L) \times (R_{out} + R_{in} - j\omega L)} + \frac{R_c(1 + j\omega C_c R_c)}{(1 + j\omega C_c R_c) \times (1 - j\omega C_c R_c)} + R_{line}$$

$$Z_{tot} = \frac{(R_{in}R_{out}^2 + R_{in}^2R_{out} - j\omega LR_{in}R_{out} + j\omega LR_{in}R_{out} + \omega^2 L^2 R_{out} + j\omega LR_{out}^2)}{(R_{out} + R_{in})^2 + \omega^2 L^2} + \frac{R_c - j\omega C_c R_c^2}{1 + \omega^2 C_c^2 R_c^2} + R_{line} \quad (C.5)$$

$$Z_{tot} = \frac{(R_{in}R_{out}^2 + R_{in}^2R_{out} + \omega^2 L^2 R_{out} + j\omega LR_{out}^2)}{(R_{out} + R_{in})^2 + \omega^2 L^2} + \frac{R_c - j\omega C_c R_c^2}{1 + \omega^2 C_c^2 R_c^2} + R_{line} \quad (C.6)$$

At resonance frequency ω_{res} the circuit reactant (imaginary part of the impedance) goes to zero. Thus setting imaginary part of equation (C.6) to zero

$$\begin{aligned}
X &= \frac{j\omega LR_{out}^2}{(R_{out} + R_{in})^2 + \omega^2 L^2} + \frac{-j\omega C_c R_c^2}{1 + \omega^2 C_c^2 R_c^2} = 0 \\
0 &= j\omega LR_{out}^2 (1 + \omega^2 C_c^2 R_c^2) - j\omega C_c R_c^2 ((R_{out} + R_{in})^2 + \omega^2 L^2) \\
LR_{out}^2 (1 + \omega^2 C_c^2 R_c^2) &= C_c R_c^2 ((R_{out} + R_{in})^2 + \omega^2 L^2) \\
LR_{out}^2 + \omega^2 C_c^2 R_c^2 LR_{out}^2 &= C_c R_c^2 (R_{out} + R_{in})^2 + C_c R_c^2 \omega^2 L^2 \\
\omega^2 (C_c^2 R_c^2 LR_{out}^2 - C_c R_c^2 L^2) &= C_c R_c^2 (R_{out} + R_{in})^2 - LR_{out}^2 \\
\omega^2 &= \frac{C_c R_c^2 (R_{out} + R_{in})^2 - LR_{out}^2}{C_c^2 R_c^2 LR_{out}^2 - C_c R_c^2 L^2} \\
\omega_{res} &= \left[\frac{C_c R_c^2 (R_{out} + R_{in})^2 - LR_{out}^2}{C_c^2 R_c^2 LR_{out}^2 - C_c R_c^2 L^2} \right]^{0.5} \tag{C.7}
\end{aligned}$$

Appendix D

Supporting Simulations Results

Figure D.1(a), (b) and (c) illustrates the relation between d , A_c and $(A_n - A_c)/d$, respectively. A_c for varying d is estimated from equation (1.15). Figure D.1(a) shows that d decreases faster compared to $(A_n - A_c)$ which is shown in Figure D.1(b). This results in an increase in $(A_n - A_c)/d$ with A_c as shown in Figure D.1(c). These relationship have the implication that contact capacitance increase with A_c , as defined by equation (2.3) with A_c . An increase in A_c is followed by a decrease in $(A_n - A_c)$, and is associated with a decrease in d . Since d decreases faster than $(A_n - A_c)$, the proportional factor of $(A_n - A_c)/d$ in equation (2.3) increases with A_c , thus contact capacitance increases with A_c .

Figure D.1: Relation of d , $A_n - A_c$, $A_n - A_c/d$ and with respect to A_c . (a) d versus A_c , (b) versus A_c , (c) $A_n - A_c/d$ versus A_c

Appendix E

Thermocompression in Silver-Indium System

E.1 Overview

Solid-liquid interdiffusion bonding consists of a multilayer of high-melting and low-melting materials to form a joint. Bonding is usually carried out at temperatures above the melting point of the low-melting material, during which the low-melting material is gradually consumed and resulted in a micro-joint containing only inter-metallic compounds. Through proper control of the multilayer film thickness and processing conditions, it is possible to form a joint free of the low-melting material [181].

