



Study on Wiring and Packaging Techniques for Miniaturizing and Integrating MEMS-Based Sensors

Aono, Takanori

(Degree)

博士 (工学)

(Date of Degree)

2018-03-25

(Date of Publication)

2019-03-01

(Resource Type)

doctoral thesis

(Report Number)

甲第7186号

(URL)

<https://hdl.handle.net/20.500.14094/D1007186>

※ 当コンテンツは神戸大学の学術成果です。無断複製・不正使用等を禁じます。著作権法で認められている範囲内で、適切にご利用ください。



博 士 論 文

Study on Wiring and Packaging Techniques for Miniaturizing and
Integrating MEMS-Based Sensors

小型・集積化 MEMS センサの配線・パッケージング技術に
関する研究

平成 30 年 1 月

神戸大学大学院工学研究科

青野 宇紀

Doctoral Dissertation

Study on Wiring and Packaging Techniques for Miniaturizing and
Integrating MEMS-Based Sensors

小型・集積化 MEMS センサの配線・パッケージング技術に
関する研究

January 2018

Department of Mechanical Engineering,
Graduate School of Engineering, Kobe University

Takanori AONO

ABSTRACT

The microelectromechanical systems (MEMS)-based sensors are applied as various applications such as automobile, robot, smartphone, medical analysis etc. These sensors are required an endurance of temperature, humidity and shock, a miniaturization for mounting on portable equipments and a precise accuracy for detecting. Therefore, these MEMS-based sensors should be improved in reliability and reduction of production size and manufacturing cost. In recent days, the post-processes of MEMS-based sensors are important to determine device integration, performance, reliability and cost.

This thesis focuses on the post-processes of MEMS-based sensors, which are wiring and packaging processes for miniaturization and integration. Chapter 1 introduces about the MEMS applications used in a market, and fabrication processes and post-processes which are generally used in manufacturing makers. In the design and the fabrication steps, atomic behaviors of materials utilized for MEMS are also important to realize the wiring and the package of MEMS-based sensors with a high reliability and a high performance. Chapter 2 describes about the molecular dynamics simulations for determining the materials or the process conditions in the post-processes of MEMS-based sensors.

In chapter 3, a method for fabricating multilevel interconnection structures using differential adhesive fracture energies between metal and silicon oxide thin films is described. When the selectivity of the adhesive fracture energies between the metal and the silicon oxide thin films sets on the wiring, the silicon oxide (SiO_2) thin film can be released on the low adhesive fracture energy area and can be held on the high adhesive fracture energy area with ultrasonic treatment. The adhesive fracture energies are calculated with a molecular dynamics (MD) simulations. The adhesive fracture energies between chromium (Cr), titanium (Ti) and nickel (Ni), and SiO_2 are larger than those of copper (Cu) and gold (Au) thin films. Cr, Ti and Ni are applied as an adhesion layer with silicon oxide, and Cu and Au are applied as a release layer from SiO_2 . The MD results are applied to the process for fabricating the multilevel interconnection structures, and the release and the adhesive areas on SiO_2 thin film can be fabricated on the wiring by applying ultrasonic treatment. With this method, the lower wiring and the contact areas of multilevel interconnection structures can be easily fabricated without lithography and etching.

In chapter 4, an eutectic-based wafer-level-packaging (WLP) technique for piezoresistive MEMS accelerometers on the basis of molecular dynamics analyses and shear tests of WLP accelerometers is described. The bonding conditions were

experimentally and analytically determined to realize a high shear strength without solder material atoms diffusing to adhesion layers. Molecular dynamics (MD) simulations and energy dispersive X-ray (EDX) spectrometry done after the shear tests clarified the eutectic reaction of the solder materials used in this research. Energy relaxation calculations in MD showed that the diffusion of solder material atoms into the adhesive layer was promoted at a higher temperature. Tensile creep MD simulations also suggested that the local potential energy in a solder material model determined the fracture points of the model. These numerical results were supported by the shear tests and EDX analyses for WLP accelerometers. Consequently, a bonding load of 9.8 kN and temperature of 300 °C were found to be rational conditions because the shear strength was sufficient to endure the polishing process after the WLP process and there was little diffusion of solder material atoms to the adhesion layer. Also, eutectic-bonding-based WLP was effective for controlling the attenuation of the accelerometers by determining the thickness of electroplated solder materials that played the role of a cavity between the accelerometers and lids. If the gap distance between the two was less than 6.2 μm , the signal gains for x- and z-axis acceleration was less than 20 dB even at the resonance frequency due to air-damping.

In chapter 5, an anodic bonding-based wafer-level-packaging (WLP) technique to simultaneously seal an accelerometer in the atmosphere and a gyroscope in vacuum with a glass cap for MEMS sensors are described. The accelerometer with a damping oscillator is necessary to be sealed in the atmosphere for its high-speed response. As the gyroscope can achieve high sensitivity with a large displacement at the resonant frequency without air-damping, the gyroscope must be sealed in vacuum. The technique consists of three processing steps: 1st bonding step in the atmosphere for the accelerometer, pressure control step and 2nd bonding step in vacuum for the gyroscope. The process conditions were experimentally determined to achieve higher shear strength at the interface of the packaging. The packaging performance of the accelerometer and gyroscope after WLP was also investigated by using a laser-doppler-velocimeter at a room temperature. The amplitude at the resonant frequency of the accelerometer was reduced by air-damping, and the quality factor of the gyroscope showed a value higher than 1000. The reliability of the gyroscope was also confirmed in a thermal cyclic test and an endurance test at high humidity and high temperature.

Contents

Chapter 1: Introduction

1.1 MEMS applications	1
1.2 MEMS fabrications	5
1.3 MEMS post processes	11
1.4 Objectives and organization of thesis	19
References	20

Chapter 2: Molecular dynamics simulations for applying MEMS post-processes

2.1 Introduction	24
2.2 MD simulations	24
2.3 Analysis method of adhesion strength	35
2.4 Conclusions	36
References	37

Chapter 3: Evaluation of Fabricating Method for Multilevel Interconnection Structures Using Differential Adhesive Fracture Energies between Metal and Silicon Oxide Thin Films

3.1 Introduction	38
3.2 Fabrication of multilevel interconnection structures	39
3.3 Design and experimental procedures	42
3.4 Results and discussions	46
3.5 Conclusions	51
References	52

Chapter 4: Eutectic-based wafer-level-packaging technique for piezoresistive MEMS accelerometers and bond characterization using molecular dynamics simulations

4.1 Introduction	53
4.2 Design and experimental procedures	54
4.3 Results and discussions	63
4.4 Conclusion	71
References	72

Chapter 5: Development of wafer-level-packaging technology for simultaneous sealing of accelerometer and gyroscope under different pressures

5.1 Introduction	74
5.2 Design and experimental methodology	75
5.3 Investigation of bonding conditions	78
5.4 Characteristics of MEMS sensors	86
5.5 Conclusion	90
References	91

Chapter 6: Conclusions	94
------------------------	----

Acknowledgements	96
------------------	----

Appendix	97
----------	----

Chapter 1: Introduction

1.1 MEMS APPLICATIONS

Recently, micro electromechanical systems (MEMS) devices such as sensors and actuators are widely applied to various fields; e. g. automobile, robotics, information technology, medical and image projection, and so on [1, 2]. The most economically interesting applications of MEMS are to sensors to measure physical parameters such as temperature, pressure or acceleration, and chemical parameters such as component or concentration of substances.

Figure 1.1 shows the general systematization of MEMS technologies [3]. The MEMS technologies are largely classified as applications, integration, elements and basic technologies. In order to utilize MEMS, it is necessary to integrate many components with various functional properties such as mechanical, chemical, fluid-dynamic, optical, biological, electrical and electronic and so on.

Several MEMS devices utilized in automobiles and smartphones are introduced as representative examples. Figure 1.2 shows the MEMS applications utilized in automobiles. The MEMS sensors are mainly mounted for driving safety and fuel management in this field. For example, accelerometers are utilized for the detection of automotive behavior or for activation of airbag in case of a collision. Pressure sensors are used for tire pressure monitoring, as well as for fuel and exhaust gas flow rate measuring in order to reduce low-fuel consumption. These sensors need to endure high temperatures and shocks for the safety driving systems, since they are mounted near the engine. Figure 1.3 shows the MEMS applications for smartphones. MEMS applications such as accelerometers, gyroscopes and microphones were applied as a user interface and communication tools in the portable device. Since the MEMS devices enable miniaturization, integration and reduction of production cost, a lot of sensors and actuators are mounted in the housing which extend the capabilities of portable equipments.

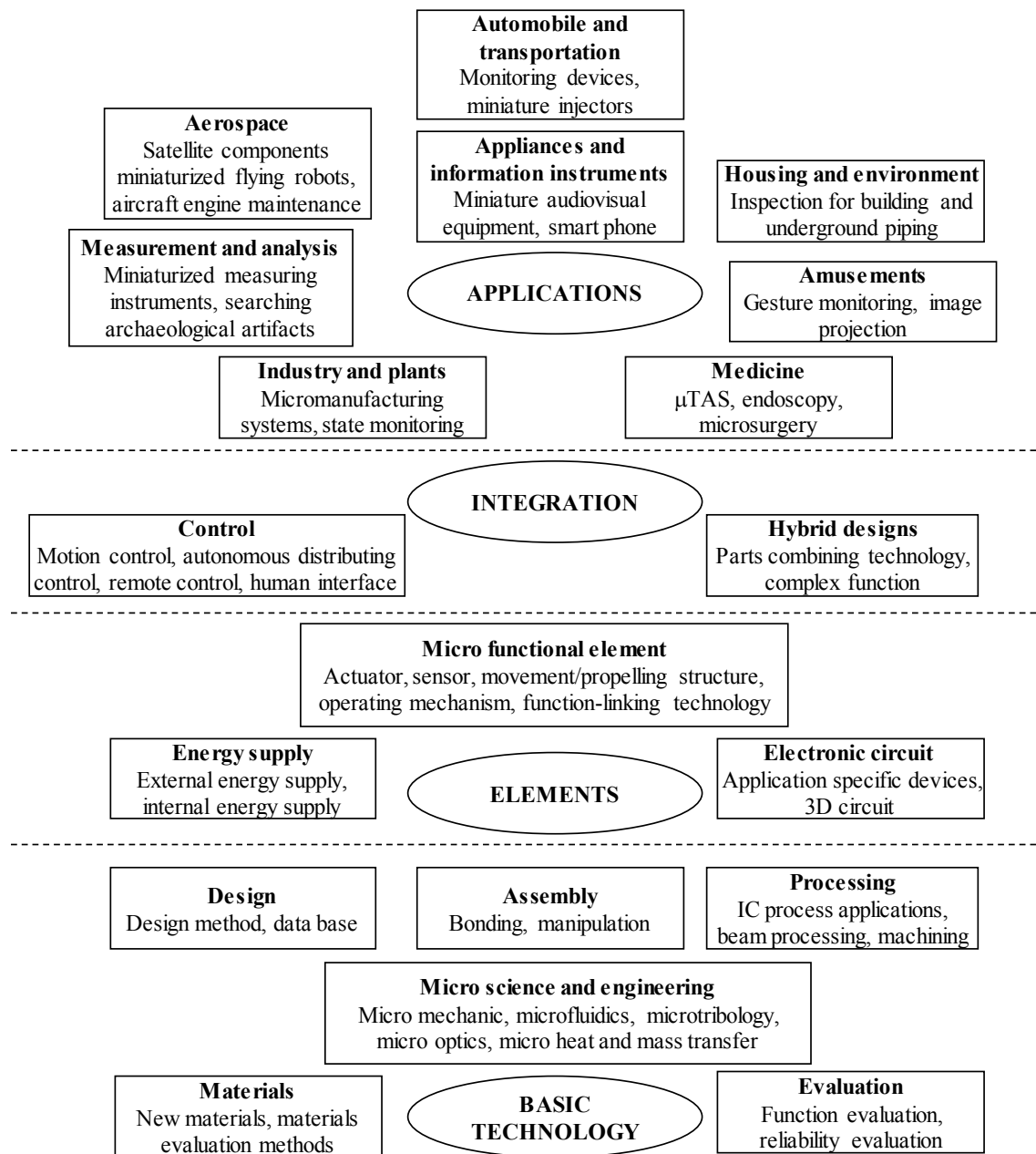


Figure 1.1 General systematization of MEMS technologies.

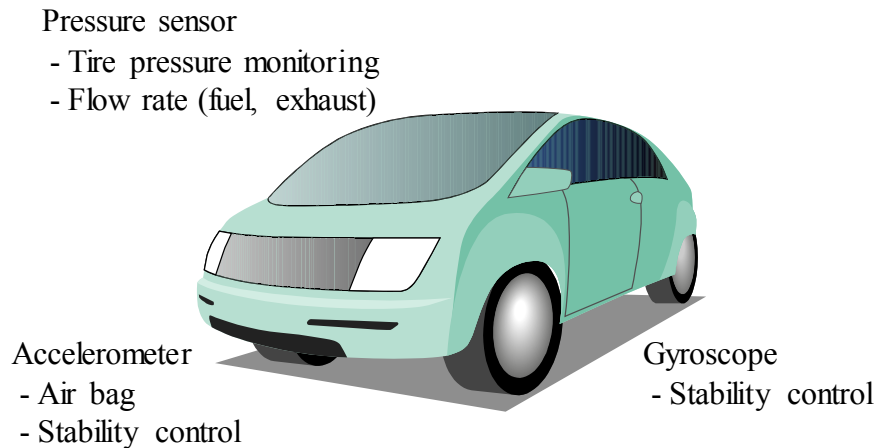


Figure 1.2 Schematic of MEMS sensors for automobile.

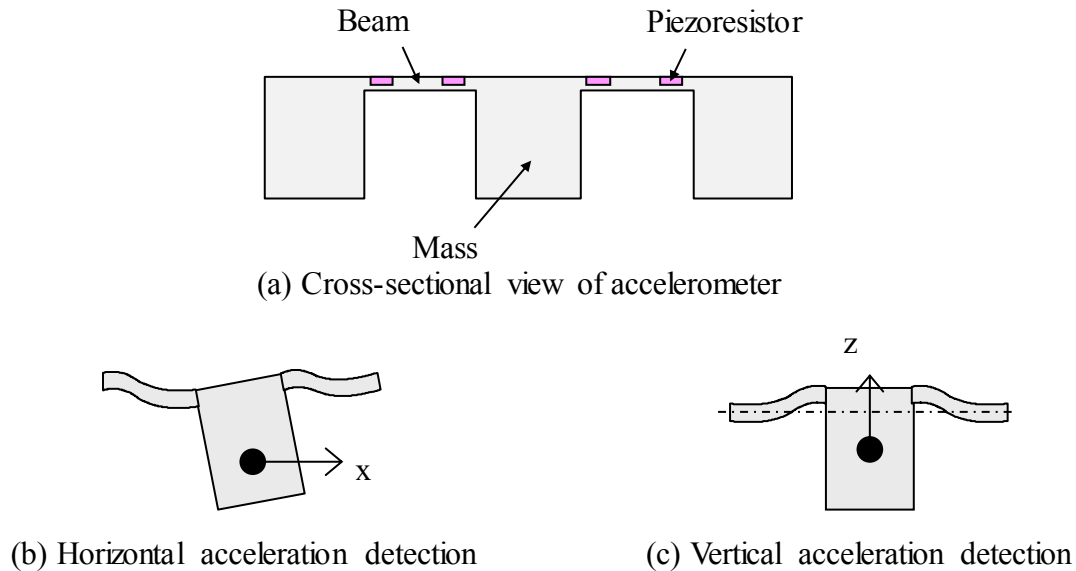


Figure 1.3 Schematic of MEMS sensors for smartphone.

