Mechanics Aspects of Wafer Thermocompression Bonding

by

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Submitted to the Department of Materials Science and Engineering
in partial fulfillment of the requirements for the degree of

Master of Science in Materials Science and Engineering

at the

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

February 2005

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Abstract

Wafer-level, thermocompression bonding is a promising technique for microelectromechanical systems (MEMS) packaging. The process is a form of solid-state joining and requires the simultaneous application of temperature and pressure to wafers patterned with metallic thin films in order to bring the mating surfaces into atomic proximity. The quality of the resulting bond is critically dependent on the interaction between flatness deviations that range from wafer bow to surface roughness, the thin film properties and the process parameters and tooling used to achieve the bonds. Hitherto there has been limited modeling applied to understand the relative contributions of these effects.

This thesis addresses the above issue through the development of a mechanics-based framework that allows the effect of flatness deviations to be assessed for typical geometries and process conditions. The strain energy release rate associated with the elastic deformation required to overcome wafer bow is calculated. A contact yield criterion is used to examine the pressure and temperature conditions required to flatten surface roughness asperities in order to achieve bonding over the full apparent area. The results are compared to experimental data of bond yield and toughness obtained from four-point bend delamination testing, microscopic observations and measurements on the fractured surfaces.

Conclusions from the modeling and experiments indicate that wafer bow has negligible effect on determining the variability of bond quality and that the well-bonded area is increased with increasing bonding pressure. The enhanced understanding of the underlying deformation mechanisms allows for a better controlled trade-off between the bonding pressure and temperature.

Thesis Supervisor: S. Mark Spearing
Title: Professor of Aeronautics and Astronautics
Acknowledgements

This thesis would not have been possible without the help from many people and organizations. I will try to name them below. First of all, I would like to thank my advisor, Professor Mark Spearing, for his patient guidance and continuous support throughout the course of this work. Mark gave me the opportunity to explore a challenging research problem and at the same time he taught me the necessary approach to address it. Being my advisor has benefited my academic life in many ways. I would like to thank Professor Carl Thompson for serving as a reader for my thesis and for his thoughtful comments. I am also grateful to the rest of the MIT faculty whom I had the privilege to be a student for enriching my academic experience over the past two years.

The help and support of all the TELAC members is greatly appreciated. In particular, I would like to thank Dr. Kevin Turner and Dr. Christine Tsau for the valuable discussions we had as well as their suggestions. Furthermore, my experimental work at MIT would have been less rewarding without Kevin’s guidance and assistance. I am also grateful for the interaction I have had with fellow students and in particular my Greek colleagues as well as Ching Au, In-Suk Choi, George Pau, Georgios Constantinides and David Quinn.

I would like to express my gratitude to the Hellenic Air Force for awarding me the graduate fellowship that allowed me to pursue my education at MIT. Also, the experimental portion of this thesis was financially supported by the Singapore-MIT Alliance.

Finally, and most importantly, I thank my parents, brother and wife for their unconditional love and support.
# Contents

1 Introduction ........................................ 13
   1.1 Motivation: Wafer-Level Thermocompression Bonding ................. 13
   1.2 Objectives ............................................. 15
   1.3 Outline of the Thesis .................................... 16

2 Background ............................................. 18
   2.1 Aspects of Solid-State Bonding .................................. 18
      2.1.1 Fundamentals of Bonding Mechanisms .......................... 18
      2.1.2 Solid-State Bonding and Process Parameters .................. 19
   2.2 Wafer-Level Gold Thermocompression Bonding .......................... 21
      2.2.1 Introduction ........................................... 21
      2.2.2 Characterization of Wafer Thermocompression Bonding .......... 23
      2.2.3 Factors under Examination and Approach ....................... 26

3 Influence of Flatness Deviations on Bond Quality ....................... 29
   3.1 Wafer Geometry and Flatness Deviations ............................ 29
   3.2 Wafer Bow .................................................. 30
   3.3 Surface Roughness Effect ...................................... 33
      3.3.1 Topography Accommodation and Deformation Mechanisms ......... 35
      3.3.2 Plastic Deformation of Surface Asperities .................... 37
4 Experimental Characterization ................................................................. 40
  4.1 Thin Film Stress Measurement .......................................................... 40
  4.2 Bond Quality Measurements and Characterization .............................. 42
    4.2.1 Specimen Fabrication .................................................................. 44
    4.2.2 Four-Point Bend Delamination Mechanics .................................. 46
    4.2.3 Mechanical Testing and Microscopic Observations Procedure ...... 49

5 Results and Discussion ............................................................................. 52
  5.1 Gold Film Yield Stress .......................................................................... 52
  5.2 Bond Quality Results and Characterization ........................................ 54
    5.2.1 Load – Displacement Data and Interface Fracture Behavior ......... 54
    5.2.2 Bond Toughness .......................................................................... 57
    5.2.3 Microscopic Observations and Measurements ............................. 60

6 Conclusions and Recommendations .......................................................... 67
  6.1 Thesis Summary and Conclusions ....................................................... 67
  6.2 Recommendations for Future Work .................................................... 68

A Slip-Line Field Analysis ........................................................................... 71

B Specimen Fabrication Process Flow ......................................................... 75

Bibliography .................................................................................................... 77
List of Figures

1-1 Conventional die-level as compared to wafer-level bonding approach ........ 14

2-1 Mechanistic model for the generic diffusion bonding process .................. 20
2-2 Gold thermocompression technique for very large array bonding .............. 23
2-3 $G_{lc}$ for all process conditions (P, T) and t=10min as a function of (n/N) .... 24
2-4 $G_{lc}$ for various bonding times and P=30 MPa, T=300°C as a function of (n/N). 25
2-5 SEM images of fractured surfaces of a delaminated specimen .................... 26

3-1 Classification of the flatness types of deviations of concern ..................... 30
3-2 The deformation process of two initially bowed wafers into a bonded pair .......... 31
3-3 AFM images and line scan of a typical gold surface prior to bonding ............ 34
3-4 The deformation process for an array of idealized asperities ..................... 35
3-5 A typical deformation mechanism map for FCC metals ............................ 36

4-1 The scanning laser method for measuring substrate curvature .................... 41
4-2 Top view of orthogonal alignment and detail of bond pads ....................... 44
4-3 Schematic of the bonding process set-up ............................................. 45
4-4 IR imaging of a bonded wafer pair ..................................................... 46
4-5 The four-point bend configuration under loading ..................................... 47
4-6 Loading modes at the interface of a bilayer ........................................... 49

5-1 Stress evolution in a 0.5 μm Au film on a Si substrate during thermal cycling .. 53
5-2 A typical load-displacement curve from the four-point bend testing ............ 56
5-3 \( G_{ic} \) (all), for various pressure conditions and \( T=200^\circ C \) as a function of \( (n/N) \)  

5-4 \( G_{ic} \) (average per specimen), for various pressure conditions and \( T=200^\circ C \) as a function of \( (n/N) \)  

5-5 The fracture failure modes associated with the corresponding interfaces  

5-6 Micrographs showing variation in failure mode  

5-7 Micrographs showing variation in plastic deformation  

5-8 Bond yield for specimens bonded under varying pressure  

5-9 Surface roughness profiles for specimens bonded under varying pressure  

5-10 AFM images from fractured surfaces of specimens bonded under various pressure conditions showing the extent of plastic deformation  

A-1 A representative element of a slip-line field  

A-2 Slip-line field and deformation during the blunting of a plastic wedge  

A-3 The evolution of the flow coefficient during the blunting of the asperities  

B-1 Specimen fabrication process flow details
Chapter 1

Introduction

1.1 Motivation: Wafer-Level Thermocompression Bonding

Microelectromechanical systems (MEMS) packaging which includes assembly and testing has been identified to be the single most challenging and critical process in successful MEMS design and commercialization [1, 2, 3]. While in the integrated circuit (IC) industry, electronic packaging must provide reliable interconnections, MEMS packaging must account for a far more complex and diverse set of requirements. For instance, devices such as pressure sensors may require functionality in harsh environments with severe variations of temperature or while contacting corrosive media; other systems such as microfluidic devices pose much more stringent operational requirements, where a vacuum packaging is often a necessity [3]. As a consequence of these diverse requirements, standards for MEMS packaging are lacking and the packaging cost is responsible for a large fraction of the total production cost, reaching up to 95% [1, 4].