Figure E.1: Ag-In Phase Diagram. Re-drawn from ASM Handbook Volum 3 [182].

Indium (In) based solders are attractive for low temperature bonding due to their low melting temperatures. In most cases, In reacts easily with a higher melting counterpart such as Cu, Au or Ag, to form a wide variety of intermetallic compounds (IMC). The resulting IMCs most of the time are having high melting temperatures. A high interdiffusion rate of In and noble metal system, intermetallic compound (IMC) formation have been reported even occur at ambient temperature [183–186]. A quick reference to Ag-In phase diagram, as shown in Figure E.1 the solid solubility of In in Ag is much higher (approximately 20 at.% In in Ag) than that of Ag in In (<1 at.% Ag in In). At temperatures between the melting points of In (156.7°C) and Ag (961.9°C), solid Ag is dissolved in the molten In to form a eutectic compound and different IMCs. The melting point of these compounds increases with the Ag content, i.e. eutectic (144°C) $<$ AgIn_2 (166°C) $<$ γ (300°C) $<$ ξ (670°C) $<$ β (695°C) [182, 187].

In the mid-nineties, Roy and Sen assessed the contact and composite resistances to monitor the evolution of interfacial reaction at different temperatures [188]. Through these measurements, it was reported that the formation of AgIn_2 phase is a diffusion-controlled process with activation energy of 0.43 eV. Lee *et al.* proposed a two-stage bonding-annealing process of the Ag-In thin layers, which consist of a short duration exposure with temperatures slightly above 200°C , followed by a lengthy heat treatment under hydrogen environment below 150°C . The high re-melting temperature of the joint was produced by consuming all the In in the bonded couple to form an IMC phase of Ag_2In [184, 185]. Although the effects of bonding temperature and time have been investigated extensively [188, 189] so far, effect of pressure during bonding to IMC phase formation has. Bonding is usually carried out at low pressures [184, 185, 187–190]. However, as the bonding temperature becomes lower, the morphology of the matting solder surface becomes more important. Microscopically rough surface is unavoidable and causes the reduction in the true contact area between the mating couple. Application of load in the form of higher pressure during bonding helps to flatten the surface, and thus may improve the true

contact area [107,114,115]. Under thermocompression bonding, metallic bonds formation could take place easier as distance between the two substrates becomes so small. In such a close distance, surface could become energetic and coalesce in order to eliminate the interfacial energy.

In this chapter, intermetallics formation from low temperature thermocompression bonding of Ag-In system is investigated. The study interested on the effects of bonding parameters, especially the applied pressure in the formation of IMCs at the bonding interface. The results could provide an alternative method to produce high temperature joints other than the heat treatment method.

E.2 Experiments

The Ag-In multilayer structure for the low temperature bonding study is shown in Figure E.2. Side A consists of a 50 nm-thick SiO₂ as the top layer, 25 nm-thick Cr (to improve the adhesion), 800 nm-thick In and 100 nm-thick Ag layer in the rear. The Ag layer was used as an oxidation prevention layer, by reacting with In to form AgIn₂ during deposition [188]. Similarly, Side B consists of a 50 nm-thick SiO₂, followed by 30nm-thick Cr, 2.6 μ m-thick Ag and 30 nm-thick Au layers. The In layer on Side A is thin enough such that it will be fully consumed to form IMCs by Ag on side B during thermocompression bonding. Upon uniform distribution of In at the bonding layer, the overall composition is approximately 17 at.% In. In other words, the average atomic ratio of a homogeneous phase depends on the layer structure thickness ratio, which is Ag/In = 83/17 in our solder system. From previous literature, it was suggested that the thickness of In on Side A and Ag on Side B determines the final phase composition of the bonding couple [190].

The 50 nm-thick SiO₂ on both A and B were deposited by Plasma Enhanced Chemical Vapor Deposition (PECVD) at 300°C on a 200 mm bare silicon wafer. The metal film stack was deposited on separate wafers for sides A and B. This was done in a single evaporation step without breaking the vacuum (10^{-5} torrs) to prevent In oxidation. Next, pre-prepared wafers of both sides A and B were cut into squares of 5

Figure E.2: Multilayer bonding couple design, In-rich on side A and Ag-rich on side B.

mm $\times$ 5 mm. Thereafter, both sides were aligned and bonded at 180°C for varying time and pressure using a Suss FC150 flip chip bonder. Temperature was only applied when the target pressure had been achieved. The thermocompression cycle was completed by cooling down the bonder to room temperature while maintaining the applied pressure.