The accelerometers for automotive airbags were one of the first commercial MEMS by Analog Devices in 1990 [4]. They are widely used in the form of a single chip containing a smart sensor or an accelerometer. When the rapid deceleration by a collision is detected with the accelerometer, the airbag immediately expands for protecting of a driver or passengers. The usage of accelerometers is not limited to automotive applications. Now, they are also applied to earthquake detection [5], motion control for industrial robot [6], motion sensing of smartphone or games [7, 8] and falling detection of disk drive [9, 10].

The accelerometer is a capacitive or piezoresistive device consisted of a proof mass suspended by beams [11-13]. Figures 1.4 shows the schematic and the detection mechanism of a piezoresistive accelerometer. When the acceleration acts on the mass toward the horizontal or vertical direction, the beams are moved and the acceleration can be sensed by the resistance change of the piezoresistor on the beams. The size of a

MEMS-based accelerometer in the recent days is less than 2 square mm and the thickness is less than 1 mm. This sensor is currently handily mounted in portable equipments.



Figures 1.4 Schematic and detection mechanism of piezoresistive accelerometer.

The pressure sensor is also an extremely successful MEMS application [14]. These sensors are applied as a tire pressure monitoring sensor (TPMS), a fuel level sensor and flow rate sensor of fuel and exhaust in the automotive field [15, 16]. Figure 1.5 shows the schematic of piezoresistive pressure sensor. The pressure sensor comprises of a thin silicon diaphragm fabricated by etching techniques. It typically measures the pressure difference, either from the absolute pressure (gauge pressure) or another defined pressure (differential pressure), by the displacement of silicon diaphragm. The pressure sensors are also utilized to monitor blood pressure in medical field [17], to measure pneumatic and hydraulic pressure of industrial robots or to measure barometric pressure to detect height difference.

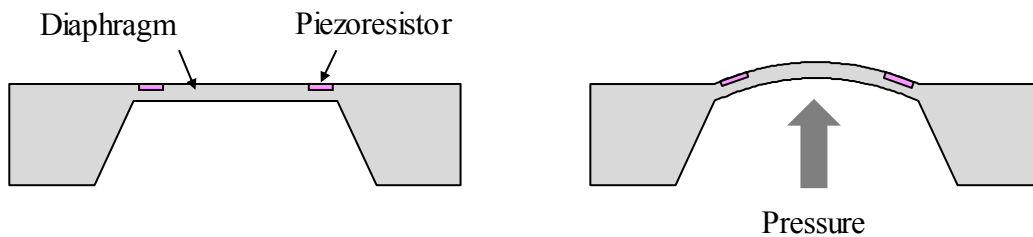


Figure 1.5 Schematic of piezoresistive pressure sensor.

Gyroscopes detect and measure the angular motion or the orientation of an object. MEMS-based gyroscopes are typically utilized to measure the angular velocity of automotive, aerospace, games or camera for motion detection and stabilization. The detecting principle exploits the exchange of energy between different axes of vibration due to Coriolis effect. The quartz tuning fork gyroscopes were commercialized by BEI technologies since 1996 [18], and silicon MEMS-based gyroscopes have been also massively produced since early 21st century [19].

Microphone is a transducer that converts sound into an electrical signal. They are used in many applications such as smartphones, hearing aids, voice recorders and ultrasonic sensing [20]. The most MEMS-based microphones are commercialized as condenser microphones with electrically biased diaphragms whose capacitance changes as sound wave vibrate it. For increasing signal to noise ratios, the piezoelectric MEMS-based microphones have also been researched and developed [21].

The digital mirror device (DMD) for digital light processing-based projector was invented by Texas Instruments in 1987 [22]. The DMD device has several million mirrors arranged in a rectangular array which correspond to the pixels in the image to be displayed. The mirrors can be individually rotated, and bright and dark images are projected on the screen. It is used in about 85 % of digital cinema projection.

These MEMS devices are miniaturizing to set on the limited space of the equipments in the same way as ICs. Although the manufacturing cost of MEMS is reduced by downsizing, the packaging cost increases due to difficulty in mounting miniaturized MEMS chips on a package. Therefore, wafer-level-packaging (WLP) techniques are one of the most important technologies to realize miniaturizing with high reliability and low cost for MEMS [23].

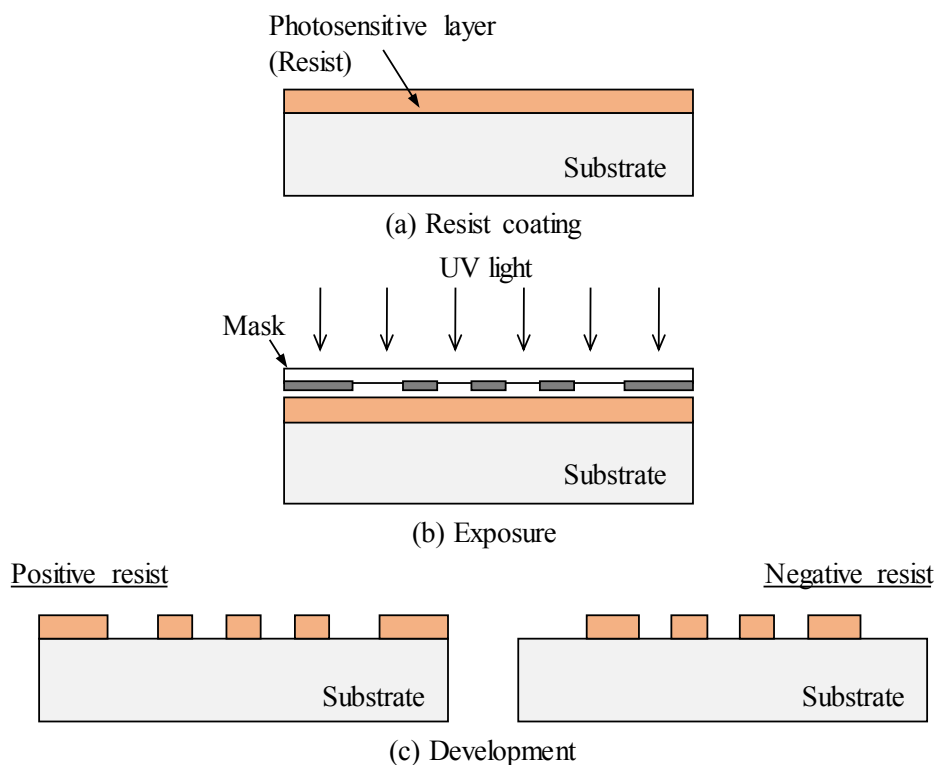
1.2 MEMS FABRICATIONS

This section introduces about MEMS fabrication processes for realizing MEMS applications shown in section 1.1. The MEMS fabrication processes are classified as preprocessing and post-processing. In the preprocessing, lithography and etching techniques of semiconductors are applied to MEMS. In chapters 3, 4 and 5, the interconnection, the accelerometer and the gyroscope are fabricated on Si substrates with this preprocessing. Lithography and etching techniques are shown below.

1.2.1 LITHOGRAPHY

Figures 1.6(a) to (c) depict the process flow of lithography [24]. Lithography is used to prepare the substrate for subsequent processing stages. In order to be able to etch desired pattern of the work piece selectively, a photosensitive layer is coated on the substrate surface by a spin or a spray coatings [see Fig. 1.6(a)]. This photosensitive resist will be lithographically structured so that specified areas of the substrate remain covered and protected. This technique is the most critical and also the most expensive single micromechanical process and plays a key role in mass-production of MEMS.

The photosensitive layer can be masked and structured with irradiating ultraviolet light [see Fig. 1.6(b)]. The mask is made of a light-transparent substrate such as a glass and a light-blocking layer on it. The light-blocking layer is generally made of chromium. Irradiation to ultraviolet light causes molecule chains to break or to cross-link, depending on the type of resist. Either the exposed area of the positive resist, or the unexposed area of the negative resist are removed in development step [see Fig. 1.6(c)]. During this step, the mask pattern is transferred to the resist for the next steps.



Figures 1.6 Process flow of lithography.

1.2.2 ETCHING

The etching methods used for MEMS must exactly remove material for obtaining micro-sized structures such as grooves, bridges, membranes or beams [25]. The etching can produce three-dimensional and surface structures for MEMS. In wet etching, the etching solution, which is acidic or alkaline, dissolves the material to be removed. Etching is carried out by dipping the substrate into the etching bath or spraying it with the etching solution. Also, the etching process can either be isotropic or anisotropic depending on the structure of the material or the etching solution.

1.2.2.1 ISOTROPIC ETCHING

When the material is amorphous or polycrystalline, chemical wet etching process is isotropic [26]. Figures 1.7 show the schematic of isotropic etching and the photographs of cavity on glass substrate isotropically etched with HF solution

In isotropic etching, the etching speed is the same for all directions, thus the cavities have rounded off edges, and are widened by undercuts under the mask. However, the round edges are usually not preferred unless they are suited to form good fragile strength in moving parts. Therefore, isotropic etching is suitable for forming a few- μm -deep cavities or wirings made by thin SiO_2 or metal films.

In chapters 4 and 5, the metal adhesion layer for eutectic bonding, and the bumps and the cavities on glass substrate for anodic bonding are fabricated with the isotropic etching techniques, respectively. Table 1.1 tabulates the representative etching solutions of materials for fabricating MEMS [27].

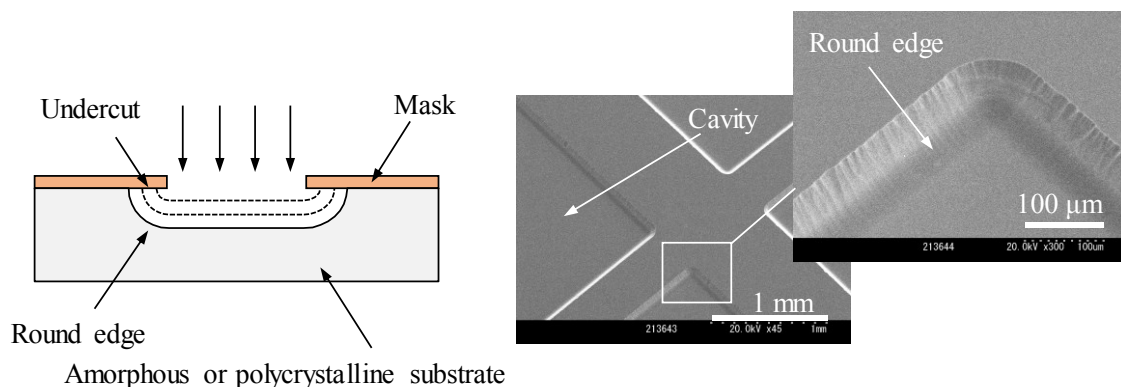


Figure 1.7 Schematic of isotropic etching and photographs of glass etched with isotropic etching technique.

Table 1.1 Etching solutions for fabricating MEMS.

Material		Etching solution
Aluminum	Al	$\text{H}_3\text{PO}_4 + \text{CH}_3\text{COOH} + \text{HNO}_3 + \text{H}_2\text{O}$
Titanium	Ti	dilute HF
Chromium	Cr	$\text{Ce}(\text{SO}_4)_2 \cdot 2(\text{NH}_4)_2\text{SO}_4 \cdot 2\text{H}_2\text{O} + \text{HNO}_4 + \text{H}_2\text{O}$
Copper	Cu	$\text{H}_3\text{PO}_4 + \text{CH}_3\text{COOH} + \text{HNO}_3 + \text{H}_2\text{O}$
Nickel	Ni	50 wt% HNO_3
Platinum	Pt	70 °C $\text{HCl} + \text{HNO}_3$
Gold	Au	$\text{I}_2 + \text{NH}_4\text{I} + \text{H}_2\text{O}$
Silicon	Si	$\text{HF} + \text{HNO}_3 + \text{CH}_3\text{COOH}$
Silicon oxide	SiO_2	$\text{HF} + \text{NH}_4\text{F}$
Borosilicate glass	SiO_2	HF
Silicon nitride	Si_3N_4	180 °C H_3PO_4

1.2.2.2 ANISOTROPIC ETCHING

Single crystal silicon can be anisotropically etched with an aqueous solutions of alkali hydroxides KOH, NaOH, LiOH, CsOH and RbOH, or TMAH (tetramethylammonium hydroxide) [28, 29]. Among them, KOH is widely utilized to the etching of silicon substrate masked with silicon dioxide or silicon nitride.

Figures 1.8(a) to (c) show the atomic arrangement of single crystal silicon. The silicon has fcc (face-centered cubic) structure. With these alkali solutions, the etching speed of silicon decreases in the order of the (110) planes, the (100) planes and the (111) planes. Especially, the etching speed of (111) planes is distinctly minimal, which brings the etching process to make a facet on this plane. Figures 1.9 show the schematic of anisotropic etching and photograph of silicon etched with KOH solution. When a silicon substrate with the surface of the (100) plane is etched with the anisotropic etching techniques, the cavities are formed as V-like rectangle shapes surrounded with the (111) planes. The walls of the structure are smooth, since the etching speed of the (111) planes is several hundred times slower than that of the perpendicular planes. Thus, anisotropic etching allows to form geometrically precise microstructures with sharp corners and edges that can be defined in a single crystal silicon.

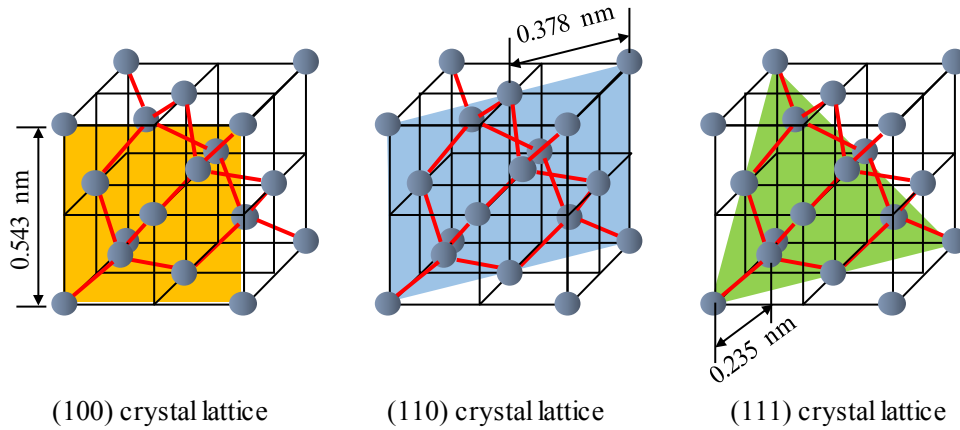


Figure 1.8 Schematics of silicon lattice structure.

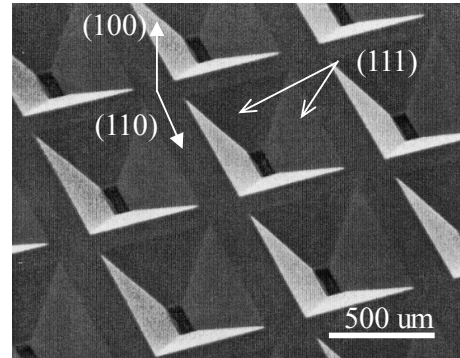
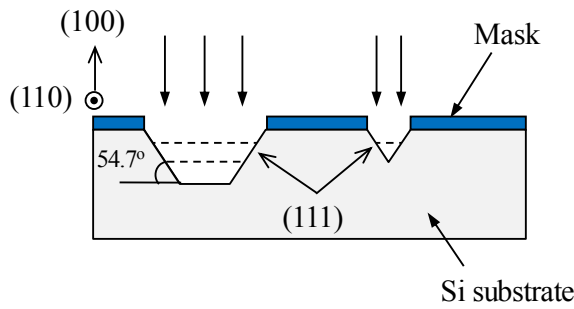


Figure 1.9 Schematic of anisotropic etching and photograph of silicon etched with anisotropic etching technique.