Wafer-level bonding offers an attractive option for MEMS packaging, as the cost of the process is distributed over the total number of devices on the wafer and at the same time, a controlled and protective environment is created, as illustrated in the schematic of Fig.1-1. Among the available wafer bonding methods, the most prominent is direct
bonding. Other, low temperature methods, such as anodic and eutectic bonding may offer advantages in some respects since diffusion in previously fabricated components is minimized, but these also have certain limitations. Gold thermocompression bonding is an alternative thin film, wafer-level joining technique, which may be performed at even lower temperatures than anodic and direct bonding and is particularly attractive since it does not involve a liquid phase or the application of high voltages. Moreover, its widespread use in die-bonding together with some highly desirable properties of gold, such as oxidation resistance and electrical conductivity, make gold thermocompression bonding a very promising technique for MEMS packaging [5]. This process is a form of solid-state joining and requires the simultaneous application of temperature and pressure to wafers patterned with metallic thin films in order to bring the mating surfaces into atomic proximity. The quality of the resulting bond is critically dependent on the interaction between flatness deviations that range from wafer bow to surface roughness, the thin film properties and the process parameters used to achieve the bonds. Hitherto there has been limited modeling applied to understand the relative contributions of these effects.

Figure 1-1: Conventional die-level bonding process flow (a) as compared to wafer-level bonding approach (b).
The feasibility of wafer-level, gold-gold thermocompression bonding, at relatively low temperature and pressure has been initially demonstrated by Tsau et al. [6]. In subsequent work [7], which is described in detail in section 2.2 of this thesis, Tsau performed a systematic characterization of this process for the effects of applied temperature, pressure and time. High bond toughness was obtained and the bond quality was found to improve with increases in the bond temperature and pressure. Nevertheless, large scatter in the bond toughness was found as plasticity was introduced into the system. Additional factors, not examined in that study, such as wafer bow and surface roughness were thought to cause the observed bond quality variability [7]. This variability has to be addressed to achieve the yield and repeatability standards required in manufacturing environments. Also, an enhanced understanding of the underlying mechanisms is necessary to allow for a controlled trade-off between the bonding pressure and temperature.

1.2 Objectives

The primary goal of this thesis is to investigate the effects of flatness deviations (wafer topography) on the resulting thermocompression bond quality. The two principal flatness deviations of concern in the current work are: 1) the overall wafer shape or bow and 2) the local surface roughness. This goal will be accomplished by modeling the deformation required to accommodate wafer topography and establish material continuity. Thus, the main objectives of this thesis are:

1) To identify the dominant deformation mechanisms that accommodate wafer topography with respect to the reference length scale and the typical process conditions.
2) To develop an analytical framework that allows the effect of wafer topography to be assessed for typical geometries and process conditions.
3) To complement modeling with experiments and microscopic observations in order to validate the suggested framework as well as to assess the relative contribution of the factors under examination.

1.3 Outline of the Thesis

This thesis addresses the objectives described in Section 1.2 and is organized into six chapters. Chapter 2 begins with a discussion of some fundamental aspects of solid-state joining and continues with a review of the previous studies on thermocompression bonding. Chapter 3 examines the wafer topography effects through the development of an analytical framework. Specifically, an interface fracture mechanics and a contact yield criterion are implemented to allow wafer bow and surface roughness effects to be assessed, respectively. Chapter 4 discusses the experimental approach which was used and also provides some theoretical background on the mechanical testing as well as the testing procedures. Chapter 5 reports and discusses the results of the current study on the effects of the wafer topography. Chapter 6 summarizes the thesis conclusions from the modeling and experiments and also provides suggestions for future work.
Chapter 2

Background

This chapter begins with a review of the fundamental aspects of solid-state joining: the bonding mechanism in its broadest context and the role of the process parameters with respect to the most notable process variations. Then, the discussion is focused on the thermocompression bonding technique and its application at the wafer-level. A review of the relevant literature and an assessment of the parameters believed to have an impact on the resulting bond are provided. This chapter concludes with the identification of the factors believed to contribute to bond quality variability which are investigated in the current thesis.

2.1 Aspects of Solid State Joining

2.1.1 Fundamentals of Bonding Mechanisms

In its broadest context, welding (bonding) is a process in which materials are brought together and caused to join through the formation of primary (and occasionally, secondary) chemical bonds, under the combined action of heat and pressure [8].

Thus, the key point is achieving material continuity by accommodating any physical disruption on an atomic scale in order to form chemical bonds. Given the context of the
current study, we will focus on the mechanisms for obtaining continuity between crystalline materials and metals, in particular. According to Granjon [9], there are three distinctive mechanisms by which this can be accomplished: 1) solid-phase plastic deformation, 2) diffusion and 3) melting and solidification. Through the application of the first mechanism, atoms comprising two pieces of crystalline metal can be brought together sufficiently close to ensure that bonds are established at their equilibrium spacing as the result of mutual attraction. On the other hand, extraneous atoms from contaminants (oxide, adsorbed gases etc) have to be excluded, by employing plastic deformation in the solid phase, with or without heat [10]. The second mechanism (diffusion) involves the transport of mass from one piece to another across an interface through atom movement and the third class of mechanisms involves gross mass and atom transport (via melting) as well as flow and microscopic transport (via solidification). The preceding three mechanisms contribute separately or in combination to the establishment of material continuity in every bonding process. All processes, in which bonds are obtained from solid-state contact between the materials, without melting, are called solid-state (non-fusion) bonding processes.

2.1.2 Solid-State Bonding and Processes Parameters

In solid state bonding, continuity is achieved by either plastic deformation or solid-state diffusion, under the simultaneous application of heat and pressure. The relative amounts of heat and pressure necessary to create bonds may vary from one extreme to the other. Very high heat and little or no pressure can produce bonds by relying on the high rate of diffusion at elevated temperatures (as in diffusion bonding). Little or no heat with very high pressures can produce bonds by forcing atoms together by plastic deformation on either the macroscopic scale (as in pressure welding) or on the microscopic scale (as in friction welding). Furthermore, when ceramics have to be bonded together or to metals, it is a common practice to introduce a metal interlayer between the components. This metal or alloy should be ductile and those used in practice are usually Al, Cu, Ag,
Au, Ni, Ti and Ni-Cr alloys [11]. The four most notable variations of solid-state (non-fusion) bonding process are: 1) pressure welding 2) roll bonding, 3) diffusion welding (bonding) and 4) hot isostatic pressing (HIP). While there are some differences regarding the procedure followed in these variations, the same underlying mechanism is relevant in all of them and may be illustrated by a three-step mechanistic model [12] shown schematically in Fig. 2-1. This process sequence consists of: (1) interface bond formation, (2) bond extension and (3) the subsequent shrinkage of the isolated pores (voids) that completes the bonding process.

Among the earlier described process variations, conventional diffusion welding (bonding) and hot isostatic pressing processes are accomplished at a temperature of at least 0.6 $T_M$ up to 0.9 $T_M$, where $T_M$ is the metal melting temperature in Kelvin, and are based on the diffusion capacity of materials [10, 11]. Among the critical process

![Figure 2-1](image)

**Figure 2-1** (After R.L. O’ Brien, [12]): Schematic of a three-step mechanistic model for the generic diffusion bonding process: (a) initial contact, (b) interface bond formation / misfit accommodation, (c) bond extension / pore elimination and (d) bonding complete.
parameters of temperature, pressure and time, temperature is by far the most important, provided there is enough pressure to cause contact between the mating surfaces. The reason for this critical dependence is that diffusion is controlled by an Arrhenius relationship with an exponential dependence on temperature. The use of diffusion bonding in this temperature regime in conjunction with superplastic forming of Ti alloys is considered as one of the most attractive solutions for the manufacture of complex structures and weight reduction in military aircraft [11].

On the other hand, there are variations of the basic process, such as deformation diffusion bonding and the cold (or warm) isostatic pressing which are accomplished with higher pressures and at much lower temperatures \( T < 0.4T_M \). In such cases the plastic deformation caused by the application of pressure is the principal deformation mechanism but the increased temperature allows the pressure requirement to be relaxed [10, 13]. Isostatic pressing, under various combinations of high pressure and temperature, has been extensively used for solid-state forming purposes and specifically for the compaction and/or sintering of fine powders [14], as well as the consolidation of metallic powders and metal matrix composites (MMC) [15].

2.2 Gold Thermocompression Bonding

2.2.1 Introduction

Thermocompression bonding is a form of solid-state joining that requires the simultaneous application of temperature and pressure in order to bring the mating surfaces into atomic proximity to form bonds. This joining technique is a variation of the generic diffusion bonding process and is essentially identical to the deformation diffusion bonding technique described in the previous section. Thermocompression has been a standard, die-level, packaging technique in microelectronics fabrication. Various ductile metals could be readily bonded under modest temperature and pressure. Nevertheless,
gold is the most commonly used material since it exhibits highly desirable properties such as oxidation and corrosion resistance, low yield point and electrical conductivity.