Figure E.3: EDX point array taken across bonding interfaces. The stars represent locations where EDX points were taken.

Several methods were used to characterize by bonded samples. Cross section elemental composition was characterized by Energy Dispersive X-Ray spectroscopy (EDX). Samples were mounted on epoxy resin and subsequently polished. Arrays of EDX spectrum were taken from Side B to Side A to measure the element composition as a function of various depths as shown in Figure E.3. X-Ray Diffraction (XRD) method was used to determine the exact phases that had formed under the various bonding conditions. Bonded samples were pulled apart by mechanical force to expose the bonded interface. X-ray diffraction spectrum was then obtained using the Bruker-General Area Detector Diffraction System (GADDS). Several selected samples were also characterized by Differential Scanning Calorimeter (DSC) to determine the melting temperature of the phase that had formed at different bonding

conditions.

E.3 Results

Figure E.4: As deposited film composition, side A is dominated by AgIn_2 with some unreacted In. Side B have no IMC formation with overlapping major Ag and minor Au peak.

It has been reported that Ag diffuses rapidly into In via an interstitial mechanism while In diffuses into Ag through grain boundaries and could forms AgIn_2 [189, 190]. Upon the film deposition, similar result had also observed that the In film at side A had start to react to form AgIn_2 with the thin Ag layer as shown in Figure E.4.

E.3.1 Effect of Bonding Duration to IMC Formation

Figure E.5: EDX cross-section scans from bonded couples at 1.4 MPa - 180°C and at different bonding time. Zero reference was taken from the Ag-Cr interface, where (a) 10 min-short bonding time, Ag had diffused further to side A comparing to In into side B; (b) 40 min-long bonding time, average composition of In in the Ag-In IMC saturates around 34 at.% In, close to composition of Ag_2In or Ag_9In_4 . Note also a pure Ag region in side B for both cases.

Figure E.5 shows the EDX scans of cross sectioned samples bonded at 1.4 MPa and 180°C at different durations (10 and 40 min). The dashed line on each of the plot indicates the original bonding interface where sides A and B initially met. The cross sections consist of pure Ag, Ag-rich and In-rich regions. It is also observed that Ag diffused further into the In-region for longer bonding time. The XRD analysis supports the observations that bonding couple is dominated by AgIn_2 phase for short bonding duration, and Ag_9In_4 for long bonding time on Side A as shown in Figure E.6.

Figure E.6: XRD surface scan from bonded couple at 1.4 MPa – 180°C at different bonding time. (a) side A: at short bonding time, simply not enough Ag to available, hence it form In-rich phase. However as longer bonding duration, more supply of Ag available to react with In and most likely to consume it entirely. (b) side B, the surface dominated by Ag-rich phase and Au-In phase as during bonding molten In react with Au to form AuIn_2 before any In supply can diffuse further to Ag-rich side.

Samples that were bonded under similar condition as Figure E.5a and Figure E.5b were prepared for XRD characterization. The bonded couple were pulled or sheared apart to expose the bonding interface. Figure E.6a and Figure E.6b shows the XRD data from side A and side B from separated chips pulled from bonded sample respectively. As shown in Figure E.6a where it was initially In-rich side, at long bonding time, majority of the phase are identified as Ag_9In_4 . Meanwhile, for short bonding time it was dominated by AgIn_2 . However, at side B where it was initially Ag-rich side as shown in Figure E.6b, only one IMC observed, i.e Ag_9In_4

E.3.2 Effect of Bonding Pressure to IMC Formation

To study the effect of bonding pressure on IMC formation, several samples were bonded at 180°C for 10 min with bond pressure varying from 1.0 MPa to 1.6 MPa. Cross sectional EDX analysis of the samples are shown in Figure E.7. It was observed that the depth of In diffusing from Side A (In-rich side) to Side B (Ag-rich side) becomes shorter as the applied bonding pressure increases. On the other hand, Ag diffusion from Side B to A seemed to be independent of the bond pressure. Although no 100% In region was found from the EDX analysis, XRD detected In phase on Side A at 1.0 and 1.2 MPa bond pressure besides AgIn_2 (Figure E.8). In-rich regions shown in Figure E.7a and Figure E.7b could be a mixture of unreacted In and AgIn_2 phases. On the other hand, the phase is dominated by Ag_9In_4 for bonding pressure of 1.6 MPa,.