1.2.2.3 DRY ETCHING

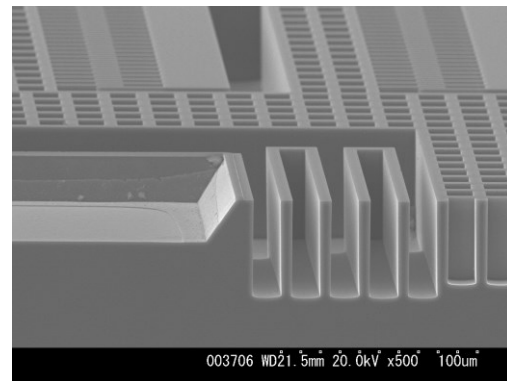
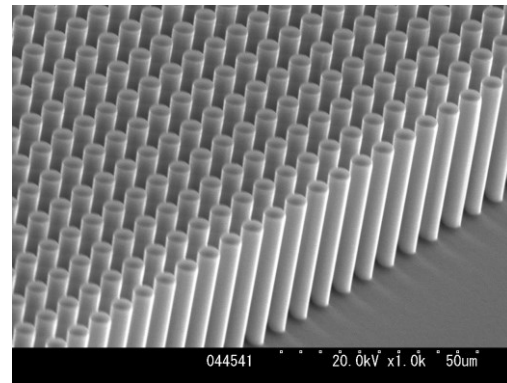
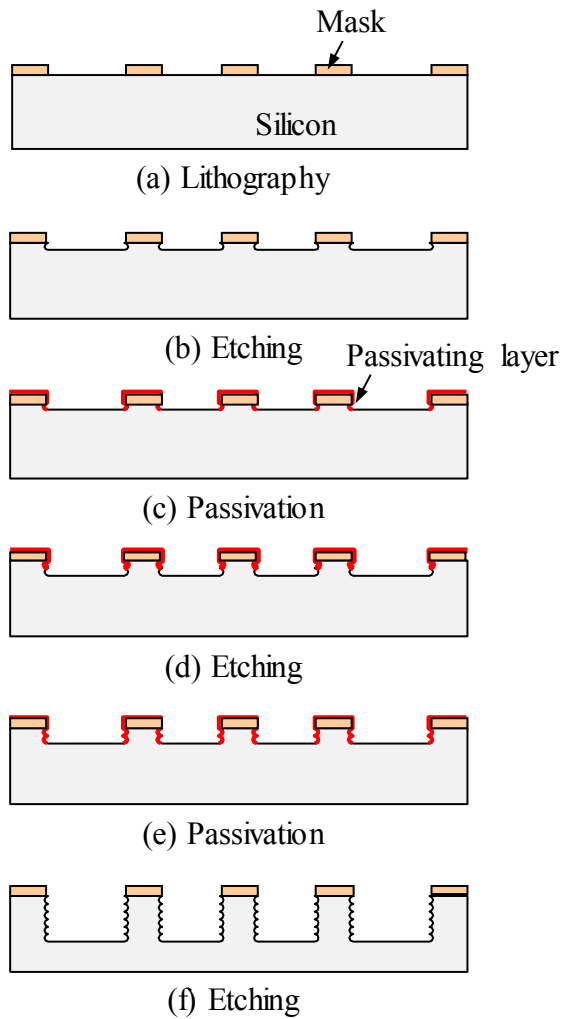
Dry etching involves the process to expose the substrate to an ionized gas or a reactive gas. Etching is carried out through chemical or physical reaction between ions in gas and atoms of substrate. Dry etching techniques can be utilized to structure almost any materials suited for MEMS devices. Figures 1.10(a) to (f) depict the schematics of dry etching process for fabricating in various high-aspect ratio silicon structure pioneered and patented by Bosch [30], where two different gases are alternated in the reaction chamber. The first gas etches the substrate, and the second gas created a polymer on the surface on the substrate. During the etching step [see Figs. 1.10(b), (d) and (f)], the silicon atoms exposed to a reactive gas are etched by the following reaction 1.1.



On the other hand, the surfaces of silicon exposed by previous etching step are covered by a polymer synthesized in the following plasma reaction 1.2 during the passivation step [see Figs. 1.10(c) and (e)].



The polymer is immediately etched, but only on the horizontal surfaces and not the sidewalls during the etching steps. Thereby a temporary etching stop layer is formed on the sidewall of remaining parts. Alternatingly repeating the etching and the polymerizing steps can fabricate a three-dimensional silicon structure with a high aspect ratio.



Figures 1.10 Schematics of dry etching and photographs of silicon etched with dry etching technique.

1.3 POST PROCESSES

This section introduces about the post processes for realizing the MEMS applications shown in sections 1.1 and 1.2. The post processes are classified as a wiring fabrication to electrically connect MEMS and packages, and packaging technologies to protect MEMS and maintain their performances.

The packaging technologies are extremely important for successful device commercialization, since MEMS devices downsizing and cost reduction are required in the market. In the conventional IC fabrication, packaging corresponds to about 60 % of manufacturing cost, and for MEMS fabrication it corresponds to same percentage. For example, vibratory MEMS such as accelerometer, gyroscopes, scanning-mirrors and micro-resonators should be packaged in vacuum suitable for each MEMS in order to fully exploit their performances. Although it is possible to seal MEMS in vacuum with the conventional ceramics packaging techniques, the manufacturing cost is not reduced since MEMS are packaged one by one in the ceramics housing. Therefore, the wafer-level packaging (WLP) technology that collectively packages the MEMS in the state of the wafer is one of the most important post processes for realizing high reliability, downsizing and cost reduction.

The fabrication of wiring for integrating MEMS is described in chapter 3, and the packaging techniques of MEMS are described in chapters 4 and 5.

1.3.1 WIRING PROCESSES

1.3.1.1 METAL THIN FILM FABRICATIONS

Metal thin films are essential to fabricate IC and MEMS, since they are utilized as an electrical signal carrier or a chemical catalyst. The metal thin films are generally fabricated with evaporation, sputtering or ion plating which processes are carried out under vacuum [31]. They are also able to be deposited by electroplating techniques.

In evaporation technique, the substrate sets over the evaporation source in a vacuum chamber. The metal materials are heated above the melting point in a crucible with a resistance heated source, an inductively heated source or an electron beam. The metal atoms can leave from the melt materials by evaporation and travel onto the substrate, whereby they condense and form a metal thin film.

In sputtering techniques, a metal target and a substrate are placed opposite to each other in a chamber filled with argon gas under low vacuum. When an electric field is applied between the target and the substrate, the argon ions are generated in the discharge and accelerated and collided to the metal target. And then, the metal atoms are released from the metal target by the argon ions collision. The metal atoms condense on

the substrate, and form a metal thin film. Furthermore, metal compound films such as oxide or nitride can be fabricated by introducing a reactive gas into the chamber.

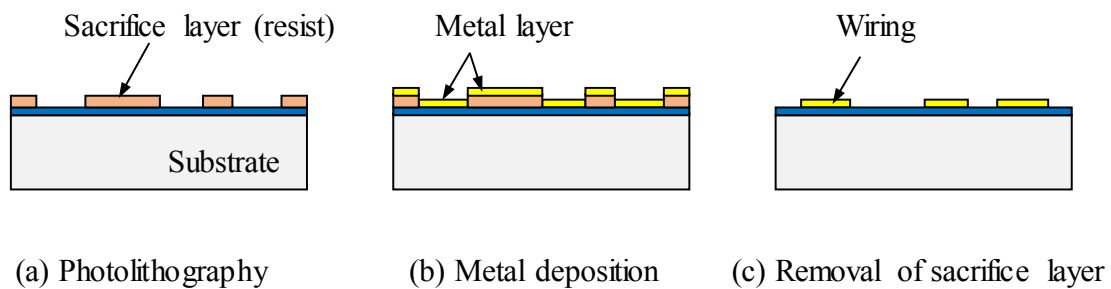
In electroplating techniques, the metal films are deposited by a redox reaction of electrolyte. The substrate as cathode and the metal plate as anode are placed opposite to each other in an electrolyte including target metal ions. At the cathode, the metal ions are reduced to metals by gaining electrons as shown an oxidation reaction 1.3. On the other hand, the metal plate is oxidized to metal ions on the anode as shown a reduction reaction 1.4. This electroplating techniques are suitable for fabricating the thick-film MEMS structures in a short time.



Wirings and electrodes are mainly fabricated by combining the metal deposition, the lithography and the etching techniques shown in above subsection.

1.3.1.2 LIFT-OFF PROCESS

Figures 1.11(a) to (c) depict the process flow for wiring with the lift-off process [32]. At first, inverse patterns of wirings are fabricated as a sacrifice layer on the substrate [see Fig. 1.11(a)]. Here, the sacrifice layer used is generally a resist as shown in Fig. 1.6. Next, the metal layer is deposited on the whole surface of substrate with evaporation or sputtering [see Fig. 1.11(b)]. Finally, the sacrifice layer is removed together with the covering metal layer [see Fig. 1.11(c)]. As a result, the metal thin films remain only on the part of the substrate without the sacrifice layer.



Figures 1.11 Lift-off process for wiring fabrication.

1.3.2 WAFER LEVEL PACKAGING

Packaged electronics is the embodiment of all electronic equipment, computers, smartphone, television, automobile and etc. It consists of active components such as semiconductor chips. The active components are interconnected, supplied with electric power and housed in packaging. Also, MEMS devices such as sensors and actuators are necessary to be housed in the package [23, 33-37]. Various packaging technologies have been developed to achieve high performance and highly reliable of MEMS devices. Table 1.2 tabulates the packaging technologies for MEMS devices. Each packaging technologies are explained as follows.

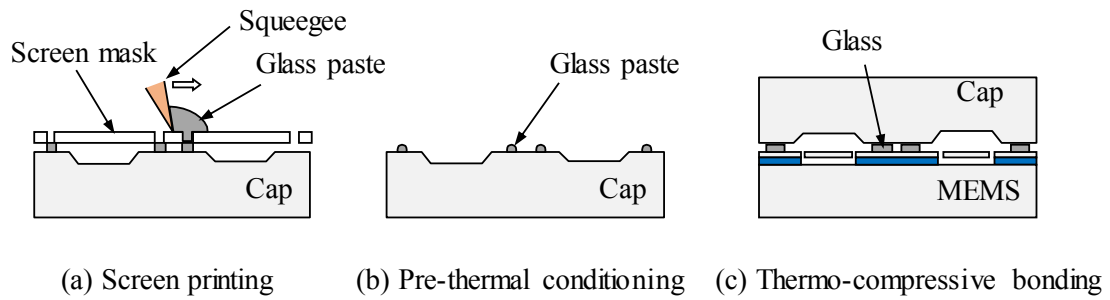
Table 1.2 Packaging technologies for MEMS devices.

Bonding methods	Temperature	Roughness	Substrate
Glass frit bonding	450-650 °C	Low	Si, glass, metal, ceramic
Silicon direct bonding	>800 °C	Highly sensitive	Si-Si
Plasma-activated bonding	r. t.	Highly sensitive	Si, glass, metal, ceramic
Eutectic bonding	200-400 °C	Low	Si, glass, metal, ceramic
Anodic bonding	250-500 °C	Highly sensitive	Si-Glass, LTCC

1.3.2.1 GLASS FRIT BONDING

Glass frit bonding is one of the wafer bonding techniques with low melting point glass as an intermediate layer [38, 39]. The glass paste which is a precursor of low melting-point glass is prepared by mixing lead, zinc and SiO₂ particles in binder and solutions. Figures 1.12(a) to (c) depict the process flow of glass frit bonding. The bonding flow is composed of three main steps; the deposition of glass paste by screen printing, the pre-thermal conditioning of glass paste, and the thermo-compressive bonding. The screen printing technique can easily make the bonding frame of glass paste on the cap substrate without fabrication process as lithography [see Fig. 1.12(a)]. During the pre-thermal conditioning of glass paste, the binder and solution is completely evaporates and burned out [see Fig. 1.12(b)]. This conditioning is important to remove the voids in the bonding flame in order to increase the bonding strength and the hermetic reliability. At last, in the thermo-compressive step, the temperature is

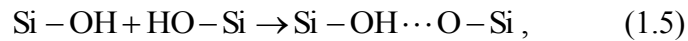
increased to melting temperature of the glass paste of range from 450 to 650 °C. The glass particles melt and form the bonding intermediate layer between the substrates [see Fig. 1.12(c)]. The glass frit bonding can even bond substrates with rough surfaces due to the deformation capability of the glass paste.



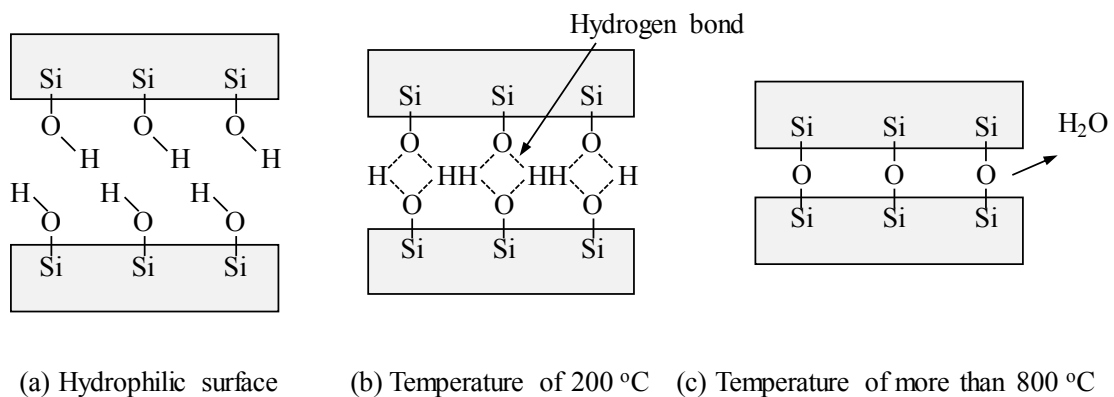
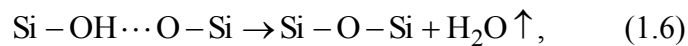
Figures 1.12 Process flow of glass frit bonding.

1.3.2.2 SILICON DIRECT BONDING

Direct bonding can bond between substrates with a dehydration chemical reaction without the need of any intermediate layer [40-42]. Figures 1.13(a) to (c) depict the mechanism of silicon direct bonding. This bonding consists of three main steps; the preprocessing, the pre-bonding at room temperature and the annealing at high temperature. This bonding requires that the surface of substrate is sufficiently clean, flat and smooth in order to contact the substrates directly. Thus, particle, organic and ionic contaminations are removed from the surface of substrates with RCA clean [see Fig. 1.13(a)]. Next, in the pre-bonding, when the substrates are brought into contact with each other, the bonding is started between water molecules chemisorbed on the surface [see Fig. 1.13(b)]. The interaction of chemisorbed water molecules is showed in the hydrogen-bond reaction 1.5.



The Si-OH (silanol) groups start to polymerize forming Si-O-Si and H₂O shown in reaction 1.6. However, this reaction is reversible at room temperature due to remaining water on the interface. Next, the annealing at a high temperature (more than 800 °C) migrates or diffuse remaining water along the interface, and Si-O-Si bond with a large bonding strength is formed on a whole interface of the wafer [see Fig. 1.13(c)].



Figures 1.13 Mechanism of silicon direct bonding.

1.3.2.3 PLASMA ACTIVATED BONDING

Plasma activated bonding utilizes sputter cleaning with noble gas such as neon, argon and xenon in vacuum to remove contamination on the surface [43-46]. This bonding can directly bond between substrates at lower temperature without any intermediate layers. Figures 1.14(a) to (c) depict the process flow for plasma activated bonding. This bonding is carried out in three main steps; the preprocessing, the plasma activation in vacuum and the bonding. In the preprocessing step, the surface of substrates are cleaned with RCA methods [see Fig. 1.14(a)]. Next, in the plasma activation step, the dangling-bonds on surface of substrates are formed by irradiating noble gas plasma [see Fig. 1.14(b)]. However, this bonding has to be carried out in high vacuum, since the dangling-bonds immediately react with various molecules in a bond chamber. Thus, the plasma activated bonding is suitable to the MEMS hermetically sealed in a high vacuum. At last, in the bonding step, the substrates with activated surfaces can be strongly bonded with only contact, since dangling-bonds between contacting substrates form chemical bonds.