Several studies have been performed on the characterization of thermocompression for wire-bonding applications. The effect of surface contamination on thermocompression bonding of gold to gold-chromium metallization has been examined by Jellison [16]. The process was found to be highly temperature dependent when organic films were present. UV-ozone treatment was effective in removing organic contaminants from gold films. For bonds where metallic bond interfaces were discontinuous, post-heat treatment resulted in their growth [17]. It was also found that the bonding may be divided into two stages. The first stage resulted from the instantaneous mechanical disruption of barrier films by shear displacements. The second stage involved the growth of the metal-metal interfaces by a sintering process (see section 2.1.2). Under high applied pressure, the rate of the second stage exhibited little temperature dependence, indicative of a stress-assisted process [18]. In another work, Condra et al. [19] evaluated the contribution of plastic flow to gold-gold thermocompression bonding by studying the deformation properties of gold. In particular, the temperature dependence of the flow stress was determined. When deformed at temperatures higher than 300°C, work hardening was negligible. Also, dispersion of surface contaminants and exposure of clean metal were promoted [16]. Panousis and Kershner [20] studied the thermocompression bondability of gold films with respect to its thickness. The results showed that it was possible to obtain acceptable bondability for the thick gold films but that the bondability window was significantly smaller than that for thin films. This large difference in bondability was thought to be due to the observations that the thick films were less dense, rougher and had more surface contaminants.

When larger arrays of bonds became desirable, studies on bump-lead bonds began. Kim et al. [21] performed experiments on a 328-lead tape automated bonding device. The effects of thermocompression bonding parameters on the bump-pad adhesion were experimentally determined. Pressure and duration rather than temperature were found to be the most significant parameters that affect adhesion. A very large array, bonding
Figure 2-2 (After Furman and Mita [22]): Schematic of the two different joining test vehicles (TV) for the gold thermocompression technique developed for very large array bonding (1992).

Technique was initially reported by Furman and Mita [22]. With this technique, gold-gold thermocompression bonding has been extended from individual or tens of connections to tens of thousands of connections over a large area in a single joining cycle. A semi-isostatic press was developed for joining metal-metal or metal-polymer arrays onto silicon substrates, as shown in Fig 2-2. A pressure ranging from 0.7 MPa to 2.8 MPa was applied for nearly three hours, with one hour at the peak temperature of 375°C. Since the total bond area was only a fraction of the total pad area, the average pressure on the gold was greater than the pressure reported.

2.2.2 Characterization of Wafer Gold Thermocompression Bonding

Hitherto, limited work has been conducted to examine the feasibility and to characterize gold thermocompression bonding at the wafer-level. Drost et al. [23] carried out experiments to find appropriate parameters for the gold thermocompression bond, at both the wafer and chip-level. An applied pressure of approximately 0.05 MPa, at 400°C, for 1
min was found to be insufficient as inspection of the gold surface of the totally metallized wafers showed that no continuous bond was formed. Instead, a lot of small, local joints have been observed which were ascribed to the low pressure used [23]. The feasibility of wafer-level, gold-gold thermocompression bonding, at relatively low temperature and pressure, 300°C and 7 MPa, respectively has been initially demonstrated by Tsau et al. [6]. The toughness of the resulting bond has been shown to closely correlate with the fracture morphology. The critical strain energy release rate for the bonds ranged between 22 to 67 J/m² and was not shown to be strongly associated with the gold bond layer thickness in the thickness range studied (0.23 to 1.4 μm) [5]. In following work [7], Tsau performed a more systematic characterization of this process investigating the effects of

Figure 2-3 (After Tsau [7]): Bond toughness quantified in $G_s$, for all tested process conditions ($P$, $T$) and fixed $t=10$ min as a function of data point rank ($n/N$), in ascending order.
applied temperature (260 and 300°C), pressure (30 to 120 MPa) and time (2 to 90 min). High bond toughness was obtained and the bond quality was found to improve with increases in the bond temperature and pressure, as shown in Fig. 2-3. The experimental results showed that bonding can be achieved at 260°C, well within the acceptable range for packaging applications. Although bonds can be formed at pressures as low as 1.25 MPa, a pressure of 120 MPa was recommended to ensure the level of repeatability and yield desired in manufacturing environments. Bond toughness was not found to improve with increasing time. In fact, virtually no difference in bond toughness was observed regardless of whether the bond was performed in 2 or 90 min, as shown in Fig. 2-4.

Nevertheless, large scatter in the bond toughness was found as plasticity was introduced into the system. This was confirmed by the wide variation in the ductility observed in the fractured surfaces of delaminated specimens, as shown in Fig. 2-5 [5, 7].
Using finite element analysis, a correlation between the mask layout and the non-uniform pressure distribution was found. Additional factors such as wafer bow, wafer and gold thickness variations and surface roughness were also thought to induce the observed bond quality variability [7].

2.2.3 Factors under Examination and Approach

The recent work of Tsau et al. [5, 6, 7] demonstrated the feasibility of gold thermocompression bonding, at the wafer-level and identified several general trends, particularly the effect of pressure, temperature and time on the bond toughness. Nevertheless, the observed bond variability has to be addressed to achieve the yield and repeatability standards required in manufacturing environments.

There exist additional factors, such as flatness deviations that range from wafer bow to surface roughness which were not examined in earlier work and at the same time are believed to have a critical interaction with the material properties and process parameters.
used on the resulting bond quality. The strategy followed in the current work is to define clearly these different types of wafer topography and to model the deformation required to accommodate them during the bonding process. Thus, the basic mechanics of the process have to be studied to allow the relative contribution of the wafer topography to be assessed according to the reference length scale and the typical geometry, and process conditions used to achieve the bonds.

The earlier applications of solid-state bonding on the macroscopic scale and thermocompression bonding on the die-level reviewed in Sections 2.1.2 and 2.2.1, respectively, provide insight into the mechanics of the generic diffusion bonding process. Specifically, the in-depth understanding of: (1) the underlying physical mechanisms and (2) the role of the process parameters on the resulting bond quality together with the previous experimental data are essential to identify the dominant deformation mechanisms that accommodate the wafer topography on either the macroscopic, wafer-scale or on the local, nano-scale. However, the process window examined in earlier experiments [7] has to be extended to lower temperatures in order to validate the suggested mechanics modeling and to result in an enhanced understanding of the wafer topography interaction with the other process parameters.
Chapter 3

Influence of Flatness Deviations on Bond Quality

This chapter begins with an overview of the flatness deviations that exist across a typical silicon wafer which may affect bonding. Then, the wafer topography effects are examined through the development of an analytical framework. Specifically, an interface fracture mechanics and a contact yield criterion are implemented to allow wafer bow and surface roughness effects to be assessed, respectively.

3.1 Wafer Geometry and Flatness Deviations

There is a range of flatness deviations that exists across a typical silicon wafer which may be classified into different types according to the reference lateral length scale, as illustrated schematically in Figure 3-1. The two principal flatness deviations of concern in the present work are 1) the overall wafer shape or bow which is characterized by one or more radii of curvature, $\rho$, and 2) the local surface roughness which is characterized by nano-scale asperities. As shown in Figure 1, another way to characterize these different types of topography is their wavelength. Thus, while wafer bow spans the whole...
Figure 3-1: Classification of the relevant flatness deviations according to their lateral length scale and wavelength.

wafer diameter, the surface roughness has a wavelength six orders of magnitude smaller (on the order of tens of nanometers). The above classification of the flatness deviations has the primary goal of allowing the accommodation of each type to be modeled individually as the dominant deformation mechanism changes with respect to the reference length scale. At intermediate length scales (amplitudes and wavelengths), flatness deviation is characterized by the surface waviness, which is not thought to be as important a factor in determining bond quality and is not examined in the current thesis.