Figure E.7: EDX cross-section scans from bonded couples at 180°C – 10 min and at different bonding pressure; (a) 1.0 MPa, (b) 1.2 MPa, (c) 1.4 MPa, (d) 1.6 MPa. Zero reference was taken from Ag-Cr interface

Figure E.8: Bonding pressure effect on the IMC formation for bonding at 180°C - 10 min, (a) on side A: Ag₉In₄ is the dominant phase as the bonding pressure increases. (b) on side B, consistent with side A, Ag₉In₄ is the dominant phase as the bonding pressure increases.

E.3.3 IMC Phase Stability

The IMC phase stability was studied by aging bonded couple (with bonding condition of 1.4 MPa and 180°C for 10 minutes) at 70°C. By aging the bonded couple, Ag and In atoms could gain energy to form more stable phase. Note that the aging temperature is lower compared to AgIn₂ transition temperature. Thus any phase transformation expected occur through solid state reaction. Figure E.9 shows the effect of aging to the IMC phase formation. Without aging, it was observed that side A (Figure E.9a), were dominated by AgIn₂. Samples with 17 and 30 hours aging at 70°C show the presence of single IMC phase of Ag₉In₄,

Figure E.9: Results of XRD scan of aged samples at 70°C versus various aging time, where these samples were bonded at 1.4 MPa - 180°C for 10 minutes. (a) side A: co-existed AgIn₂ and Ag₉In₄ in the samples with 30 hours aging treatment, while Ag₉In₄ is dominant IMC phase in the samples with 17 hours aging treatment; (b) side B: the Ag₉In₄ is preferred dominant IMC phase in all cases.

Figure E.10a shows the EDX result of a sample cross section bonded at 1.4 MPa – 10 mins – 180 °C with an additional aging at 70°C for 17 hours. It was observed that the cross section consists of pure Ag and Ag-rich regions. With no aging, Side A of the bonding couple is mostly dominated by AgIn_2 while samples of 17 hours aging at 70 °C contain only the IMC phase of Ag_9In_4 . With further aging up to 30 hours, AgIn_2 phase was detected again .

Figure E.10: (a) Results of EDX scans of aged samples at 70°C for 17 hours where it shows the preferred Ag-rich phase. (b) Results of EDX scans of aged samples at room temperature for six months compared with just bonded sample, where this samples were bonded at 1.4 MPa - 180°C - 10 min.

Figure E.10 shows the EDX result of another sample that was kept at room temperature for six months. It is also observed that the cross section consists of pure Ag region and Ag-rich region, similar to those aged at 70 °C for 17 hours. Figure E.11 shows the XRD data of a sample which underwent an additional six months of room temperature storage, exhibiting a coexistence of AgIn_2 and Ag_9In_4 phases.

Figure E.11: Results of XRD scan of aged samples at room temperature for six month, where these samples were bonded at 1.4 MPa - 180°C - 10 min.

From DSC characterization, the Ag_9In_4 phase has a re-melting temperature of

more than 400°C. Figure E.12 shows the comparison between the two DSC results. Fully AgIn₂ in Figure E.12a samples shows two distinct endothermic peaks at 145.10°C and 176.78°C. The first endothermic reaction is the melting of the mixture consist of residual In and AgIn₂ [191] mentioned as ϕ phase. The later peak corresponds to the peritectic decomposition of the ϕ phase according to the reaction of $\phi \longrightarrow \text{In}(\text{Ag})_1 + \gamma$ [191]. Whereas for sample that are fully Ag₉In₄ in E.12b there were no phase transition was observed. This results suggest, that the Ag₉In₄ phase is having melting temperature higher than 400°C. Base on phase diagram, Ag₉In₄ compositions is pretty close to γ phase (Ag₂In).