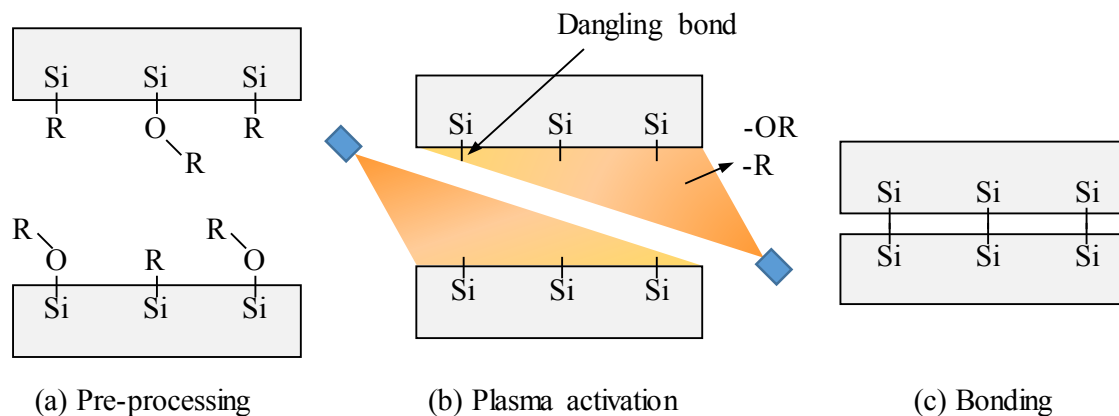


Figure 1.14 Process flow for plasma activated bonding.

1.3.2.3 EUTECTIC BONDING

Eutectic bonding is one of the wafer bonding techniques with eutectic metals as an intermediate layer [47-49]. The eutectic metals directly transform from solid to liquid states at or over the eutectic temperature. Table 1.3 tabulates the representative eutectic metals, their composition and their eutectic temperature [50].

Figures 1.15(a) to (c) depict the process flow for eutectic bonding. This bonding is carried out in three main steps; the eutectic metals deposition, the preprocessing and the bonding at or over eutectic temperature. The eutectic metals are deposited by sputtering, evaporation or electroplating techniques. In the deposition, the metal layers are necessary to consider for not only eutectic reaction and diffusion between metal layers but also adhesion with base substrate [see Fig. 1.15(a)]. As a general deposited structure, adhesion layer, diffusion prevention layer and eutectic reaction layer are deposited in this order. Generally, the eutectic metals tend to be oxidized the surface in atmosphere. When the oxide layer exists at the bonding interface, the eutectic reaction is prevented and a bonding strength is not enough. Thus, the preprocessing is necessary to remove the oxide layer with plasma treatment or wet etching for achieving a large bonding strength [see Fig. 1.15(b)].

At last, the substrates are aligned and fixed on a fixture, and bonded at or over the eutectic temperature in a bond chamber [see Fig. 1.15(c)]. During the bonding step, warp of substrate is corrected by adding contact load. At or over eutectic temperature, eutectic metals form liquid phase, and bond between substrates.

The eutectic bonding can produce not only sealing but also electrical interconnection in order to utilize conductive metals. For example, the eutectic bonding of Al-Ge has applied to both hermetic sealing and electric connection between MEMS and ICs, and commercially realized the gyroscopes sealed in vacuum [19].

Table 1.3 Eutectic metals, compositions and temperatures.

Eutectic metals	Eutectic composition [wt%]	Eutectic temperature [°C]
Au-In	0.6Au-99.4In	156
Sn-Pb	60Sn-40Pb	183
Ag-Sn	3.5Ag-96.5Sn	221
Cu-Sn	5Cu-95Sn	227
Au-Sn	80Au-20Sn	278
Au-Si	97.15Au-2.85Si	356
Au-Ge	72Au-28Ge	363
Al-Ge	87.5Al-12.5Si	419

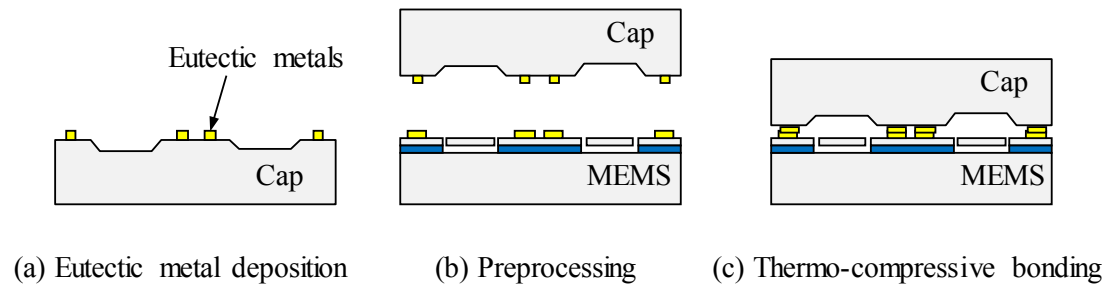
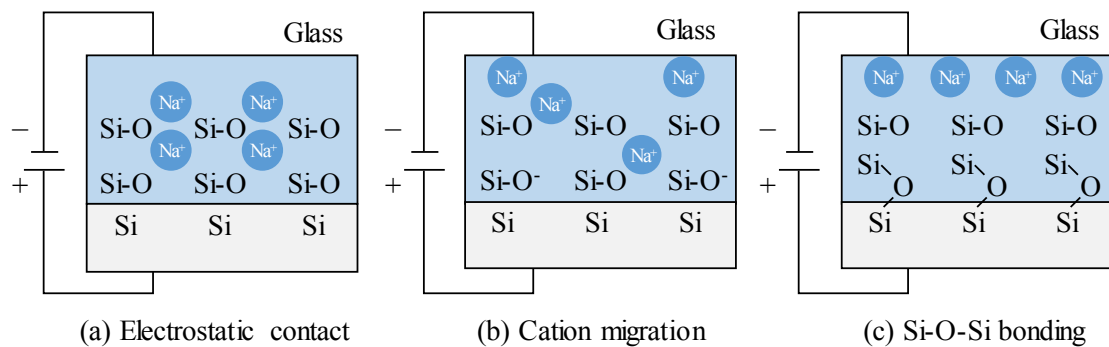


Figure 1.15 Process flow of eutectic bonding.

1.3.2.4 ANODIC BONDING

Anodic bonding is to electrostatically bond between glass and silicon or metal without an intermediate layer [51-55]. Generally, the glass has to use borosilicate glass containing a high concentration of alkali ions. The glass and silicon are connected with cathode and anode electrodes, respectively. This bonding is carried out at a temperature range from 250 °C to 400 °C with a voltage range from 400 V to 1000 V.

Figures 1.16(a) to (c) show the anodic bonding mechanism in the case of glass and silicon substrates. At first, the glass and silicon substrates are electrostatically contacted by adding a high voltage [see Fig. 1.16(a)]. The cations of Na^+ or K^+ in glass migrate to cathode electrode by a high voltage at bonding temperature [see Fig. 1.16(b)]. At that time, the Si-O^- as depleted layer is formed on the interface between the glass and silicon substrates. The Si-O^- chemically reacts with silicon atoms and can covalently bond between glass and silicon with a large bond strength than a fracture strength of glass or silicon [see Fig. 1.16(c)].



Figures 1.16 Anodic bonding mechanism.

1.4 OBJECTIVES AND ORGANIZATION OF THESIS

This doctoral dissertation is composed by a total of six chapters, and the contents of each chapter is organized as follows.

Chapter 1 explains the MEMS applications, the fabricating processes and the post-processes for MEMS.

Chapter 2 explains the description of molecular dynamics (MD) simulating methods in order to consider the materials or the process conditions of post-processes of MEMS.

Chapter 3 develops the fabricating method of multilevel interconnection of MEMS with the difference of adhesion fracture strength between metal and SiO₂ layers. First, the adhesion fracture energy is estimated with the MD simulations. Next, the adhesion fracture strength is evaluated with ultrasonic treatment.

Chapter 4 develops the eutectic-based WLP technique for piezoresistive MEMS accelerometers on the basis of MD analysis and shear tests of WLP accelerometers. The bonding conditions are analytically and experimentally determined to realize a high shear strength without solder material atoms diffusing to adhesion layers.

Chapter 5 develops the anodic bonding-based WLP technique to simultaneously seal an accelerometer in the atmosphere and a gyroscope in vacuum with a glass cap for MEMS sensors. The process conditions are experimentally determined to achieve higher shear strength at the interface of the packaging. The packaging performance of the accelerometer and gyroscope after WLP is also investigated with a laser-doppler-velocimeter.

Finally, chapter 6 shows the summarized conclusion of this thesis.

REFERENCES

- [1] M. Tilli, T. Motooka, V. M. Airaksinen, S. Franssila, M. P. Krockel and V. Lindroos, Handbook of silicon based MEMS materials and Technologies, Elsevier, 2015
- [2] M. Esashi and S. Tanaka, "Stacked Integration of MEMS on LSI", *Micromachine*, Vol. 7, No. 8, 137, 2016
- [3] S. Fatikow and U. Rembold, "Microsystem Technology and Microrobotics", Springer Verlag Berlin Heidelberg, 1997
- [4] Analog Devices
- [5] F. Murakami, H. Sato, T. Kuroda, S. Abe and N. Kato, "Evaluation of MEMS accelerometer Sensor for Earthquake Observations", *Bull. Earthq. Res. Inst.*, Vol. 84, pp. 251-256, 2009
- [6] P. Neto, J. N. Pires and A. P. Moreira, "Accelerometer-Based Control of Industrial Robotic Arm", *The 18th IEEE International Symposium on Robot and Human Interactive Communication*, Toyama, Japan, pp. 1192-1197, 2009
- [7] K. Sato, "Accelerometer-based controller", US20090005166 A1, 2006
- [8] G. Zalewski, R. Marks. X. Mao, "Scheme for detecting and tracking user manipulation of game controller body", US20060256081 A1, 2006
- [9] K. S. Chae, H. J. Kim, G. Hahm, S. W. Cho, H. J. Park, Y. Lee and Y. S. Oh, "Development of 3D Motion Sensor Module", *IEEE Sensors2006*, pp. 666-670, 2006
- [10] A. Gola, E. Chiesa, E. Lasalandra, F. Pasolini, M. Troncoli, T. Ungaretti and A. Baschiroto, "Interface for MEMS-Based Rotational Accelerometer for HDD Applications With 2.5 rad/s² Resolution and Digital Output", *IEEE Sen. Jour.*, Vol. 3, No. 4, pp. 383-392
- [11] K. Okada, "Tri-axial piezoelectric accelerometer", *The 8th International Conference on Solid-State Sensors, Actuators & Microsystems, Transducers'95*, pp. 25-29, 1995
- [12] F. Han, B. Sun, L. Li and Q. Wu, "Performance of a Sensitive Micromachined Accelerometer With Electrostatically Suspended Proof Mass", *IEEE SENSORS JOURNAL*, Vol. 15, No. 1, pp. 209-217, 2015
- [13] S. Tez, U. Aykutlu, M. M. Torunbalci and T. Akin, "A Bulk-Micromachined Three-Axis Capacitive MEMS Accelerometer on a Single Die", *J. Microelectromech. Sys.*, Vol. 24, No. 5, pp. 1264-1274, 2015
- [14] Pressure, Acceleration and Angular Velocity Sensor Market 2012-2013, Yano Research Institute Ltd. (in Japanese)

- [15] W. J. Fleming, "New Automotive Sensors - A Review", *IEEE SENS. J.*, Vol. 8, No. 11, pp. 1900-1921, 2008
- [16] S. J. Prosser, "Automotive sensors: past, present and future", *J. Phys: Conf.*, 76, 012001, 2007
- [17] R. A. Wolthuis, G. L. Michell, E. Saaski, J. C. Hartl and A. Afromowitz, "Development of Medical Pressure and Temperature Sensors Employing Optical Spectrum Modulation", *IEEE Trans. Bio. Eng.*, vol. 38, No. 10, pp. 974-981, 1991
- [18] A. M. Mandi, L. Costlow and S. J. Knowles, "Common Design Techniques for BEI GyroChip Quartz Rate Sensors for Both Automotive and Aerospace/Defense Markets", *IEEE SENS. J.*, Vol. 3, No.5, pp. 569-578, 2003
- [19] J. Seeger, M. Lim and S. Nasiri, "DEVELOPMENT OF HIGH-PERFORMANCE, HIGH-VOLUME CONSUMER MEMS GYROSCOPE", *Solid-State Sensors, Actuators and Microsystems Wksp., Hilton Head, SC*, pp. 61-64, 2010
- [20] K. F. Becker, M. Koch, T. Braun, V. Bander, P. Meier, E. Jung, R. Aschenbrenner and H. Reichl, "MEMS Packaging–Technological Solutions for a Si-Microphone", *CFA/DAGA'04*, Strasbourg, pp. 405-406, 2004
- [21] M. D. Williams, B. A. Griffin, T. N. Reagan, J. R. Underbrink and M. Sheplak, "An AlN MEMS Piezoelectric Microphone for Aeroacoustic Applications", *J. Microelectromech. Syst.*, Vol. 21, No. 2, pp. 270-283, 2012
- [22] P. F. van Kessel, L. J. Hornbeck, R. E. Meier and M. R. Douglass, "A MEMS-Based Projection Display", *Proc. IEEE*, Vol. 86, No. 8, pp. 1687-1704, 1998
- [23] A. C. Fischer, F. M. Lapisa, S. J. Bleilker, G. Stemme, N. Roxhed and F. Niklaus, "Integrating MEMS and ICs", *Microsyst & Nanoeng.*, 1, 15005, 2015
- [24] H. K. Levinson, *Principles of Lithography*, SPIE Press, 2005
- [25] K. E. Petersen, "Silicon as a Mechanical Material", *Proc. IEEE*, Vol. 70, No. 5, pp. 420-456, 1982
- [26] R. Ghodssi and P. Lin, *MEMS Materials and Processes Handbook*, Springer, 2011
- [27] J. L. Vossen and J. J. Cuomo, *Thin Film Processes*, Academic Press, 1978
- [28] H. Seidel, L. Csepregi, A. Heuberger and H. Baumgartel, "Anisotropic Etching of Crystalline Silicon in Alkaline Solutions", *J. Elechem. Soc.*, Vol. 137, No. 11, pp.3613-3626, 1990
- [29] P. Pal and K. Sato, *Silicon Wet Bulk Micromachining for MEMS*, Pan Stanford Publishing Pre, Ltd., 2017
- [30] F. Laermer and A. Schilp, "Method of anisotropic etching silicon", US5501893A, 1996