3.2 Wafer Bow

Wafer bow may be the result of either the manufacturing process, or the residual stress caused by the deposition of a thin film on the wafer, or both. The process of bonding two initially bowed wafers under the application of uniform pressure and temperature is
considered in this section and is illustrated schematically in Figure 3-2. As the process conditions are applied, the wafers are deformed into a common final curvature, $\kappa_f$. The mechanics-based framework employed here is based on the previous work of Turner and Spearing [24] on the modeling of direct wafer bonding. While the underlying physical mechanism in that technique is very different to that which operates in thermocompression bonding, the wafer deformation that occurs during the process is relevant in both of them. Given that, the ratio of film thickness to wafer thickness used in the typical thermocompression configuration, as well as in the current experiments is approximately $10^{-3}$, the deformation of the film may be ignored compared to the overall wafer pair deformation considered here. Thus, the wafer deformation can be determined using the classical thin plate theory for the case of an axisymmetric configuration. The governing differential equation for wafer deflection, denoted as $w$ in Figure 3-2, expressed here for conditions of uniform load $P$ and temperature $T$, is given by:

$$\frac{d}{dr} \left[ \frac{1}{r} \frac{d}{dr} \left( r \frac{dw}{dr} \right) \right] = \frac{Pr}{2D}$$

(3.1)

where $D$, is the wafer flexural rigidity, defined in terms of the wafer elastic properties $E$, $\nu$ and thickness $h$, as:
\[
D = \frac{Eh^3}{12(1-v^2)}
\] (3.2)

Taking into account the clamped configuration of the thermocompression bonding set-up, which is described in detail, in Section 4.2.1, we note that the deformation is subject to the following boundary conditions (at \(r = 0, b\)):

\[
w = 0, \quad \frac{dw}{dr} = 0
\] (3.3)

Then, the integration of Equation (3.1) and application of the boundary conditions of Equation (3.3) yields an expression for the pressure, \(P_b\), required to deform the wafers sufficiently in order to overcome the initial bow and to establish a macroscopic interface contact:

\[
P_b = \frac{16Eh^3\delta}{3b^4(1-v^2)}
\] (3.4)

where \(b\) is the wafer radius. Moreover, the resulting effective bending moments acting on each wafer, \(M_1\) and \(M_2\), assuming common elastic properties are determined by:

\[
M_1 = M_2 = \frac{P_b}{16}\left[(1+\nu)b^2 - (3+\nu)r^2\right]
\] (3.5)

\(M_1\) and \(M_2\) are equal since the two wafers are identical. Once the wafers are bonded and the external loads are released, these moments have to be balanced by another effective moment acting over the complete bonded pair [25], \(M_3\), in order that: \(M_1 + M_2 + M_3 = 0\)

Thus, \(M_3\), is given by:
Then, the elastic strain energy stored in the bonded pair, as an outcome of the above deformation, may be determined using the interface fracture mechanics framework for layered materials, developed by Suo and Hutchinson [26]. In the current work the two wafers have the same thickness and thus, the strain energy release rate, $G$, at the bonded interface, is determined by:

$$G = \frac{E h^3 (1+\nu)^2}{(1-\nu^2)} \frac{\delta^2}{b^4} \left[ 1 + N\left(\frac{r}{b}\right) \right]$$  \hspace{1cm} (3.7)$$

where $N(r/b)$, is a non-dimensional parameter. For the wafer material studied here, we use the effective isotropic elastic properties of (100) Si ($E=148\text{GPa}$ and $\nu=0.18$) for a 4 inch wafer with $525\mu\text{m}$ thickness and a $50\mu\text{m}$ bow in order to estimate $G$. For the given parameters, the portion of $G$, which is associated with the wafer bow accommodation, was found to be on the order of $10^{-2}$ J/m$^2$. This value compared to previous experimentally measured values of bond toughness [6, 7], is substantially lower, by up to four orders of magnitude and thus is unlikely to be the critical factor affecting bond quality, suggesting that surface roughness may be the dominant factor.

### 3.3 Surface roughness effect

As discussed in section 3.1, surface roughness is characterized by a lateral length scale and wavelength on the order of nanometers for the geometry and materials under examination. Figure 3-3 shows an AFM image and line scan of a typical gold surface prior to bonding, where the root mean square (RMS) roughness and wavelength were
Figure 3-3: AFM images of a 1x1μm² region of a deposited gold film surface (a, b) and surface profile plot (c). RMS roughness and wavelength were measured to be approximately 5 and 100 nm, respectively.

measured to be approximately 5 and 100 nm, respectively. This section focuses on assessing the effect of the surface height variations (see also surface asperities) on bonding by modeling the deformation required to accommodate them.
3.3.1 Topography Accommodation and Deformation Mechanisms

Achieving full interfacial contact between the two mating surfaces requires that local deformation overcome the surface roughness. The mechanistic model for the generic diffusion bonding process, discussed in section 2.1.2, provides the necessary insight for the modeling of the surface roughness accommodation process. Bonding is assumed to be between two blocks of the same purely ductile material whose mating surfaces are ideally clean and uncontaminated but covered by an array of identical small topographic features such as pyramids or spheres, whose peaks make the initial contact. The asperities of the two surfaces are considered to be aligned with respect to each other, which provides an upper bound on the actual required deformation. The deformation caused by the externally applied pressure flattens the peaks, creating isolated bonded neck areas that are progressively extended as the asperities are crushed and the ductile material is redistributed. This mechanism is illustrated schematically in Fig. 3-4.

The misfit due to the surface roughness has to be accommodated by elastic or plastic deformation or by creep and diffusion [27, 28, 29]. Generally, the dominant mechanisms of deformation change with respect to stress, temperature and strain rate [30]. This is clearly illustrated in Fig. 3-5, where a typical deformation mechanism for an FCC metal is shown. Here, the strain rate is plotted as a function of stress and temperature, for a fixed grain size. While the map shown is for fine-grained aluminum, the same basic trends are expected for gold. In general, as the grain size and film thickness are reduced, diffusion-controlled processes will become more significant. Plasticity, creep and

![Figure 3-4: (a) (After Pullen et al. [33]) The manner in which metal is redistributed during the crushing of the asperities. (b) The deformation process for an array of idealized asperities.](image-url)
Figure 3-5: (After H.J. Frost and M. F. Ashby [30]) A typical deformation mechanism map for an FCC metal. The regime in which time-independent plasticity is the dominant deformation mechanism is denoted with the dotted line. This map is only given as a general reference. While it is anticipated that the map for thin-film gold would be broadly similar, the small grain size of gold leads to the expansion of the diffusional-flow field to much lower homologous temperature.

diffusion mechanisms are dominant in different regimes [30]. As discussed in section 2.1.2, in solid-state bonding variations, the relative amounts of heat and pressure necessary to create bonds may vary from one extreme to the other. Nevertheless, for the current thermocompression process conditions, which are characterized by low to moderate temperatures \((T \leq 0.4T_M)\) and high stresses, well above the rate-independent yield stress \((\sigma \geq \sigma_y)\), plasticity is considered as the dominant deformation mechanism. Mass transport mechanisms such as creep and volume diffusion are considered to be very slow and have a negligible contribution, taking into account the typical bonding temperature and time, respectively. On the other hand, surface diffusion that occurs during the last phase of the bonding process (see 2.1.2) is relatively fast as compared to the typical bonding time range and consequently does not constitute a contributing factor.
to the bond quality variability. Previous experiments [7] confirm this assessment as they have shown no correlation between the bonding time ranged from 2 to 90 min and the bond quality in terms of toughness for the process conditions of interest as discussed in section 2.2.2. Also, the modeling of isostatic pressing processes at low temperatures \( T \leq 0.4T_m \) for metal consolidation applications have showed that the inelastic deformation at the contact of metals occurs predominantly by time-independent plasticity [15, 31].

### 3.3.2 Plastic Deformation of Surface Asperities

Previous studies of the plastic contact of rough surfaces have shown that the behavior of the surface asperities is not dependent on their exact geometry and is essentially the same whether they are modeled as pyramids, wedges, spheres or with an irregular shape [32, 33]. Moreover, those treatments were based on the concept that the total volume of metal is not changed by plastic deformation and that the displaced material when the asperities are crushed is redistributed as a uniform rise in the non-contacting surface, as shown in Fig. 3-4(a). The driving force for the growth of the bonded area and subsequent elimination of the non-contacting surface is the plastic deformation of the gold film which accommodates the externally applied pressure.

The complexity of the inelastic constitutive equations precludes analytical treatment for this group of problems. However, provided that the gold does not strain-harden to a large extent, it may be idealized as a rigid perfectly plastic solid which yields at a constant stress during the applied compression. Approximate solutions are then available with the use of slip-line field analysis for the blunting of perfectly plastic materials [28, 34] and result in the simple yield criterion (see Appendix A):

\[
\sigma_c \geq F \cdot \sigma_y
\]  

(3.8)
where $\sigma_c$ is the average normal contact stress (or pressure) at the interface, $\sigma$, the yield strength and $F$ the flow coefficient, usually treated as a constant and given by an upper bound of:

$$F = \frac{2 + \pi}{\sqrt{3}} = 2.97$$  \hfill (3.9)

where this value for $F$ was determined with the use of the Mises yield criterion. However, if appreciable work hardening does occur, this will increase further the pressure required to achieve full interfacial contact. This treatment has been previously applied to the modeling of the plastic deformation of asperities during solid-state forming processes [15, 35]. While the additional use of FEM analysis permits the examination of complexities such as the evolving asperity shape and the redistribution of stresses, as shown in Appendix A, Fig.A-3, the onset of fully plastic deformation which is relevant to the current modeling occurs at approximately the pressure plateau (three times the yield strength) that slip-line theory predicts [15, 36].
Chapter 4

Experimental Characterization

The objectives of the current experimental study are to obtain a basic understanding of the gold film mechanical behavior as well as to perform further bond quality characterization at a bonding temperature lower than the typical process regime already explored in Tsau’s studies [6, 7]. Thus, the gold film flow stress at the bonding temperature, and the interface fracture toughness and yield of the bonded surfaces have been measured. The ultimate goal is to complement the modeling study which was described in Chapter 3 and was based on existing experimental data with further measurements and observations in order to examine a wider range of parameters and to result in an enhanced understanding of the flatness deviations interaction with the other process parameters.