Figure E.12: DSC scan profile up to 400°C. (a) Side A of sample that bonded at 1.4 MPa-180°C for 10 minutes. (b) Ag₉In₄ on the side A, bonded at 1.4 MPa for 10 minutes with temperature of 180°C. Sample also annealed for 17 hours at 70°C

E.4 Discussions

From the result presented above, we deduce that there are several relationships between IMC formation and the bonding parameters. During the bonding process at 180°C, the In film melts while Ag remains as a solid and dissolves into the molten In. Since the solubility limit of Ag in In is low (<1 at.% Ag in In), further supply of Ag is expected to drive the formation of Ag-In IMC [182].

E.4.1 Effect of Bonding Time

The duration of bonding determines the IMC that will form through the super saturation of Ag in molten In. At temperatures above the In melting point, the melt erodes the solid Ag. Given sufficient bonding time, Ag dissolves in the molten

In and attains the solubility limit. Further supply of Ag would drive the formation of IMC that is preferred at the particular temperature. From the phase diagram, a Ag-rich IMC is the preferred phase at bonding temperature of 180 °C. Thus, the majority of the phases formed at long bonding time (40 min) is Ag_9In_4 . This is in agreement with an earlier published result in which a Ag-rich preferred phase was formed at higher annealing temperature over longer duration [190, 192].

On the other hand, for short bonding duration, some regions in the bonded couple may not exceed the Ag solubility limit at the particular bonding temperature. Thus no IMC formation can be initiated. This is especially true for regions that are relatively far from the Ag reservoir with insufficient time for In diffusion and Ag dissolution. However, as the temperature is being lowered (during cooling), the Ag become less soluble in In, and the extra Ag solute would eventually lead to the formation of an IMC. From Figure E.1, an In-rich AgIn_2 phase would tend to form first for liquid transition temperature lower than 166°C. AgIn_2 IMC was also detected for samples bonded for short bonding time (10 min), which may have formed during cooling.

E.4.2 Effect of Bonding Pressure

There are three factors that could drive a Ag-rich IMC phase formation at high pressure. First, there is a reduction in In supply as pressure increases. The reduction in In supply caused increase in melting temperature of pure In. The second factor, increase in pressure also decrease in the AgIn_2 to Ag_9In_4 transition temperature [193]. Finally, an increase in force with higher pressure that flattened more asperities on a rough surface, thus increasing contact between the two mating surfaces [112]. With assumption of true contact area proportional to the shear strength of bonding integrity, the final factor confirmed by the shear test results of bonded couple as shown in Figure E.13.

The applied pressure was found to change the melting temperature of the metal stack during the bonding process. In turn, changes in the pure melting temperature

Figure E.13: *Shear test*

of In would affect the quantity of the melt, thus affecting the reaction kinetics. The pressure dependent melting temperature of materials is thermodynamically defined in the Clapyeron equation [193],

$$T \propto T_1 \exp \left(\frac{\Delta V}{\Delta H} P \right) \quad (\text{E.1})$$

where T is the phase changes temperature, P is the pressure, T_1 is the phase transition temperature at standard pressure (1 atm), ΔH is the change in enthalpy of fusion in solid-liquid transition and ΔV is the change in system volume. ΔH is usually considered to be weakly dependent on pressure. ΔH and ΔV are both positive for solid-to-liquid transition. These positive parameters in the exponential factor of equation (E.1) translates to an increase in the transition temperature as the pressure increases. With the increase in In melting temperature, there would be less supply of molten In, leading to a reduction of solid-liquid reaction and In diffusion. Furthermore, as the supply of Ag is virtually unlimited, liquid In quickly become Ag-saturated which may initiate a Ag-rich IMC nucleation (Ag_9In_4).

Thus, with increasing bond pressure and decreasing melting temperature of pure In, only regions that are near the In-Ag interface are able form IMCs. If the In film is too thick, regions that are further from the bonding interface may only form an In-rich solid solution or even pure In, and a Ag-rich phases would form near the bonding interface. As shown in Figure E.7d, EDX confirms that high concentrations of In phase were detected at locations further from the bonding interface even as

the XRD characterization (Figure E.8) determines that a Ag-rich phase tends to dominate at high bonding pressure.