- [31] W. Menz, J. Mohr and O. Paul, *Microsystem Technology*, WILEY-VCH, 2001
- [32] D. W. Widmann, "Metallization for integrated circuits using a lift-off technique, *J. Solid-State Circuits*, 11, pp. 466-471, 1976
- [33] R. R. Tummala, E. J. Rymaszewski and A. G. Klopfenstein, *Microelectronics Packaging Handbook*, Springer Science, 1997
- [34] M. A. Schmidt, "Wafer-to-Wafer Bonding for Microstructure Formation", *Proc. IEEE*, Vol. 86, No. 8, pp. 1575-1585, 1998
- [35] L. Lin, "MEMS Post-Packaging by Localized Heating and Bonding", *IEEE Trans. Adv. Pack.*, Vol. 23, No. 4, pp. 608-616, 2000
- [36] M. Esashi, "Wafer level packaging of MEMS", *J. Micromech. Microeng.*, 18, No. 7, 073001, 2008
- [37] S. Tanaka and M. Esashi, "Wafer-level MEMS Package and Its Reliability Issues", *MICROELECTRONICS RELIABILITY*, Vol. 54, pp. 875-881, 2014
- [38] R. Knechtel, "Glass frit bonding: an universal technology for wafer level encapsulation and packaging", *Microsyst. Technol.*, 12, pp. 63-65, 2005
- [39] R. Knechtel, M. Wiemer and J. Fromel, "Wafer level encapsulation of microsystems using glass frit bonding", *Microsyst. Technol.*, 12, pp. 468-472, 2006
- [40] J. B. Lasky, "Wafer bonding for silicon-on-insulator technologies", *App. Phys. Lett.*, Vol. 48, No. 1, pp. 78-80, 1986
- [41] R. Stengel, T. Tan and U. Gosele, "A Model for the Silicon Wafer Bonding Process", *Jpn. J. Appl. Phys.*, Vol. 28, No. 10, pp. 1735-1741, 1989
- [42] H. Moriceau, F. Rieutord, F. Fournel, Y. L. Tiec, L. D. Cioccio, C. Morales, A. M. Carvet and C. Deguet, "Overview of recent direct wafer bonding advances and applications", *Adv. Nat. Sci.: Nanosci. Nanotechnol.*, 1, 043004, 2010
- [43] S. Kuhne and C. Hierold, "Wafer-level packaging and direct interconnection technology based on hybrid bonding and through silicon vias", *J. Micromech. Microeng.*, 21, No.8, 085032, 2011
- [44] H. Takagi and R. Maeda, "Aligned room-temperature bonding of silicon wafers in vacuum by argon beam surface activation", *J. Micromech. Microeng.*, 15, No. 2, pp. 290-295, 2005
- [45] C. Wang, E. Higurashi and T. Suga, "Void-Free Room-Temperature Silicon Wafer Direct Bonding Using Sequential Plasma Activation", *Jap. J. Appl. Phys.*, Vol. 47, No. 4, pp. 2526-2530, 2008
- [46] V. Masteika, J. Kowal, N. St. J. Braithwaite and T. Rogers, "A Review of Hydrophilic Silicon Wafer Bonding", *ESC J. Solid State Science and Technology*,

Vol. 3, No. 4, Q42-Q54, 2014

- [47] T. A. Tollefsen, A. Larsson, O. M. Lovvik and K. Aasmundtveit, “An-Sn SLID Bonding-Properties and Possibilities”, *Metallurgical and Materials TRANS. B*, Vol. 43, pp. 397-405, 2012
- [48] J. S. Mitchell and K. Najafi, “ A DETAILED OF YIELD AND RELIABILITY FOR VACUUM PACKAGES FABRICATED IN A WAFER-LEVEL AU-SI EUTECTIC BONDING PROCESS”, *The 15th International Conference on Solid-State Sensors, Actuators & Microsystems, Transducers 2009*, pp. 841–844, 2009
- [49] C. C. Lee, C. Y. Wang and S. Matijasevic, “A New Bonding Technology Using Gold and Tin Multilayer Composite Structures”, *IEEE Trans. Comp. Hybrids. Manuf. Technol.*, Vol. 14, No. 2, pp. 407-412, 1991
- [50] K. J. Puttlitz and K. A. Stalter, *Handbook of Lead-Free Solder Technology for Microelectronic Assemblies*, Mercel Dekker, 2004
- [51] G. Waillis and D. I. Pomerantz, “ Field Assisted Glass Metal Sealing”, *J. App. Phys.*, Vol. 40, No.10, pp. 3946-3949, 1969
- [52] U. Hofmann, H. J. Quenzer, C. Eisermann, J. Janes, C. Schroeder, B. Jensen, J. Hagge, F. Soerensen, F. Senger, D. Vick, O. Schhwarzelbach, L. Rantzmann, B. Wagner and W. Benecke, “A NOVEL VACUUM-PACKAGED LOW-POWER SCANNING MIRROR WITH INCLINED 3D-SHAPED WINDOW”, *The 16th International Conference on Solid-State Sensors, Actuators & Microsystems, Transducers 2011*, pp. 1527–1530, 2011
- [53] S. Tez, U. Aykutlu, M. M. Torunbalci and T. Akin, “A Bulk-Micromachined Three-Axis Capacitive MEMS Accelerometer on a Single Die”, *J. Microelectromech. Syst.*, Vol. 24, No. 5, pp. 1264-1274, 2015
- [54] H. Tachibana, K. Kawano, H. Ueda and H. Noge, “VACUUM WAFER LEVEL PACKAGED TWO-DIMENSIONAL OPTICAL SCANNER BY ANODIC BONDING”, *Proc. 22th IEEE International Conference on Micro Electro Mechanical Systems, MEMS2009*, pp. 959–962, 2009
- [55] R. M. Haque and K. D. Wise, “A Glass-in-Silicon Reflow Process for Three-Dimensional Microsystems”, *J. Microelectromech. Syst.*, Vol. 22, No. 6, pp. 1470-1477, 2013
- [56] J. Liu, J. Shang, J. Tang and Q. A. Hung, “Micromachining of Pyrex 7740 Glass by Silicon Molding and Vacuum Anodic Bonding”, *J. Microelectromech. Syst.*, Vol. 20, No. 4, pp. 909-915, 2011

Chapter 2: Molecular dynamics simulations for applying MEMS post-processes

2.1 INTRODUCTION

In physical or chemical fields, molecular dynamics (MD) simulations have been developed as methods for clarifying molecular behaviors in liquid phase or conformation of proteins [1, 2]. Now the MD simulations are also applied to solve material designs, material physics or microscopic phenomena in mechanical or metal engineering fields due to the increase of computational capabilities. Computer simulations can fill the gap between theory and experiment. Some quantities and behaviors may be impossible or difficult to measure in an experiment.

2.2 MD SIMULATION

2.2.1 SUMMARY OF MD SIMULATIONS

The properties of objects experimentally measured are generally macroscopic, and have time or space averaged properties. Macroscopic and microscopic properties are defined as X and x , respectively. The microscopic property x is theoretically described as a function of time $x(t)$. This microscopic phenomena almost occur in short time of less than 10^{-12} sec. On the other hand, measuring time of macroscopic properties is much longer than the varying time of microscopic properties. Thus, the macroscopic property is expressed with the aggregate of microscopic properties by the following equation 2.1.

$$X = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T x(t) dt, \quad (2.1)$$

where right-hand side means that time average of $x(t)$ ranged from time of 0 to T , when the time T becomes infinite. However, it is extremely difficult to calculate the right-hand side in Eq. 2.1, since it is necessary to calculate all molecular behaviors in the object to acquire the macroscopic properties. Accordingly, statistical mechanics methodology is proposed for calculating macroscopic properties X from microscopic properties x under several general and universal presumptions. In particular, the logic of statistical mechanics concerned macroscopic property in thermal equilibrium is known as statistical thermodynamics and is representative by theory of Gibbs' ensemble.

For a real object in thermal equilibrium, a large number of groups with exactly the same thermodynamic boundary conditions and the same constituent particles are

considered as one ensemble. The microscopic properties of all the constituent particles included in this group are decided by the thermodynamic conditions. Therefore, the microscopic property x for each group shows various values. However, since each group is composed of a large number of constituent particles, the variation of the microscopic property x throughout the group has a certain distribution. Thus, Gibbs proposed that measured macroscopic property X can be expressed with statistical microscopic properties x including variations by the following equation 2.2.

$$X = \langle x \rangle, \quad (2.2)$$

where the right-hand side represents the statistical average of microscopic properties x in the whole ensemble. In MD simulation, the microscopic behaviors of constituent particles in the target are directly calculated with the right-hand side of Eq. 2.1 with a large number of particles.

2.2.2 ANALYSIS METHODS

MD simulation has been considered to be effective tool in monitoring microscopic properties such as atomic positions, velocities and forces as well as macroscopic properties such as deformation, profile and slip velocity.

In well-defined microscopic properties x , MD simulation calculates macroscopic properties X with the right-hand side of Eq. 2.1. The motion of each constituent atom in the object is calculated with classical Newton's equation of motion. Then, dynamic processes and phenomena are calculated as atomic motions, and various structures and physical properties can be considered. If mass m and number of atoms N exist in a system with a potential energy, motion equation of atoms is expressed in Eqs. 2.3 and 2.4.

$$m \frac{d^2 r_i(t)}{dt^2} = F_i(t) \quad (i=1, 2, 3, \dots, N), \quad (2.3)$$

$$F_i(t) = -\frac{\partial \Phi}{\partial r_i}, \quad (2.4)$$

where $r_i(t)$ is positional vector of atom i at a time t , $F_i(t)$ is an adding force to atom i at the time t and Φ is all potential energies in the system. Here, a two-body potential energy is considered as an interaction between atoms i and j energy is described in Eq.

2.5.

$$F_i(t) = \sum_{\substack{j=1 \\ j \neq i}}^N F(r_i(t), r_j(t)), \quad (2.5)$$

Furthermore, if this two-body potential energy $\Phi(t)$ is defined by a function $\phi(r)$ of only distance between atoms, Eq. 2.5 is described in Eq. 2.6.

$$\Phi = \frac{1}{2} \sum_{i=1}^N \sum_{\substack{j=1 \\ j \neq i}}^N \phi(r_{ij}), \quad (2.6)$$

In MD simulation, the position and velocity of atoms in a time are acquired by approximately solving the above motion equations.

There are several algorithms to integrate the equations of motion in MD simulation. The algorithms assume that the positions and dynamic properties (velocities, accelerations, and so on) can be approximated with finite difference methods. Next, the Verlet algorithm [3] and the Gear predictor-corrector algorithm [4] are introduced. Both of them calculate the atomic motions with finite difference methods, and are widely used in MD simulations.

2.2.2.1 VERLET ALGORITHM

This method is a direct solution of the second-order Eq. 2.3. The method is based on the current and previous positions, as well as on the accelerations.

The position of atom i at time t is expressed as $r_i(t)$. The current and previous positions $r_i(t \pm \Delta t)$ at time $t \pm \Delta t$ are described in Eqs. 2.7 as a second-order of Taylor series expansion of $r(t)$.

$$\begin{aligned} r_i(t + \Delta t) &= r_i(t) + \frac{dr_i(t)}{dt} \Delta t + \frac{1}{2} \frac{d^2 r_i(t)}{dt^2} (\Delta t)^2 \\ r_i(t - \Delta t) &= r_i(t) - \frac{dr_i(t)}{dt} \Delta t + \frac{1}{2} \frac{d^2 r_i(t)}{dt^2} (\Delta t)^2 \end{aligned} \quad (2.7)$$

The summation and difference of Eq. 2.7 are calculated in Eq. 2.8, respectively.

$$\begin{aligned}
r_i(t + \Delta t) + r_i(t - \Delta t) &= 2r_i(t) + \frac{d^2 r_i(t)}{dt^2} (\Delta t)^2 \\
r_i(t + \Delta t) - r_i(t - \Delta t) &= 2 \frac{dr_i(t)}{dt} \Delta t
\end{aligned}
\tag{2.8}$$

Next, the velocity $v_i(t)$ and acceleration $a_i(t)$ of atom i at time t are expressed in Eq. 2.9, respectively.

$$\begin{aligned}
v_i(t) &= \frac{dr_i(t)}{dt} \\
a_i(t) &= \frac{d^2 r_i(t)}{dt^2}
\end{aligned}
\tag{2.9}$$

When the velocity $v_i(t)$ and acceleration $a_i(t)$ are substituted into Eq. 2.8, and the resulting equations are expressed in equations 2.10 and 2.11, respectively.

$$v_i(t) = \frac{r_i(t + \Delta t) - r_i(t - \Delta t)}{2\Delta t}, \tag{2.10}$$

$$r(t + \Delta t) = 2r(t) - r(t - \Delta t) + a(\Delta t)^2. \tag{2.11}$$

Verlet algorithm uses the positions and accelerations at time t , and the positions from the previous step $r(t - \Delta t)$ to calculate the new positions $r(t + \Delta t)$ at time $t + \Delta t$ (see Eq. 2.11). Also, the velocities are calculated by dividing the difference in positions at times $t + \Delta t$ and $t - \Delta t$ by $2\Delta t$ as shown in Eq. 2.10.

2.2.2.2 GEAR PREDICTOR-CORRECTOR ALGORIHM

The predictor-corrector methods have three basic steps. First, new positions, velocities, accelerations and high-order terms are predicted by the Taylor series expansions. Second, the forces are evaluated at the new positions to give accelerations $a^c(t + \Delta t)$. These accelerations are compared with the accelerations that are predicted from Taylor series expansion $a^p(t + \Delta t)$. The difference between the predicted and calculated accelerations is used to correct the positions, velocities and so on, in correction step. The position of atom at time t is expressed as $r(t)$. The new position $r^p(t + \Delta t)$, velocity $v^p(t + \Delta t)$, acceleration $a^p(t + \Delta t)$ and differential acceleration $b^p(t + \Delta t)$ at time $t + \Delta t$ is predicted by Taylor series expansion about $r(t)$ and showed as Eqs. 2.12.

$$\begin{aligned}
r^P(t + \Delta t) &= r(t) + v(t)\Delta t + \frac{1}{2}a(t)(\Delta t)^2 + \frac{1}{6}b(t)(\Delta t)^3 + \frac{1}{24}c(t)(\Delta t)^4 + \dots \\
v^P(t + \Delta t) &= v(t) + a(t)\Delta t + \frac{1}{2}b(t)(\Delta t)^2 + \frac{1}{6}c(t)(\Delta t)^3 + \dots \\
a^P(t + \Delta t) &= a(t) + b(t)\Delta t + \frac{1}{2}c(t)(\Delta t)^2 + \dots \\
b^P(t + \Delta t) &= b(t) + c(t)\Delta t + \dots
\end{aligned} \tag{2.12}$$

Here, accelerations $a^c(t+\Delta t)$ calculated with forces is compared with $a^P(t+\Delta t)$ predicted by Taylor series expansions, and positions, velocities and accelerations are corrected with $\Delta a(t+\Delta t)$. The corrected equations are shown as follows;

$$\Delta a(t + \Delta t) = a^c(t + \Delta t) - a^P(t + \Delta t), \tag{2.13}$$

and

$$\begin{aligned}
r^c(t + \Delta t) &= r^P(t + \Delta t) + c_0 \Delta a(t + \Delta t) \\
v^c(t + \Delta t) &= v^P(t + \Delta t) + c_1 \Delta a(t + \Delta t) \\
a^c(t + \Delta t) &= a^P(t + \Delta t) + c_2 \Delta a(t + \Delta t) \\
b^c(t + \Delta t) &= b^P(t + \Delta t) + c_3 \Delta a(t + \Delta t)
\end{aligned} \tag{2.14}$$

Gear has suggested the best values of the coefficients c_0 , c_1 , c_2 and c_3 . These coefficients are dependent on the order of Taylor series expansion. In Gear predictor-corrector algorithm, if the time step is finely divided, the calculated results of positions, velocities and accelerations can be precisely obtained.

2.2.3 STATISTIC ENSEMBLE

2.2.3.1 MICROCANONICAL (NVE) ENSEMBLE

In the microcanonical ensemble, the number of particles N , the volume V and the energy E are conserved. It means that a microcanonical molecular dynamics trajectory can be seen as an exchange of kinetic energy and potential energy.

$$H_0 = \sum_{i=1}^N p_i^2 / 2m_i + \Phi(r) = \text{const.}, \tag{2.15}$$

where p_i is momentum of particle i , m_i is mass and $\Phi(r)$ is the potential energy as shown

in Eq. 2.6.