4.1 Thin Film Stress Measurement

The yield strength of the gold film at the bonding temperature is the most important material property in this modeling approach.

Yield strength may be obtained using a curvature measurement technique [37]. A film-substrate system is subjected to thermal cycling with the objective of inducing a
Figure 4-1 (After L.B. Freund and S. Suresh, [37]): Schematic of the scanning laser method for measuring substrate curvature.

thermal mismatch strain in the film. The radii of spherical curvature of the system are measured with respect to the applied temperature and the average film stress can be then obtained by use of the Stoney formula [38], [37]:

\[ K = \frac{6 \cdot f}{M_s \cdot h_s^2}, \quad f = \sigma_m \cdot h_f \quad (4.1) \]

Temperature-curvature measurements were performed using a Tencor FLX-2320 instrument by recording variations in the intensity of a laser beam originating from a fixed source and deflected from the surface of the wafer, as shown in Figure 4-1. The heating rate was approximately 5°C/min while the cooling rate was not actively controlled. Measurements indicated that the rate was 5°C/min initially, but then dropped to 2°C/min at 100°C, due to limited forced cooling. Since the latter phenomenon was suggested in the instrument manual [39], as well as in relevant literature [40, 41], an
additional number of measurements were selected and performed for the cooling cycle to compensate for the decreased rate. Thus, the gold film was thermally cycled between room temperature and 300°C in approximately three hours. Since the response in the first thermal cycle is complicated due to the multiple mechanisms involved (such as grain growth) and the following cycles are often different than the first but similar to each other [42], the film-substrate system was subjected to a second thermal cycle. Finally, another curvature measurement was performed at room temperature after removing the metal layer in order to account for the initial (inherent) film stress.

For the blanket gold film on the Si wafer, that was used here, the film stress can be calculated as follows [37]:

\[
\sigma_f = \frac{M_{Si}}{6} \cdot \frac{h^2_{Si}}{h_{Au}} \left( \frac{1}{\rho} - \frac{1}{\rho_o} \right),
\]

where \( M_{Si} \) is the biaxial elastic modulus of the \(<100>\) Si substrate, \( h_{Si} \) is the thickness of the Si substrate, \( h_{Au} \) is the thickness of the Au film, \( 1/\rho_o \) is the inherent curvature (before deposition) of the Si substrate and \( 1/\rho \) is the induced curvature of the Si substrate at the applied temperature.

### 4.2 Bond Quality Measurements and Characterization – An Interface Fracture Mechanics Approach

In order to further understand the interaction of the flatness deviations with the other process parameters on the resulting bond quality, an interface fracture toughness measurement technique has been used.

The fracture mechanics-based techniques, which have been developed to quantify bond strength, are primarily concerned with the measurement of the macroscopic, or effective, work of fracture per unit area required to separate the interface of interest [43]. This work may be quantified in terms of the interface strain energy release rate, \( G_I \) which
is a function of material properties such as the elastic-plastic constitutive behavior as well as mechanical parameters such as the loading mode mixture, \( \psi \) near to the crack tip. This quantity is equated to the effective interface fracture resistance (or toughness), \( \Gamma_i \), which provides a measure of the bonding energy at the interface. Contributions to \( \Gamma_i \) arise from the chemical bonding and other processes associated with the fracture mechanism including crack tip plasticity. Thus, the driving force for interfacial debonding is the strain energy release rate, \( G_i \) and this occurs when [44]:

\[
G_i \geq \Gamma_i \quad (4.3)
\]

In order to obtain the interface toughness, \( \Gamma_i \), the critical load, \( P_c \) that is just sufficient for crack growth has to be determined experimentally. Then, at this critical load, the corresponding critical strain energy release rate, \( G_{ic} \) equals the interface fracture energy, by definition:

\[
G_{ic} = \Gamma_i \quad (4.4)
\]

Therefore, by evaluating the critical driving force, \( G_{ic} \) the interface fracture energy is obtained.

Among the available methods to measure \( \Gamma_i \) [45, 46], the four-point bend delamination technique, proposed by Charalambides et al. [47], has been used in several recent studies. It has the advantage that the strain energy release rate for the interface crack is independent of the crack length, as long as the latter significantly exceeds the thickness of the upper layer of the beam [47]. This feature eliminates the difficulties involving crack length measurements and facilitates more accurate measurements of \( \Gamma_i \). The above technique which is employed in this experimental study has been previously used in the characterization of wafer gold thermocompression bonds [6] as well as wafer fusion bonds [48].
4.2.1 Specimen Fabrication

For the testing approach followed in the current work, four-point bend specimens were prepared by bonding a pair of gold coated silicon wafers and then dicing them into beam-like specimens. The fabrication process followed here was developed by Tsau et al. [5] and the main steps included silicon substrate preparation, gold deposition on the silicon substrates, thermocompression bonding and dicing for mechanical testing.

Each of the three bonding pairs that were used for specimen fabrication consisted of two 4-inch, n-type, silicon wafers with an average thickness of 525µm and 450µm respectively. The former wafer was single-side polished, while the latter was double-side polished (DSP). A 60µm deep and 500µm wide central notch was formed by KOH etching in the DSP wafer. Then, a 0.3µm thick silicon oxide diffusion barrier was formed by thermal oxidation at 1100°C and a 10nm titanium adhesion layer followed by a 0.5µm gold bonding layer was e-beam deposited onto both wafers. The gold was patterned using a lift-off mask technique that resulted in seven sets of 50µm by 60mm parallel gold

Figure 4-2: (a) Top view of orthogonal alignment. (b) Discrete bond pads were formed at the intersection of the gold lines (process developed by Tsau et al., [5]).
lines, with the pattern on one wafer rotated by 90° with respect to the other (orthogonal alignment). Thus, 49 groups of 50x50 μm², discrete square pads were formed, at the intersection of the gold lines¹, as shown in Figure 4-2. The use of this pattern achieves an increased applied pressure to the individual gold pads with a fixed bonding load. A schematic of the fabrication process flow details may be found in Appendix B.

The wafer pair was then aligned and clamped on a stainless steel chuck with the use of a quartz plate, as shown in Figure 4-3. Bonding was achieved with the use of a commercial Electronic Visions™ 501 bonder, under a nitrogen atmosphere. The temperature was progressively raised up to 200°C and three different loads of 1600, 3900 and 6400N were applied at each of the three different wafer pairs for a fixed time of 10 minutes. These loads resulted in nominal bonding pressures on the gold pads of 30, 73 and 120MPa respectively.

A first macroscopic inspection of the bonded wafer pairs was performed directly in the clean room, with the use of an IR Imaging System. Any unbonded region generates a

¹Among the 49 groups, there are 42 with 441 pads and 7 with 399 pads (the latter belong to the central trench area).
characteristic interference pattern, analogous to “Newton’s rings”. This was mostly observed near the edges of the wafer pairs, as shown in Figure 4.4(a).

Finally, to form the four-point bend testing specimens, the bonded wafers were first diced into 8mm wide strips and then a central notch was cut using a dicing saw, into the DSP wafer, as shown in Figures 4-4(b) and 4-5(b) respectively.

4.2.2 Four-Point Bend Delamination Mechanics

The strain energy release rate, $G$, of any linear elastic fracture system may be obtained by [49]:

$$G = \frac{P^2}{2b} \frac{dC}{d\alpha},$$

where $P$, is the applied load, $C$, the compliance of the system, $b$, the width of the sample and $2\alpha$, the length of the crack.
Figure 4-5: (a) Schematic of the four-point bend configuration under loading. (b) Micrograph of specimen showing the geometry of the notch in the DSP wafer.