The second factor is the change in the AgIn_2 to Ag_9In_4 transition temperature. In Ag-In system bonding, AgIn_2 has a lower mass density (8.23 g/cm^3) than Ag_9In_4 (9.90 g/cm^3) which translates into a negative ΔV . From equation (E.1), the phase transition temperature from AgIn_2 to Ag_9In_4 will decrease as the bonding pressure increases.

From the perspective of contact mechanics, the application of pressure will flatten the asperities on rough surfaces, and lead to an increase in the contact area and diffusion paths between the two bonded couples. Both sides of the bonding couple are expected to be microscopically rough. At low bonding pressure, less force was applied to flatten the asperities, which resulted in a low contact area. Conversely at higher bonding pressure, the contact area would be higher and improve the diffusion paths for In and Ag inter-diffusion.

E.4.3 Effect of Aging

Post-treatment aging process allows a system to obtain its most stable phase formation. Unlike bonding process, all reactions during aging are controlled by solid state diffusion. During the initial bonding, molten In in contact with the Au layer on Side B forms a highly stable AgIn_2 phase which is unlikely to dissociate or further react with In or Ag, up to 300°C . However, this stability could also reduce the In and Ag inter-diffusion from Side A to B and vice versa, respectively. In diffusion is further inhibited due to the larger In atomic size as compared to Ag. Thus, with a larger flux of Ag from Side B into Side A, all the In will be converted into the a Ag-rich phase (Ag_9In_4) first.

According to T. H. Chuang *et. al.*, Ag_9In_4 is energetically unstable for long-term aging at temperature lower than 75°C . Thus, Ag_9In_4 tends to evolve back into AgIn_2 to maintain a lower energy state with sufficient supply of In [190]. As the supply of In in our specimens is limited, only a portion of the Ag_9In_4 phase is converted into

AgIn_2 . Hence as a compromise, the two phases of Ag_9In_4 and AgIn_2 co-exist and remain stable for a long duration, as demonstrated in our 6 month study at room temperature in E.11.

E.5 Conclusions

A low temperature soldering process can avoid the concern of residual stresses that is typically introduced by thermal expansion mismatch during the cooling step from a high temperature soldering process. Since the resulting joints need to withstand higher post-bonding temperature processing, a solder system that can form high temperature intermetallic compound (IMC) at the joint at low bonding temperature is required. We have studied pressure, temperature and bonding time parameters and their effects on the IMC formation in the Ag-In solder system. We observed that the bonding duration determines the supply of Ag in the molten state. For long bonding time, Ag reaches supersaturation in the In melt and drives the formation of a Ag-rich IMC phase. In contrary, an In-rich phase during cooling for short bonding durations. The results show that the bond condition of 180°C - 1.4 MPa – 40 min is sufficient to fully consume all the In so as to give the final major phase of Ag_9In_4 . Higher bonding pressure under solid-liquid reaction was also found to enhance the formation of Ag_9In_4 . Three factors that could drive a Ag-rich IMC phase formation at high pressure are proposed. They are (1) a reduction in In supply as pressure increases due to changes in the melting temperature of pure In, (2) a decrease in the AgIn_2 to Ag_9In_4 transition temperature as pressure increases, and (3) an additional applied force to flatten the asperities on a rough surface, thus creating more contact area between the two mating surfaces. This also implies that Ag_9In_4 can be obtained within a shorter duration at higher pressure as well. We have proved that the bonding pressure is an important factor that thus needs to be considered and optimized for low temperature solder bonding.

In conclusion, complete consumption of low melting temperature In to form a high melting temperature IMC phase, in this case Ag_9In_4 , can be achieved by two

major approaches. First of all, bonding at 180°C under pressure higher than 1.4 MPa with sufficient time can lead to Ag_9In_4 being the dominant phase. Secondly, a film thickness ratio $\text{Ag}/\text{In} = 83/17$, a joint that consists of a mixture of AgIn_2 and Ag_9In_4 phases can be converted into a joint Ag_9In_4 as dominant phase after long term room temperature storage and/or a few days of low temperature aging. These findings may lead to the formation of bonded joints with high temperature resistant IMCs at relatively low bonding process temperature for applications in IC and MEMS packaging.