2.2.3.2 CANONICAL (NVT) ENSEMBLE

The macroscopic properties are often measured under a constant temperature or a constant pressure. In the canonical ensembles, the number of particles N , the volume V and the temperature T , or the pressure P are treated as constants. This subsection summarizes the NVT ensemble proposed by Nose and Hoover [4, 5]. Their approaches add to the energy function a fictitious degree of freedom s , which represents a heat bath. The simultaneous equations are indicated with Eq. 2.16,

$$\begin{aligned} \frac{dr_i}{dt} &= \frac{p_i}{m_i} \\ \frac{dp_i}{dt} &= -\frac{\partial \Phi}{\partial r_i} - \mathcal{P}_i \\ \frac{d\zeta}{dt} &= \frac{1}{Q} \left\{ \sum_{i=1}^N \frac{p_i^2}{m_i} - 3NkT \right\} \\ \frac{1}{s} \frac{ds}{dt} &= \zeta \end{aligned} \tag{2.16}$$

The Hamiltonian of this system and the time-scale variable s in terms of the variables is postulated as

$$H = \sum_{i=1}^N p_i^2 / 2m_i + \Phi(r) + (N+1)kT \ln s + \frac{p_s^2}{2Q}, \tag{2.17}$$

where p_i is momentum of particle, s is position degree of freedom for hot bath, Q is a parameter of dimension energy and behaves as a mass for motion of s , k is Boltzmann's constant. Here, the system is coupled to a heat bath with N degree of freedom.

2.2.4 POTENTIAL ENERGIES WITH UNIVERSAL FORCE FIELDS

Verlet algorithm uses the positions and accelerations at time t , and the positions from the previous step $r(t-\Delta t)$ to calculate the new positions $r(t+\Delta t)$ at time $t+\Delta t$ (see Eq. 2.11). Also, the velocities are calculated by dividing the difference in positions at times $t+\Delta t$ and $t-\Delta t$ by $2\Delta t$ as shown in Eq. 2.10. The potential energies of the system are calculated with the results of positions and accelerations with Verlet algorithm. The

universal force field can be calculated in a lot of atoms. Table 2.1 shows the atomic data with UFF.

Table 2.1 Atomic Data [6]

atom type	valence		nonbond			effective charge Z_1^{*d}	atom type	valence		nonbond			effective charge Z_1^{*d}
	bond r_1^a	angle θ_0^b	distance x_1^c	energy D_1^c	scale ζ			bond r_1^a	angle θ_0^b	distance x_1^c	energy D_1^c	scale ζ	
H ₁	0.354	180.0	2.886	0.044	12.0	0.712	Ru6+2	1.478	90.0	2.963	0.056	12.0	3.40
H _{1b}	0.460	83.5	2.886	0.044	12.0	0.712	Rh6+3	1.332	90.0	2.929	0.053	12.0	3.508
He4+4	0.849	90.0	2.362	0.056	15.24	0.098	Pd4+2	1.338	90.0	2.899	0.048	12.0	3.21
Li	1.336	180.0	2.451	0.025	12.0	1.026	Ag1+1	1.386	180.0	3.148	0.036	12.0	1.956
Be3+2	1.074	109.47	2.745	0.085	12.0	1.565	Cd3+2	1.403	109.47	2.848	0.228	12.0	1.65
B ₁	0.838	109.47	4.083	0.180	12.052	1.755	In3+3	1.459	109.47	4.463	0.599	11.0	2.07
B ₁	0.828	120.0	4.083	0.180	12.052	1.755	Sn3	1.398	109.47	4.392	0.567	12.0	2.961
C ₁	0.757	109.47	3.851	0.105	12.73	1.912	Sb3+3	1.407	91.6	4.420	0.449	13.0	2.704
C _{1R}	0.729	120.0	3.851	0.105	12.73	1.912	Te3+2	1.386	90.25	4.470	0.398	14.0	2.882
C ₁	0.732	120.0	3.851	0.105	12.73	1.912	I ₁	1.382	180.0	4.50	0.339	15.0	2.65
C ₁	0.706	180.0	3.851	0.105	12.73	1.912	Xe4+4	1.267	90.0	4.404	0.332	12.0	0.556
N ₁	0.700	106.7	3.660	0.069	13.407	2.544	Cs	2.570	180.0	4.517	0.045	12.0	1.573
N _{1R}	0.699	120.0	3.660	0.069	13.407	2.544	Ba6+2	2.277	90.0	3.703	0.364	12.0	2.727
N ₁	0.685	111.2	3.660	0.069	13.407	2.544	La3+3	1.943	109.47	3.522	0.017	12.0	3.30
N ₁	0.656	180.0	3.660	0.069	13.407	2.544	Ce6+3	1.841	90.0	3.556	0.013	12.0	3.30
O ₁	0.658	104.51	3.500	0.060	14.085	2.300	Pr6+3	1.823	90.0	3.606	0.010	12.0	3.30
O ₁	0.528	146.0	3.500	0.060	14.085	2.300	Nd6+3	1.816	90.0	3.575	0.010	12.0	3.30
O _{1R}	0.680	110.0	3.500	0.060	14.085	2.300	Pm6+3	1.801	90.0	3.547	0.009	12.0	3.30
O ₁	0.634	120.0	3.500	0.060	14.085	2.300	Sm6+3	1.780	90.0	3.520	0.008	12.0	3.30
O ₁	0.639	180.0	3.500	0.060	14.085	2.300	Eu6+3	1.771	90.0	3.493	0.008	12.0	3.30
F ₁	0.668	180.0	3.364	0.050	14.762	1.735	Gd6+3	1.735	90.0	3.368	0.009	12.0	3.30
Ne4+4	0.920	90.0	3.243	0.042	15.440	0.194	Tb6+3	1.732	90.0	3.451	0.007	12.0	3.30
Na	1.539	180.0	2.983	0.030	12.0	1.081	Dy6+3	1.710	90.0	3.428	0.007	12.0	3.30
Mg3+2	1.421	109.47	3.021	0.111	12.0	1.787	Ho6+3	1.696	90.0	3.409	0.007	12.0	3.416
Al3	1.244	109.47	4.499	0.505	11.278	1.792	Er6+3	1.673	90.0	3.391	0.007	12.0	3.30
Si3	1.117	109.47	4.295	0.402	12.175	2.323	Tm6+3	1.660	90.0	3.374	0.006	12.0	3.30
P ₁ +3	1.101	93.8	4.147	0.305	13.072	2.863	Yb6+3	1.637	90.0	3.355	0.228	12.0	2.618
P ₁ +5	1.056	109.47	4.147	0.305	13.072	2.863	Lu6+3	1.671	90.0	3.640	0.041	12.0	3.271
P ₁ +q	1.056	109.47	4.147	0.305	13.072	2.863	Hf3+4	1.611	109.47	3.141	0.072	12.0	3.921
S ₁ +2	1.064	92.1	4.035	0.274	13.969	2.703	Ta3+5	1.511	109.47	3.170	0.081	12.0	4.075
S ₁ +4	1.049	103.20	4.035	0.274	13.969	2.703	W ₁ +6	1.392	90.0	3.069	0.067	12.0	3.70
S ₁ +6	1.027	109.47	4.035	0.274	13.969	2.703	W ₁ +4	1.526	109.47	3.069	0.067	12.0	3.70
S _{1R}	1.077	92.2	4.035	0.274	13.969	2.703	W ₁ +6	1.380	109.47	3.069	0.067	12.0	3.70
S ₁	0.854	120.0	4.035	0.274	13.969	2.703	Re6+5	1.372	90.0	2.954	0.066	12.0	3.70
Cl	1.044	180.0	3.947	0.227	14.866	2.348	Re3+7	1.314	109.47	2.954	0.066	12.0	3.70
Ar4+4	1.032	90.0	3.868	0.185	15.763	0.300	Os6+6	1.372	90.0	3.120	0.037	12.0	3.70
K ₁	1.953	180.0	3.812	0.035	12.0	1.165	Ir6+3	1.371	90.0	2.840	0.073	12.0	3.731
Ca6+2	1.761	90.0	3.399	0.238	12.0	2.141	Pt4+2	1.364	90.0	2.754	0.080	12.0	3.382
Sc3+3	1.513	109.47	3.295	0.019	12.0	2.592	Au4+3	1.262	90.0	3.293	0.039	12.0	2.625
Ti3+4	1.412	109.47	3.175	0.017	12.0	2.659	Hg1+2	1.340	180.0	2.705	0.385	12.0	1.75
Ti6+4	1.412	90.0	3.175	0.017	12.0	2.659	Tl3+3	1.518	120.0	4.347	0.680	11.0	2.068
V ₁ +5	1.402	109.47	3.144	0.016	12.0	2.679	Pb3	1.459	109.47	4.297	0.663	12.0	2.846
Cr6+3	1.345	90.0	3.023	0.015	12.0	2.463	Bi3+3	1.512	90.0	4.370	0.518	13.0	2.470
Mn6+2	1.382	90.0	2.961	0.013	12.0	2.43	Po3+2	1.50	90.0	4.709	0.325	14.0	2.33
Fe3+2	1.270	109.47	2.912	0.013	12.0	2.43	At	1.545	180.0	4.750	0.284	15.0	2.24
Fe6+2	1.335	90.0	2.912	0.013	12.0	2.43	Rn4+4	1.420	90.0	4.765	0.248	16.0	0.583
Co6+3	1.241	90.0	2.872	0.014	12.0	2.43	Fr	2.880	180.0	4.90	0.050	12.0	1.847
Ni4+2	1.164	90.0	2.834	0.015	12.0	2.43	Ra6+2	2.512	90.0	3.677	0.404	12.0	2.92
Cu3+1	1.302	109.47	3.495	0.005	12.0	1.756	Ac6+3	1.983	90.0	3.478	0.033	12.0	3.90
Zn3+2	1.193	109.47	2.763	0.124	12.0	1.308	Th6+4	1.721	90.0	3.396	0.026	12.0	4.202
Ga3+3	1.260	109.47	4.383	0.415	11.0	1.821	Pa6+4	1.711	90.0	3.424	0.022	12.0	3.90
Ge3	1.197	109.47	4.280	0.379	12.0	2.789	U ₁ +4	1.684	90.0	3.395	0.022	12.0	3.90
As3+3	1.211	92.1	4.230	0.309	13.0	2.864	Np6+4	1.666	90.0	3.424	0.019	12.0	3.90
Se3+2	1.190	90.6	4.205	0.291	14.0	2.764	Pu6+4	1.657	90.0	3.424	0.016	12.0	3.90
Br	1.192	180.0	4.189	0.251	15.0	2.519	Am6+4	1.660	90.0	3.381	0.014	12.0	3.90
Kr4+4	1.147	90.0	4.141	0.220	16.0	0.452	Cm6+3	1.801	90.0	3.326	0.013	12.0	3.90
Rb	2.260	180.0	4.114	0.04	12.0	1.592	Bk6+3	1.761	90.0	3.339	0.013	12.0	3.90
Sr6+2	2.052	90.0	3.641	0.235	12.0	2.449	Cf6+3	1.750	90.0	3.313	0.013	12.0	3.90
Y ₁ +3	1.698	109.47	3.345	0.072	12.0	3.257	Es6+3	1.724	90.0	3.299	0.012	12.0	3.90
Zr3+4	1.564	109.47	3.124	0.069	12.0	3.667	Fm6+3	1.712	90.0	3.286	0.012	12.0	3.90
Nb3+5	1.473	109.47	3.165	0.059	12.0	3.618	Md6+3	1.689	90.0	3.274	0.011	12.0	3.90
Mo6+6	1.467	90.0	3.052	0.056	12.0	3.40	No6+3	1.679	90.0	3.248	0.011	12.0	3.90
Mo3+6	1.484	109.47	3.052	0.056	12.0	3.40	Lw6+3	1.698	90.0	3.236	0.011	12.0	3.90
Tc6+5	1.322	90.0	2.998	0.048	12.0	3.40							

^aÅ. ^bDegrees. ^ckcal/mol. ^dCharge.

2.2.4.1 FORCE FIELD

The potential energy of an arbitrary geometry for a molecule is written as a superposition of two, three and four body interactions. The potential energy is expressed as bonded and nonbonded interactions [6];

$$E = E_R + E_\theta + E_\phi + E_\omega + E_{vdw} + E_{el} , \quad (2.18)$$

where E_R is the bond stretching term, E_θ is the bond angle bending term, E_ϕ is the dihedral angle torsion term, E_ω is the inversion term, E_{vdw} is the van der Waals term, and E_{el} is the electrostatic term. The E_R , E_θ , E_ϕ and E_ω show the potential energy of bonded interactions in the molecule, and the E_{vdw} and E_{el} show that of nonbonded interactions of the intermolecular.

2.2.4.2 BOND STRETCHING

Figure 2.1 shows the schematic of bond stretch interaction between the atoms i and j . This potential energy E_R is described as Morse function in Eq. 2.19.

$$E_R = D_{ij}(e^{-\alpha(r-r_{ij})} - 1)^2 , \quad (2.19)$$
$$\alpha = \sqrt{k_{ij} / 2D_{ij}}$$

where k_{ij} is the force constant, r_{ij} is the standard or natural bond length, and D_{ij} is the bond dissociation energy shown in Figure 2.1. The Morse function is a more accurate description than the function with a harmonic oscillator, since it implicitly includes harmonic terms near equilibrium (r_{ij}) and leads to a finite energy (D_{ij}) for breaking bonds.

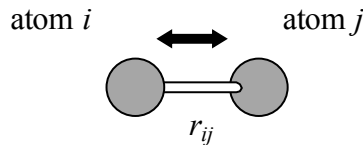


Figure 2.1 Schematic of bond stretch interaction between atoms i and j .

2.2.4.3 BOND ANGLE BENDING

Figure 2.2 shows the schematic of bond angle bending composed of atoms i, j and k . The bond angle θ is positioned between bonds ij and ik . In UFF, all angular distortions are described with General Fourier expansions as shown in Eq. 2.20. The expansions can express to have derivatives that are singularity free, to have the appropriate distortions for the large amplitude motions in MD, and so the coefficients C_n can be straightforwardly chosen to satisfy appropriate boundary conditions. The angle bend term is expressed with a cosine Fourier expansion in θ .

$$E_\theta = K_{ijk} \sum_{n=0}^m C_n \cos n\theta, \quad (2.20)$$

where the coefficients C_n are chosen to satisfy appropriate boundary condition including that the function have a minimum at the natural bond angle θ_0 .

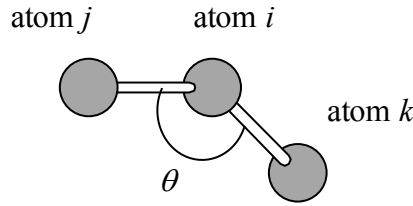


Figure 2.2 Schematic of bond angle bending between bonds ij and ik .

2.2.4.4 DIHEDRAL ANGLE TORSION

The torsional terms for two bond ij and kl connected via a common bond jk is described with a small cosine Fourier expansion in ϕ . Figure 2.3 shows the schematic of dihedral angle torsion with the angle ϕ_{ijkl} between the planes ijk and jkl .

$$E_\phi = K_{ijkl} \sum_{n=0}^m C_n \cos n\phi_{ijkl}, \quad (2.21)$$

where K_{ijkl} and C_n are determined by the torsional barrier V_ϕ , the periodicity of potential and equilibrium angle. Here, the rotational term E_ϕ is expressed with DREIDING force field [7] with modifications to the torsional barrier V_ϕ into Eq. 2.22.

$$E_\phi = \frac{1}{2} V_\phi [1 - \cos n\phi_0 \cos n\phi], \quad (2.22)$$

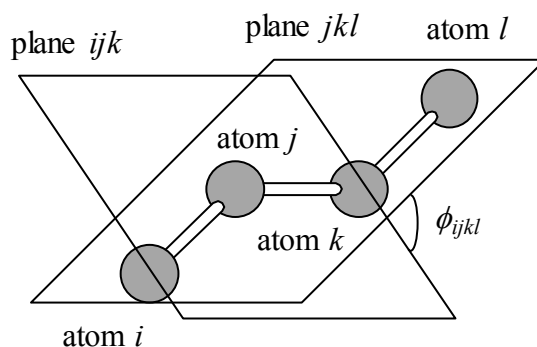


Figure 2.3 Schematic of dihedral angle torsion between planes ijk and jkl .