Once the crack length is sufficiently longer than the thickness of the notched beam, the strain energy release rate is independent of crack length for a fixed moment [47]. In the four-point bend geometry, shown schematically in Figure 4-4(a), the bending moment per unit width, between the inner loading points, is \( M_b = Pl/2b \), where \( l \) is the spacing between the inner and outer loading points of the apparatus. If the same material is used in both layers, as in the current case, the strain energy release rate may be expressed as [47]:

\[
G = \frac{M_b^2(1 - v^2)}{2E} \left( \frac{1}{I_2} - \frac{1}{I_c} \right),
\]

(4.6)
where \( E \) and \( v \) are the beam (silicon) elastic modulus and Poisson's ratio, respectively, and \( I_2, I_c \) are the second moments of area per unit width of the unnotched and composite beams, respectively. Noting that the subscripts 1 and 2 refer to the notched and unnotched beam, respectively, and \( h \) refers to the corresponding beam thickness, the second moments are given, by definition, as:

\[
I_c = \frac{h_1^3}{12} + \frac{h_2^3}{12} + \frac{h_1 h_2 (h_1 + h_2)}{4} = \frac{(h_1 + h_2)^3}{12}, \quad I_2 = \frac{h_2^3}{12}
\]  

(4.7)

Then, for simplicity, Eq. (4.6) can be restated in the general form of Eq. (4.5), taking into account Eq. (4.7):

\[
G = \frac{P^2}{2b} \left( \frac{1-v^2}{4 Eb} \right) I^2 \left( \frac{12}{h_2^3} - \frac{12}{(h_1 + h_2)^3} \right).
\]  

(4.8)

The application of the above formula for the case of the discrete gold pads, at the interface of the current specimen, requires an appropriate area correction, as described in Section 4.2.1 and applied in Chapter 5.

Moreover, the loading conditions at the interface, between the inner rollers of the apparatus, result in mixed mode fracture, with a mode mixture \( \psi \approx 41^\circ \) [47], given the geometry and material properties employed in the current study. This indicates slightly more tensile than shear loading with respect to the direction of crack propagation (\( \psi = 0^\circ \) for pure mode I and 90\(^\circ \) for pure mode II). The characterization of the mode mixture is important because the strain energy release rate that is required for crack growth along an interface is very sensitive to the loading mode of the stress field around the crack tip, as shown in Figure 4-6. It typically takes several times as much energy for a crack to propagate under mode II than under mode I conditions. Thus, it is essential that the experimental results for the interface toughness are reported along with the respective
Finally, the validity of using the results of Charalambides et al. [47], which were originally developed for an homogeneous, bilayer specimen, but here applied to a sandwich specimen which includes a thin interlayer of a second material, has been investigated by Suo and Hutchinson [45, 50]. Similar results were found for both stress intensity factor and mode mixture at the crack tip.

4.2.3 Mechanical Testing and Microscopic Observations Procedure

Mechanical testing was performed using an Instron™, model 1332, servo-hydraulic test machine fitted with a commercial four-point bending fixture, which had symmetrically positioned inner and outer loading cylinder pins, as shown in the schematic of Figure 4-4(a). A 100 N, Instron™ load cell was used to monitor the applied load in the range of interest, while the testing machine was operated in displacement-controlled mode, at a rate of 0.075mm/min. Both load and displacement data were acquired and recorded by a

Figure 4-6: Schematic of the loading modes at the interface. (a) Mode I (tensile loading). (b) Mode II (shear loading).
computer system with a data acquisition board and LabVIEW™ software. Also, a Questar™ long distance microscope has been used for in situ observations of crack initiation and propagation events. Tests were conducted in a laboratory air environment at approximately 25°C.

An important procedure that was performed prior to actual testing was the alignment of the four-point bending fixture, in order to ensure uniform loading of the specimen. The proper alignment was initially checked with the use of two piezoresistive strain gages, located below the inner rollers and aligned with them [51]. The correction of any observed misalignment was possible with the use of a custom alignment fixture, mounted on the top of the upper portion of the four-point bend fixture. This alignment fixture was originally designed and employed by Turner [51], in an experimental characterization of silicon wafer fusion bonds.

Following mechanical testing, the fracture surfaces were examined using optical microscopy to characterize the failure mode, and subsequently measure the bond yield. Furthermore, scanning white light interferometry and atomic force microscopy (AFM) were used to compare and quantify respectively, the extent of the plastic deformation during fracture. The former technique was performed using a Zygo™, New View 5000 system in order to image and measure the microstructure and topography of the fracture surfaces. This system divides light into one portion that reflects from the test surface and another portion that reflects from an internal, reference surface in the interferometric objective. Both portions are then directed onto a solid-state camera and the interference between the two light wavefronts results in an image of light and dark fringes, which indicate the surface structure of the sample being tested. Finally, the AFM images and measurements were obtained from a Veeco™, D3000 metrology system operating in tapping mode.
Chapter 5

Results and Discussion

5.1 Gold Film Yield Stress

The yield strength of the gold film at the bonding temperature has been obtained using a curvature measurement technique as described in Section 4.1. A blanket Au film and Ti adhesion layer were e-beam deposited on a Si wafer following the thermal growth of a SiO$_2$ diffusion barrier. The film-substrate system was subjected to thermal cycling and the radii of spherical curvature of this system were measured with respect to the applied temperature. Then, the film stress was calculated as follows [37]:

\[
\sigma_f = \frac{M_{Si} \cdot h_{Si}^2}{6 \cdot h_{Au}} \left( \frac{1}{\rho} - \frac{1}{\rho_o} \right),
\]

where $M_{Si} = 180.5$ GPa is the biaxial elastic modulus of the (100) Si substrate, $h_{Si} = 525$ μm is the thickness of the Si substrate, $h_{Au} = 0.5$ μm is the thickness of the Au film, $1/\rho_o$ is the inherent curvature (before deposition) of the Si substrate and $1/\rho$ is the induced curvature of the Si substrate at an applied temperature.

The results of the above calculations are shown in Figure 5-1, where the gold film biaxial stress is plotted as a function of the applied temperature. Initially, at room temperature, the gold film is under a low biaxial tensile stress. Upon heating, the stress
Figure 5-1: Stress evolution in a nominally 0.5 μm thick Au film on a Si substrate during the first and second thermal cycles.

decreases along a thermo-elastic line. Then, at approximately 110°C, the gold film starts to undergo a stress relaxation or more accurately the rate of plastic relaxation exceeds the applied loading rate, as noted by Thouless et al. [40]. The gold stress exhibits a plateau of 25±5 MPa, between 180°C and 220°C, suggesting a nearly constant flow stress of 25 MPa in this temperature regime. At higher temperatures the stress decreases again along an elasto-plastic line. Upon subsequent cooling, a tensile stress is induced, which finally
reaches a maximum value of approximately 210 MPa, at room temperature. Since the first thermal cycle is complicated due to multiple mechanisms involved (such as grain growth) and the following cycles are often different than the first but similar to each other [42, 52], the film-substrate system was subjected to a second thermal cycle. Stress relaxation, that is apparent during the first cycle, is not observed during the second cycle. However, the stress evolution in the cooling portion of the second cycle closely matches the corresponding portion of the first cycle, indicating the repeatability of the thermo-mechanical behavior of the gold film [52].

The thermo-mechanical behavior of thin metal films has been widely studied with the use of dislocation-based models. However, the underlying mechanisms and their inherent size effects are not yet well understood [41, 52, 53]. Nevertheless, regarding the modeling approach followed in the current work, only the approximate value of the flow stress (25 MPa) in the temperature regime of interest (around 200°C) is relevant. The observed value of stress is also consistent with previous experimental characterization results for a nominally 0.5 μm thick Au film [7], where a fairly constant flow stress of 30 MPa has been reported, when the applied temperature was between 200°C and 300°C.

5.2 Bond Quality Results and Characterization

This section includes the presentation and interpretation of the mechanical testing raw data and calculations, as well as the microscopic observations and measurements obtained from the application of techniques which were presented in Chapter 4.

5.2.1 Load – Displacement Data and Interface Fracture Behavior

The four-point bending system mechanics (described in Section 4.2.2) predicts that the strain energy release rate should exhibit steady-state characteristics once the crack length is sufficiently longer than the thickness of the notched beam [47]. Given a constant value
of the interfacial toughness, the analysis suggests that, ideally, crack propagation should begin at some critical load and then propagate at a constant load along the uniform moment region between the inner loading points.

However, the observed load-displacement behavior depends on how the critical strain energy release, $G_{ic}$, varies with position along the interface. Howard et al. [54] and Klingbeil et al. [55], after studying experimental load-displacement data from Ti/Ti and NiAl/steel interfaces respectively, observed many cases of unstable crack propagation immediately following initial debonding. As the critical load was reached, rapid crack extension occurred (or else crack bursting, as described in [54]) causing a large drop in the load. Possible explanations given for this phenomenon were the non-uniform interface properties and an asymmetrical crack advance on either side of the notch.