2.2.4.5 INVERSION

Figure 2.4 shows the schematic of an inversion with angle ω_{ijkl} between the plane ijk and the bond il . A one- or two-term cosine Fourier expansion in w is used for atom i bonded exactly to three other atoms j , k and l . Here, the inversion term E_ω is expressed with Eq. 2.23.

$$E_w = K_{ijkl}(C_0 + C_1 \cos w_{ijkl} + C_2 \cos 2w_{ijkl}), \quad (2.23)$$

where K_{ijkl} is the force constant and w_{ijkl} is the angle between the il axis and the ijk plane. The central atom i has three axes (il , ij and ik) which present each inversion barrier being divided by the number of inversions for central atom i .

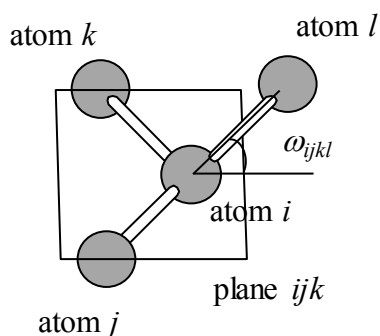


Figure 2.4 Schematic of inversion between plane ijk and bond il .

2.2.4.6 VAN DER WAALS

Distance-dependent interactions between atoms or molecules are van der Waals forces. The forces include attraction and repulsion between atoms or molecules, which are described with the Lennard-Jones type expression in UFF. Figure 2.5 shows the schematic of van der Waals with the distance x_{ij} between the atoms i and j .

$$E_{vdw} = D_{ij} \left\{ -2 \left(\frac{x_{ij}}{x} \right)^6 + \left(\frac{x_{ij}}{x} \right)^{12} \right\}, \quad (2.24)$$

where D_{ij} is the well depth and x_{ij} is the van der Waals bond length. The general x_{ij} and D_{ij} are obtained from the homonuclear parameter through the use of combination rules as shown in Eqs. 2.25.

$$x_{ij} = \frac{1}{2}(x_i + x_j), \quad (2.25)$$

$$D_{ij} = \sqrt{D_i \times D_j},$$

where x_i is the atomic van der Waals distance, and D_i is the atomic van der Waals energy.

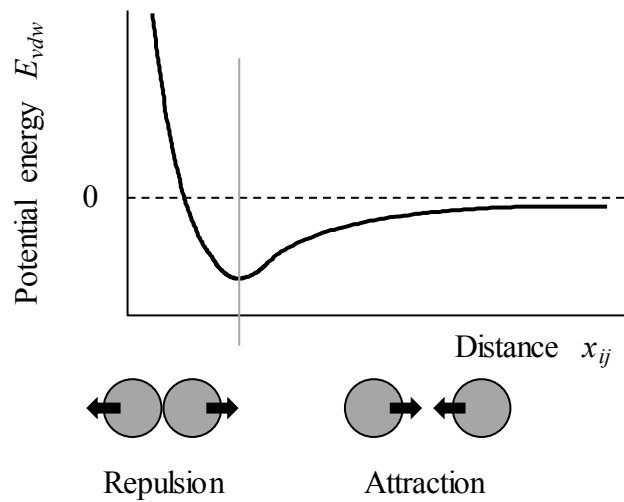


Figure 2.5 Schematic of van der Waals forces.

2.2.4.7 ELECTROSTATIC INTERACTIONS

Figure 2.6 shows the schematic of electrostatic force of the distance x_{ij} between the atoms i and j with charges of Q_i and Q_j , respectively. The electrostatic interactions without the bond interaction are calculated based-on Coulomb's law and expressed by Eq. 2.26.

$$E_{el} = \frac{332.0637Q_iQ_j}{\epsilon r_{ij}}, \quad (2.26)$$

where Q_i and Q_j are charges in electron units, r_{ij} is the distance between atoms i and j , and ϵ is the dielectric constant. The dielectric constant is defaulted to 1 for UFF.

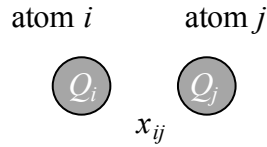


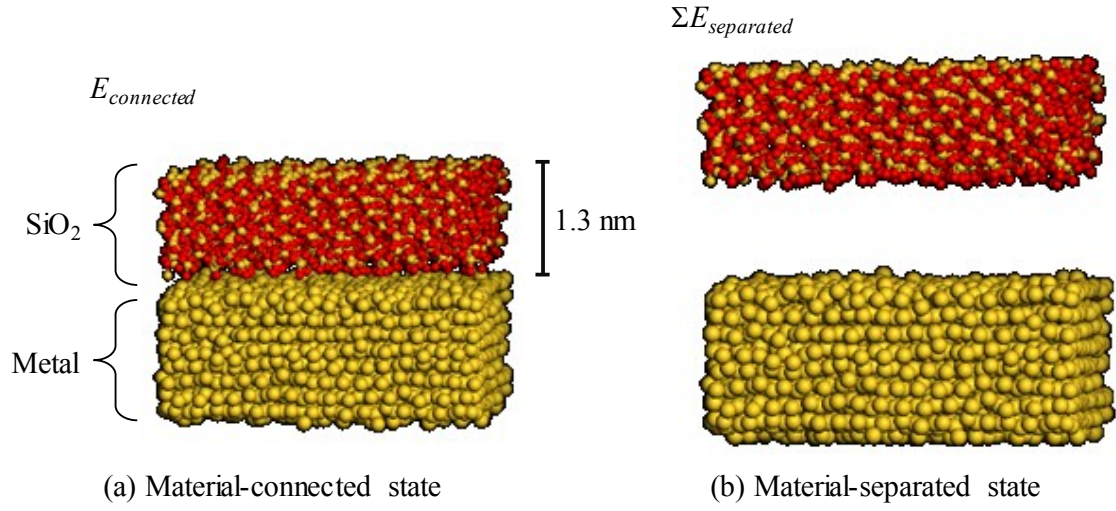
Figure 2.6 Schematic of electrostatic force.

2.3 ANALYSIS METHOD OF ADHESION STRENGTH

Figures 2.7 show an example MD model used for adhesion analysis of metal and silicon oxide layers. The adhesion strength is estimated by calculating the adhesion fracture energy E_{local} defined as the difference between the total potential energy of the material-connected state in Fig. 2.7(a), $E_{connected}$ and that of the material-separated state in Fig. 2.7(b), $E_{separated}$, expressed by Eq. 2.27 [8, 9]. These potential energies are calculated with UFF and Vertlet algorithm.

$$-E_{local} = E_{connected} - \sum E_{separated}, \quad (2.27)$$

$E_{connected}$ is equivalent to the total potential energy after the 1st relaxation calculation. $E_{separated}$ is defined as the sum of potential energies obtained from the 2nd relaxation calculation for MD models separated at one interface between the layers after the 1st relaxation calculation. E_{local} is defined with the interaction energy between separated atomic segments.



Figures 2.7 MD models of adhesive fracture energy E_{local} .

2.4 CONCLUSIONS

In this chapter, the MD simulations were summarized. The adhesive fracture energy between metal and silicon oxide layers is analytically and experimentally shown in chapter 3. In chapter 4, MD simulations were utilized to find a reasonable eutectic bonding condition to establish a reliable eutectic-based WLP accelerometer hermetically sealed in atmospheric pressure.

REFERENCES

- [1] D. W. Heermann, "Computer Simulation Methods in Theoretical Physics", Springer-Verlag Berlin Heidelberg, 1986 and 1990
- [2] L. Verlet, "Computer "Experiments" on Classical Fluids. I. Thermodynamic Properties of Lenard-Jones Molecules", *Phy. Review*, Vol. 159, No. 1, pp. 98-103, 1967
- [3] C. W. Gear, "The Automatic Integration of Ordinary Differential Equations", *Num. Math.*, Vol. 14, No. 3, pp. 176-179, 1971
- [4] S. Nose, "A unified formulation of the constant temperature molecular dynamics methods", *J. Chem. Phys.*, Vol. 81, No. 1, pp. 511-519, 1984
- [5] W. G. Hoover, "Canonical dynamics: Equilibrium phase-space distributions", *Phy. Review A*, Vol. 31, No. 3, pp. 1695-1697, 1985
- [6] A. K. Rappe, C. J. Casewit, K. S. Colwell, W. A. Goddard III and W. M. Skiff, "UFF, a Full Periodic Force Field for Molecular Mechanics and Molecular Dynamics Simulation", *J. Am. Chem. Soc.*, 114, pp. 10024-10035, 1992
- [7] S. L. Mayo, B. D. Olafson and W. A. Goddard, "DREIDING: A Generic Force Field for Molecular Simulations", *J. Phys. Chem.*, 94, pp. 8897-8909, 1990
- [8] T. Iwasaki, "Molecular dynamics study of adhesion strength and diffusion at interfaces between interconnect materials and underlay materials", *Comput. Mech.*, 25, pp. 78-86, 2000
- [9] T. Iwasaki, "Molecular dynamics study of diffusion and atomic configuration layered structures for Al circuit interconnects", *Comput. Mech.*, 24, pp. 148-154, 1999

Chapter 3: Evaluation of Fabricating Method for Multilevel Interconnection Structures Using Differential Adhesive Fracture Energies between Metal and Silicon Oxide Thin Films

3.1 INTRODUCTION

With the increasing integration of functional elements, the recent micro electromechanical systems (MEMS) used as communication devices [1, 2], fluidic devices [3, 4], and the like are designed with multilevel space-wired interconnections to output electrical signals to external devices connected to the device electrodes.

When fabricating multilevel interconnection structures in semiconductor processes, an insulating film is deposited on the lower aluminum (Al) wiring, and contact vias are formed to connect the lower and upper wiring. A seed layer is then deposited on the entire substrate, and damascene process is employed to form contact areas by copper electroplating and chemical mechanical polishing (CMP) [5]. To improve the performance of functional elements in MEMS devices, metal materials other than Al are often used for elements and interconnections from the viewpoint of low resistance, heat resistance and catalytic functions. However, this raises the problem of insufficient adhesive strength (adhesive fracture energy) between the substrate and insulating film. Low-adhesion materials can be used in combination with high-adhesion materials in layered metal films [6].

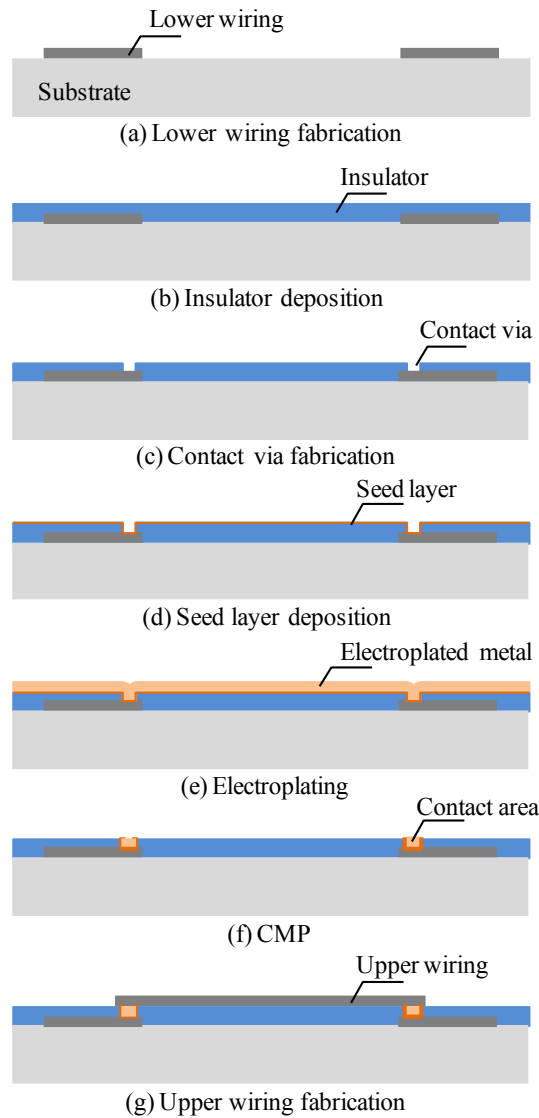
In addition, in conventional semiconductor processes, contact vias are filled by electroplating, which is likely to result in seams and voids in the contact areas. Bottom-up plating, in which metal films are grown from the lower wiring, has been used to reduce such seams and voids [7]. In that method, metal films can also grow from the sidewalls of contact vias, depending on the concentration of additives in the plating solution, its agitation conditions, and so on, which may cause seams and voids.

The purpose of this investigation was the fabrication of multilevel interconnection structures for MEMS devices using various metal materials. In particular, we devised a new fabrication process that includes (1) the use of lower wiring in which a metal with low adhesion to the SiO₂ film is placed between high-adhesion metals, (2) a method of reducing seams and voids by bottom-up growth of contact areas on the lower wiring by electroplating, and (3) a method of easily removing only the SiO₂ film on the contact areas by providing the lower wiring and the contact areas with selective adhesion to SiO₂ film.

3.2 FABRICATION OF MULTILEVEL INTERCONNECTION STRUCTURES

3.2.1 CONVENTIONAL FABRICATING METHOD

The conventional fabrication process for multilevel interconnection structures is illustrated in Figures 3.1. In the conventional process, the Al wiring is first formed on the substrate [see Fig. 3.1(a)], and then the insulating film is deposited [see Fig. 3.1(b)]. Next, contact vias are formed by lithography and etching where the lower wiring is to be connected to the upper wiring [see Fig. 3.1(c)]. A seed layer is deposited on the contact vias [see Fig. 3.1(d)], and a metal film is formed by electroplating [see Fig. 3.1(e)]. This metal film is then polished by CMP down to the contact vias to form contact areas [see Fig. 3.1(f)]. Finally, the upper wiring is deposited to connect the contact vias, thus forming a multilevel interconnection structure [see Fig. 3.1(g)].



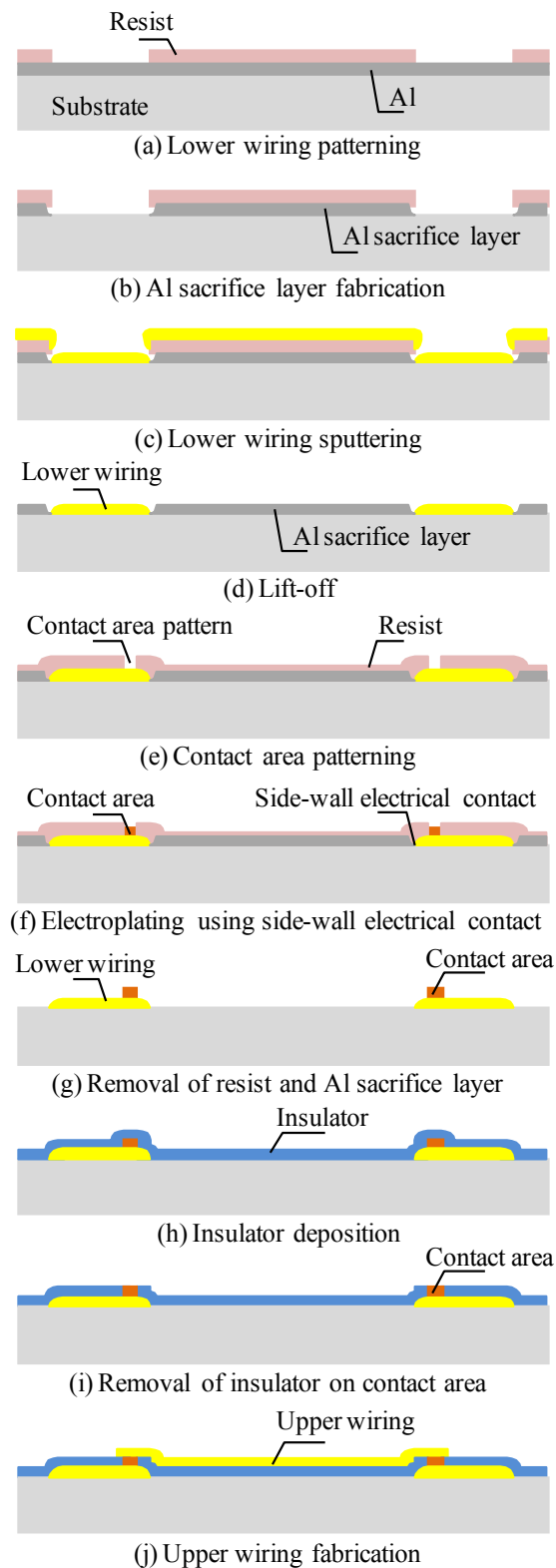
Figures 3.1 Conventional process flow of multilevel interconnection structure.