A typical load-displacement curve obtained from the current experimental study is shown in Figure 5-2. Initially, the load rises linearly with increasing displacement, as the specimen deforms elastically. Once the critical load for interface crack initiation is reached, at approximately 3.5N, the curve exhibits an abrupt change in slope. At this point, a load drop is observed indicating rapid crack propagation. The same behavior is then repeated twice, at loads slightly higher than 4N. Then, immediately after a fourth peak is reached, a short load plateau (constant load regime) is obtained, at approximately 4.5N, corresponding to stable crack propagation. Loading further than this point results in a linear but more compliant curve than the initial elastic regime, indicating that the crack has propagated over the full distance between the inner loading points. The decrease in the compliance of the system is also apparent from the slope of the curve, during unloading.

The observed unstable crack propagation is consistent with the behavior reported in previously discussed four-point bend experimental studies [54, 55]. Similar non-ideal behavior was also reported by Tsau [7] who originally characterized Au/Au thermocompression bonded specimens with the same technique. A possible interpretation of the above fracture behavior may be associated with variations in the plastic dissipation that occurs, as the crack propagates along the discontinuous ductile interface. The dominant contribution of the plasticity in the measured fracture toughness along a ductile
interface has been extensively reported in previous studies [56, 57]. Microscopic observations and corresponding measurements on the gold fracture surfaces, described in Section 5.2.3, support this argument. Moreover, the asymmetrical crack advance on either side of the notch that was originally suggested by Howard et al. [54], was confirmed in current study by real-time observations with the use of a long distance microscope (Section 4.2.3) in most cases. Thus, it may be inferred that the variation in plastic deformation along with the discontinuous configuration of this interface result in the appearance of four different peak loads which could be associated with the four discrete bonded pads regions (out of the total eight) that are included in the uniform moment.
region of the tested specimens [7]. Due to the lack of a single load plateau, both the load peaks and the averaged critical load were used for the calculation of the interface fracture toughness. None of these two approaches captures accurately the actual released fracture energy, but both provide macroscopic metrics of the bond toughness.

5.2.2 Bond Toughness

The experimentally measured $G_{ic}$ values for all tested specimens (four data points per specimen) range from 2 to 190 J/m$^2$, ranked in ascending order, as shown in the plot of Figure 5-3. Nevertheless, the majority of the measured values fall between 40 and 100 J/m$^2$.

![Figure 5-3](image)

Figure 5-3: The experimentally measured $G_{ic}$ values for all tested bonded regions (four data points per specimen) as a function of data point rank (n/N) in ascending order.
Despite the overall large scatter of the data points per bonded wafer pair, the amount of scatter is similar for each individual wafer pair. Similar scatter was also observed by Tsau [7] who characterized the process for the same range of applied pressure, but for higher temperatures (260° to 300°C). However, the upper bound of the toughness range reported in Tsau’s work [7] was considerably higher, up to approximately 400 J/m². Another plot of the $G_{ic}$ values obtained from current mechanical testing is shown in Figure 5-4. There, the averaged bond toughness values per specimen have been calculated (see Section 5.2.1) and the scatter of the data per wafer pair has been reduced.

![Figure 5-4: The average $G_{ic}$ values per specimen as a function of data point rank (n/N) in ascending order.](image-url)
A key result from these experimental data for $G_k$, is that even at bonding temperatures, as low as 200°C, the lowest achieved bond toughness is three orders of magnitude higher than the elastic strain energy associated with overcoming wafer bow (which was calculated in Equation 3.7). Thus, it can be clearly seen that wafer bow has negligible effect on determining the variability of bond quality. Also the data in the plot of Figure 5-4 suggest that almost all of the tested specimens from the wafer pair that corresponds to the highest applied pressure exhibit higher toughness values than those of the other specimens. However, both plots of bond toughness values do not conform to the expected overall trend of monotonically increasing toughness with increasing bonding pressure. It seems likely that a number of fabrication issues involved in the specimen preparation and described in Section 4.2.1 (such as substrate preparation and gold deposition) may have contributed to the lack of a clear correlation between bond toughness and applied pressure or possibly to the lower $G_k$ values as well. This argument is further supported by the fact that only a single wafer pair was used per individual process condition. Furthermore, it is not yet clear if the suggested influence of nanotopography, which is analyzed in Chapter 3 and is consistent with the previous experimental data for 260° to 300°C [7] is proved here to be sensitive to the bonding temperature decrease (200°) or whether other factors not taken into account in current modeling approach may be more significant than thought to be. Thus, these data points are proved to be inadequate in sufficiently exploring the effect of surface asperities.

The mechanical testing data presented above provide a macroscopic metric of the bond quality (due to the averaging of the toughness of each discrete gold bonded pad). Despite the limitations of this characterization in capturing local or subtle variations of bond quality, it provides a useful measure of the overall response of the bonded area. Thus, the macroscopic fracture results do substantiate the conclusion that overall wafer shape is a negligible contributor to bond quality. However, microscopic observations and measurements have to be employed in order that the actual extension of the plastic deformation on the gold pads be identified and quantified as a micro-scale metric of the bond quality.
5.2.3 Microscopic Observations and Measurements.

As discussed earlier in Sections 5.2.1 and 5.2.2 the measured $G_{ic}$ values are substantially larger compared to the intrinsic surface energy of the metal layers. This is due to the dominant contribution of plasticity in the measured interface toughness [56, 57]. A larger plastic dissipation during fracture for the fixed gold thickness of current specimens is expected to be associated with a cohesive failure within the gold layer. On the other hand, limited ductility and lower $G_{ic}$ values are normally related to the adhesive failure mode, which corresponds to delamination along the Ti/SiO$_2$ interface for the multi-layer films used in the current configuration, as shown in the schematic of Figure 5-5.

The large variation of $G_{ic}$ values that was observed in the current work, manifested itself in the simultaneous appearance of fully adhesive, fully cohesive or combined failure modes. Two characteristic cases of combined failure modes are shown in the optical micrographs at Figure 5-6. In these images, it can be seen that the non-uniformity
Figure 5-6: (a) Both failure modes observed in neighboring gold pads (cohesive to the left and adhesive to the right). (b) Variation in failure mode within the gold pad: Cohesive failure within the bonded layer appears darker, while adhesive failure at the Ti/SiO$_2$ interface appears brighter.

In failure mode may occur between neighboring pads as in micrograph (a) or even within individual gold pads, as appears in (b). The areas of the gold pads which were plastically deformed during fracture appear darker than the unbonded gold line on either side of the pads as well as the adhesive failure areas. This visual distinction is a result of the increased roughness of the gold due to the plastic deformation and may be used to characterize a well-bonded pad, without resorting to higher resolution imaging.

A straightforward comparison of fractured areas with the use of this optical contrast is shown in Figure 5-7, where a poorly bonded area is characterized by almost uniform color appearance with only little signs of plastic deformation visible at the edges of the pads (as shown in the zoom view). Since this optical comparison captures the actual extension of the plastic deformation on the gold pads, it was used as a micro-scale criterion to quantify the bond quality in terms of yield. A gold pad was defined as successfully bonded if more than approximately 75% of its surface appears darker than the unbonded gold on either side of it.
Figure 5-7: Comparison of bond quality in fractured areas with the use of optical contrast observations: (a) Only little signs of plastic deformation are visible at the edges of the gold pads. (b) The pads which were plastically deformed and successfully bonded during the process appear darker than the unbonded gold line on either side of the pads.

Given that the macroscopic metric of bond toughness failed to provide a clear correlation between bond quality and applied pressure for the current experimental conditions, this micro-scale criterion was employed to compare the bond quality of specimens which have comparable $G_{ic}$ values (but at the same time are corresponding to different process conditions), in terms of yield. Such is the case for most of the specimens which were bonded at 30 and 120 MPa respectively (see Figure 5-4). Thus, these specimens were selected as more appropriate to measure the bond yield rather than those bonded at 73
Figure 5-8: The bond yield for specimens which were bonded at 30 and 120 MPa respectively. Despite the fact that they have comparable $G_{ic}$ values, the yield measured is clearly increased with the application of higher pressure.

MPa which were clearly exhibit lower $G_{ic}$ values, given also the limited available time and the time consuming process required for the optical observations. The data obtained are presented in the graph of Figure 5-8, and clearly show that the bond yield is increased by the application of the highest pressure as expected from the analysis of Chapter 3. Also, this trend is consistent with the suggested effect of surface roughness on the bond quality which is described in Section 3.3.
However, despite the correlation with the applied pressure, even these yield data are scattered. Moreover, the highest measured yield value of approximately 65% is far from the nearly 100% yield which was reported by Tsau [7] for the same bonding pressure, but at higher temperature (260°-300°C). This implies that even an applied pressure that exceeds more than three times the temperature-dependent gold yield stress appears to be insufficient to result in full interfacial contact over the total gold area. Thus, the reported yield data constitute evidence of the improved bond quality, with increasing pressure, manifested in extended plasticity. On the other hand, the current data are inadequate in defining whether or not surface roughness is the dominant factor determining thermocompression bond quality.

In order to complement the optical observations and predominantly to quantify the extension of the plastic deformation of the gold pads, scanning white-light interferometry and atomic force microscopy were employed. With the use of those techniques, surface roughness profile plots were obtained and compared with respect to the corresponding bonding pressure used. Initially, extensive qualitative comparisons were performed with the use of interferometry, as shown in two typical plots obtained, in Figure 5-9. Then,

![surface profile plots](image.png)

**Figure 5-9:** Typical surface roughness profile plots for specimens which were bonded at 30 (a) and 120 MPa (b) respectively. The gold ductility manifested in surface roughness is increased with increasing applied pressure.
AFM measurements were performed to quantify the plastic deformation on the fractured gold surfaces with respect to the process conditions. Higher plastic deformation on the fractured surfaces is expected to be associated, in principle, with cohesive failure mode and initially well-bonded pads. The RMS value for surface roughness was measured to increase from 30-50 nm to 130-150 nm, corresponding to specimens bonded at 30 and 120 MPa, respectively. Furthermore, for the latter, the peak to valley distance was measured from 480-510 nm suggesting that the entire gold layer had plastically deformed. Also, the examination of some specimens bonded at 73 MPa shows that their ductility lay, qualitatively, between those bonded at 30 and 120 MPa respectively. Again, the overall trend suggested by the optical observations was confirmed. Gold ductility, during fracture, manifested in surface roughness, is increased with increasing applied pressure, as shown in the images of Figure 5-10.
Chapter 6

Conclusions and Recommendations

6.1 Thesis Summary and Conclusions

This thesis documents mechanics modeling of the effect of flatness deviations on gold thermocompression bonds. The main achievements and conclusions of this work are:

1) An analytical framework that allows the effect of wafer topography to be assessed for typical geometries and process conditions has been developed. This has been accomplished by modeling the deformation required to accommodate wafer topography and to establish material continuity. Specifically: (a) An analytical expression for the strain energy release rate, which is associated with the elastic deformation required to overcome wafer bow and establish an interface contact, has been developed and (b) A contact yield criterion has been used to examine the pressure and temperature conditions required to flatten surface roughness asperities in order to achieve bonding over the full apparent area.

2) The bond toughness of gold thermocompression bonded specimens has been measured with the use of the four-point bending delamination technique, under a useful range of process parameters, in order to validate the suggested framework as well as to assess the relative contribution of the factors under examination.
3) A micro-scale bond characterization has been conducted based on microscopic observations and AFM measurements in order to complement the macro-scale bond toughness measurements by quantifying the bond yield and the extent of the plastic deformation on the fractured gold surfaces.

4) The analytical results combined with experimental data for the bond toughness clearly suggest that wafer bow has a negligible effect on determining the variability of bond quality.

5) Microscopic observations and AFM measurements on the fractured surfaces of the thermocompression bonded specimens have shown that the well-bonded area is increased with increasing bonding pressure.

6.2 Recommendations for Future Work

Wafer-level, thermocompression bonding is a promising technique for microelectromechanical systems (MEMS) packaging. However, the quality of the resulting bond is critically dependent on the interaction between flatness deviations that range from wafer bow to surface roughness, the thin film properties and the process parameters and tooling used to achieve the bonds. While this work has made some advances in order to understand the relative contributions of these effects, it has also highlighted some issues that require further investigation before gold thermocompression bonding can be widely used for MEMS packaging applications.

The current experimental study validated several general trends between bond quality metrics and process conditions. For instance, the well-bonded area has been showed to increase with increasing bonding pressure through the local deformation of the surface asperities. Nevertheless, the current experimental data are inadequate in defining whether or not surface roughness is the dominant factor determining the observed bond quality variability. A more systematic experimental study has to be performed as compared to the limited process window examined in the current work. Also, given the interesting results
obtained from the current micro-scale characterization based on microscopic observations and measurements, the use of appropriate micro-mechanical testing may provide improved measurements and effective characterization of the local contact processes. Other factors, not taken into account in current modeling approach, such as the crystallographic orientation at the bonding interface, may also play a role in determining the bond quality. The employment of a more comprehensive constitutive model for the gold film thermomechanical behavior may capture effectively the influence of both nanotopography and microstructure, which may contribute to the observed bond quality variability.

Finally, there are other interesting aspects of gold thermocompression bonding, not studied in the current work, which have to be investigated such as the possibility of hermetic sealing. This property is very important in MEMS packaging manufacture and could make the thermocompression bonding technique very attractive for a class of applications.
Appendix A

Slip-Line Field Analysis

When the plastic deformation is sufficiently severe so that the plastic strains are large compared with the elastic strains, the elastic deformation may be neglected. Then, assuming plane strain deformation and idealizing the material as a rigid perfectly plastic solid, a large class of solutions to complex plasticity problems (e.g. metal forming) is available with the use of slip-line field analysis.

A loaded body of rigid perfectly plastic material comprises regions in which plastic flow is taking place and regions in which, on account of the assumption of rigidity, there is no deformation. The state of stresses within the regions of flow can be represented by a slip-line field [28]. The slip lines are drawn parallel to the directions of principal shearing stress at every point in the field, i.e. at 45° to the directions of principal direct stress. Thus, they consist of an orthogonal curvilinear net of “α” and “β” slip lines. A representative element of a slip-line field is sketched in Figure A-1(a). The stress state in the plastic zone consists of a hydrostatic stress denoted by \( \sigma \) together with the shear yield stress in the plane of deformation denoted by \( k \). It is convenient to represent this state of stress by a Mohr’s circle, as shown in Figure A-1(b), which relates \( \sigma \), \( k \) and \( \varphi \). Then, by considering the equilibrium of the element in Fig. A-1(a), in the direction of an \( \alpha \) line and \( \beta \) line respectively, we obtain:
Figure A-1 (After K. L. Johnson [28]): A representative element of a slip-line field (a) Stresses acting on the element bounded by slip lines. (b) The state of stress represented by a Mohr's circle.

\[ \frac{\partial \sigma}{\partial \alpha} - 2k \frac{\partial \varphi}{\partial \alpha} = 0, \quad \frac{\partial \sigma}{\partial \beta} + 2k \frac{\partial \varphi}{\partial \beta} = 0 \]  

(A.1)

which may be also expressed as:

\[ \sigma - 2k \varphi = \text{constant}, \quad \sigma + 2k \varphi = \text{constant} \]  

(A.2)

where \( k = \sigma_y / \sqrt{3} \) or \( \sigma_y / 2 \), with the use of the Mises or the Tresca yielding criterion, respectively.

Thus, by starting at a point of known stress (e.g. at some boundary), equations (A.2) enable the variation in \( \sigma \) throughout the field to be found from the directions of the slip lines. In the particular case of plastic blunting of surface asperities, given the idealization of section 3-3, the contact stress (or pressure), \( \sigma_c \) may be expressed by the pressure during the blunting of plastic wedges shown in Figure A-2 [28, 34]:

\[ \sigma_c = F \sigma_y \]  

(A.3)
where the flow coefficient, $F$ is given by an upper bound of $F = 2 + \pi / \sqrt{3} = 2.97$ or $F = 2 + \pi / 2 = 2.57$, with the use of the Mises or the Tresca yield criterion, respectively.

While the additional use of FEM analysis [15, 36], permits the examination of complexities such as the evolving asperity shape and the redistribution of stress, as shown

Figure A-3 (After A. R. Akisanya [36]): The evolution of the flow coefficient during the blunting of the asperities, for different modes of deformation (FEM analysis)
in Figure A-3, the onset of fully plastic deformation which is relevant to the current modeling occurs at approximately the pressure plateau \( (3\sigma_y) \) that slip-line theory predicts.
Appendix B

Specimen Fabrication Process Flow

Figure B-1 (After Tsau [5]): Schematic of fabrication process flow details, with cross sections taken along A – A’ for (a)–(d), and along B – B’ for (e). (a) Bonding pair. Detail shows notch region in DSP wafer (bottom) after KOH and shallow anisotropic etching. (b) Thermal oxidation. (c) Metal deposition. (d), (e) Aligned bonding. (f), (g) Top view of DSP and regular wafers after lift-off, respectively. Dashed central rectangle in (f) indicates the location of the etched trench.
Bibliography