3.2.2 NEW PROPOSAL FABRICATING METHOD

Figures 3.2(a) to (j) depict a new process for fabrication of multilevel interconnection structures by using the difference in adhesive fracture energy (adhesive strength) between the insulating film and the contact areas as proposed in this paper.

Al is sputtered onto the substrate, and then a lower wiring pattern is formed by lithography [see Fig. 3.2(a)]. Then, the Al film is etched to create an Al-sacrificing layer [see Fig. 3.2(b)]. Next, a metal with high adhesion to the substrate, a conductive metal film and a metal with high adhesion to the insulating film are sputtered in sequence [see Fig. 3.2(c)], and the lower wiring is formed by liftoff [see Fig. 3.2(d)]. Here, the Al-sacrificing layer and the lower wiring are in contact at the sidewalls, and electroplating on the lower wiring can be performed via Al-sacrificing layer using sidewall electrical contact [8]. Then, a contact area pattern is formed by lithography [see Fig. 3.2(e)], and contact areas are created on the lower wiring by electroplating [see Fig. 3.2(f)]. Here, the contact areas are grown from the bottom up on the conductive lower wiring by electroplating, which can prevent seams and voids. After that, the resist and Al-sacrificing layer are removed to obtain the lower wiring with contact areas [see Fig. 3.2(g)]. Next, an insulating film is deposited [see Fig. 3.2(h)], and ultrasonic treatment is applied to remove the insulating film from the contact areas [see Fig. 3.2(i)]. Here, the insulating film can be removed only from the contact areas with low adhesion to the insulating film, while remaining on the lower wiring with high adhesion. Finally, the upper wiring is deposited to connect the contact vias, thus forming a multilevel interconnection structure [see Fig. 3.2(j)].

In the conventional method, a seed layer was formed above all contact vias when they were filled by electroplating. Thus, the metal film was deposited conformally, and seams and voids could easily occur. In the proposed method, the contact areas are grown bottom-up from the lower wiring, which can prevent the formation of seams and voids. In addition, the insulating film on the contact areas can be easily removed by ultrasonic treatment.

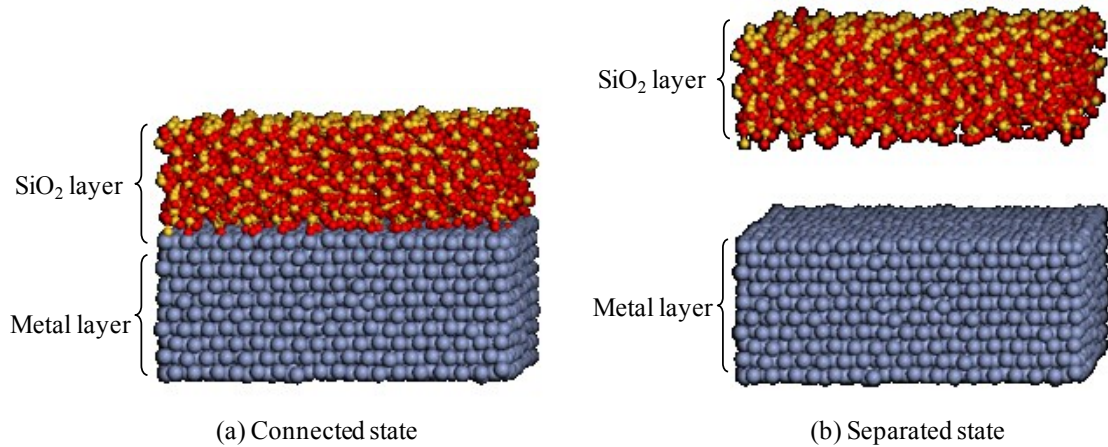


Figures 3.2 Concept of process flow of multilevel interconnection structure using differential adhesive fracture energy.

3.3 DESIGN AND EXPERIMENTAL PROCEDURES

3.3.1 ADHESIVE FRACTURE ENERGY BETWEEN METAL AND SiO₂ FILMS

To examine the adhesive fracture energy between the metal film and the SiO₂ films, we used a molecular dynamics method [9-11] that makes possible the direct analysis of bonds between atomic elements. Figures 3.3 depict the analytical model of interface between the metal and the SiO₂ films.



Figures 3.3 Interconnection model used for molecular dynamics simulations.

In order to calculate the adhesive fracture energy, a metal film and an insulating film are brought into contact as shown in Figure 3.3(a), and a relaxation calculation is performed until the equilibrium state is achieved so as to determine the potential energy in the connected state. This relaxation calculation is based on Newton's equation of motion ($\text{mass} \times \text{acceleration} = \text{force}$). Then, the metal and the insulating films are separated as shown in Figure 3.3(b) to eliminate interaction on the interface, and a relaxation calculation is performed to determine the potential energy in the separated state, again. After that, the difference in potential energy between the connected state and the separated state is found, which gives the energy required to detach the insulating film from the metal film, that is, the adhesive fracture energy. Finally, the different potential energy is divided by the area to obtain the adhesive fracture energy per unit area. In this study, we calculated the adhesive fracture energy between the metals and the SiO₂ films used for the contact areas, namely, Cr, Ti, Cu, Ni and Au.

3.3.2 REMOVAL OF SiO₂ FILM BY ULTRASONIC TREATMENT

We investigated how the metal material and pattern size affect the process of removal of the SiO₂ film from the contact areas by ultrasonic treatment [see Fig. 3.2(i)]. In particular, we considered $100 \times 100\text{-}\mu\text{m}$ patterns of electroplated $1.0\text{-}\mu\text{m}$ -thick Au,

Cu and Ni films and sputtered 1.0- μm -thick SiO_2 . As regards the plating solutions, we used MICROFAB Au310, MICROFAB Cu300 and MICROFAB Ni200 produced by Electroplating Engineers of Japan. Then, the substrates were immersed in pure water and treated for 5 min in an ultrasonic bath (W-338 BAKUSEN by Honda Electronics). This ultrasonic cleaner is provided with a Dyna Shock system, featuring fast switching between three oscillation frequencies (28 kHz, 40 kHz and 100 kHz). The power output was set at its maximum of 600 W. After ultrasonic cleaning, the state of removal of the SiO_2 film from the contact areas was observed by scanning electron microscopy (SEM) and energy dispersive X-ray spectrometry (EDX). The pattern size of contact areas was 10×10 to 50×50 - μm ; 1.0- μm -thick Au film was electroplated, and 1.0- μm -thick SiO_2 film was sputtered. Next, the silicon substrates were immersed in pure water and the state of removal of the SiO_2 film in the contact areas after ultrasonic treatment was observed by SEM.

3.3.3 FABRICATION OF MULTILEVEL INTERCONNECTION STRUCTURES

A schematic illustration and the fabrication process of the multilevel interconnection structure are shown in Figure 3.4 and Figures 3.5, respectively. The multilevel interconnection structure is composed of lower wiring, SiO_2 film, contact areas and upper wiring. The upper wiring and lower wiring are connected via the contact areas, and the crossing parts are insulated by the SiO_2 film.

A 1.0- μm -thick Al film is formed on an Si substrate with a thermal-oxide layer [see Fig. 3.5(a)]. The resist pattern for the electrodes and lower wiring is formed by lithography, and an Al-sacrificing layer is formed by etching of the Al film with a mixed aqueous solution of H_3PO_4 (75 %), CH_3COOH (15 %), and HNO_3 (5 %) [see Fig. 3.5(b)]. Next, a metal film for the electrodes and lower wiring is formed by sputtering Ti 50 nm/Pt 200 nm/Au 200 nm/Pt200 nm/Ti 50 nm [see Fig. 3.5(c)], and the electrodes and lower wiring are formed by liftoff [see Fig. 3.5(d)]. Here, Ti is an adhesion layer, Pt is a diffusion prevention layer and Au is a conductive layer. Adhesion to the Si substrate and the SiO_2 film is improved by placing the conductive layer between the adhesion layers. Next, the resist pattern for contact areas connecting the electrodes and lower wiring with upper wiring is formed, while leaving the Al-sacrificing layer unaltered [see Fig. 3.5(e)]. Because electroplating is difficult to perform on the Ti adhesion layer, the Ti film is removed by etching with 1-wt% HF solution, and 1.0- μm -thick Au (MICROFAB Au310) is electroplated onto the Pt diffusion prevention layer by sidewall electrical contact using the Al-sacrificing layer [see Fig. 3.5(f)]. After removing the resist and the Al-sacrificing layer [see Fig. 3.5(g)], an SiO_2 film is sputtered to insulate

the lower wiring and the upper wiring [see Fig. 3.5(h)]. The substrate is immersed in pure water, and ultrasonic treatment is performed to remove the SiO_2 film from the electrode and the contact areas [see Fig. 3.5(i)]. Next, a 1.0- μm -thick Al film is deposited and the resist pattern for upper wiring is formed by lithography. After that, the Al-sacrificing layer formed by etching of the Al film with a mixed aqueous solution of H_3PO_4 (75 %), CH_3COOH (15 %), and HNO_3 (5 %) [see Fig. 3.5(j)]. The metal film of the upper wiring formed by sputtering of Ti 50 nm/Pt 200 nm/Au 200 nm (Figure 3.5(k)), and the upper wiring is formed by liftoff [see Fig. 3.5(l)]. Next, the resist pattern is formed on the upper wiring [see Fig. 3.5(m)], and 1.0- μm -thick Al is deposited by sidewall electrical contact [see Fig. 3.5(n)]. Finally, the resist and Al-sacrificing layer are removed to obtain the multilevel interconnection structure [see Fig. 3.5(o)].

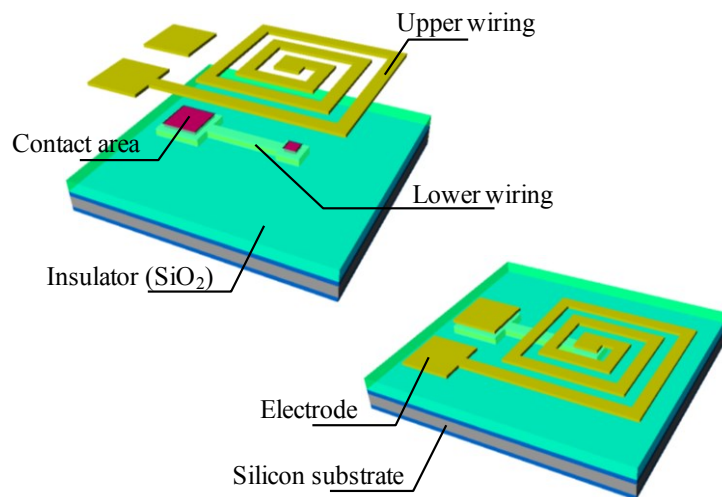
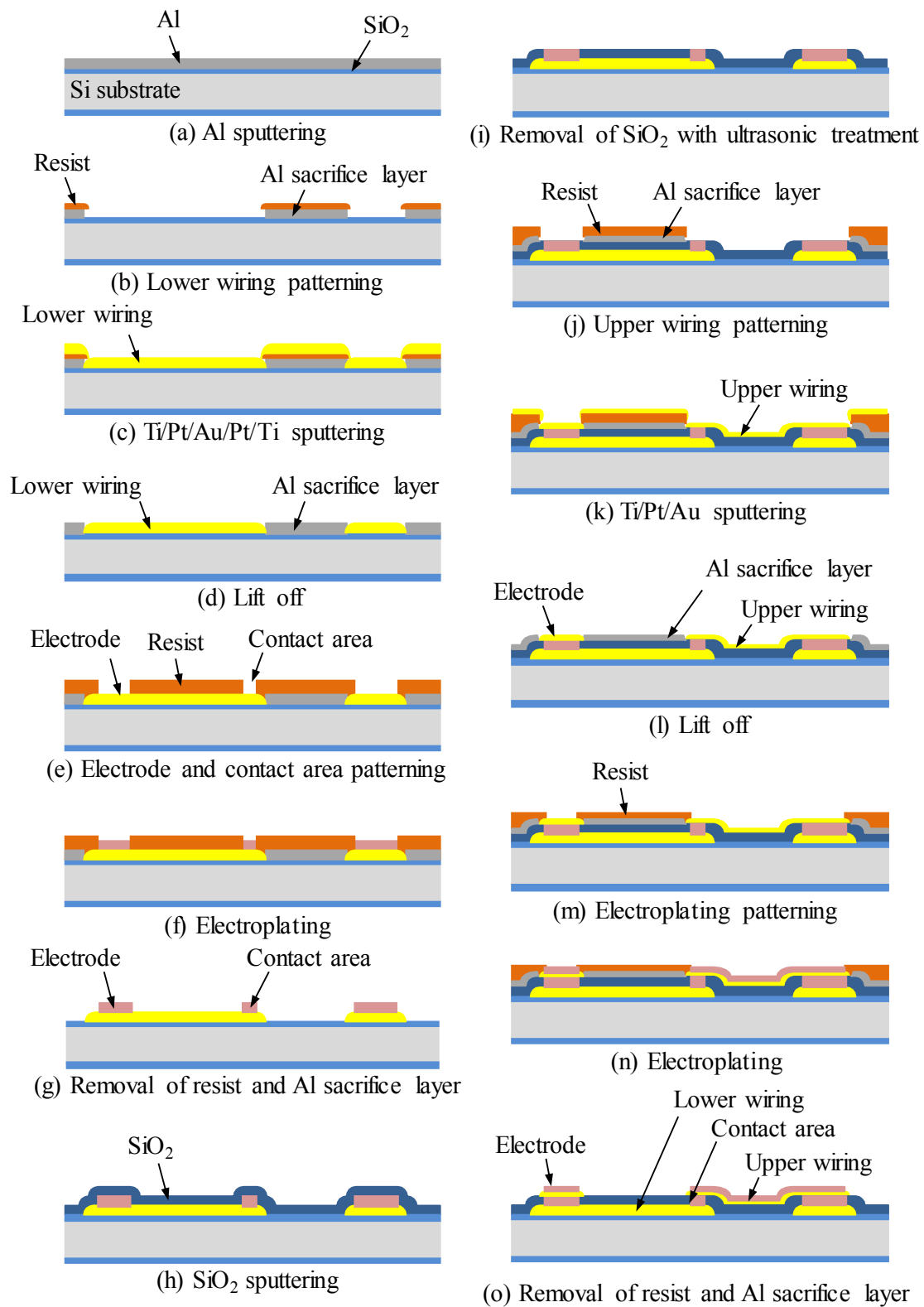


Figure 3.4 Schematic illustration of multilevel interconnection structure.



Figures 3.5 Process flow of multilevel interconnection structure.

3.4 RESULTS AND DISCUSSIONS

3.4.1 ADHESIVE FRACTURE ENERGY BETWEEN METAL AND SiO₂ FILMS

The adhesion strength (adhesive fracture energy) between the metal films and SiO₂ film calculated by the molecular dynamics method is shown in Figure 3.6. In particular, the adhesive fracture energy was 0.562 J/m² for Cr, 0.369 J/m² for Ti, 0.247 J/m² for Ni, 0.134 J/m² for Cu and 0.100 J/m² for Au. Thus, the adhesive fracture energy decreases Cr, Ti, Ni, Cu and Au in this order, which has adhesion strength shown in references [11, 12]. These results provide guidelines for selecting appropriate materials for the lower wiring and contact areas. The Ni, Cu and Au contact areas were prepared with electroplating on the lower wiring [see Fig. 3.2(c)], and were evaluated the process of removing the SiO₂ film from the contact areas by ultrasonic treatment [see Fig. 3.2(f)].

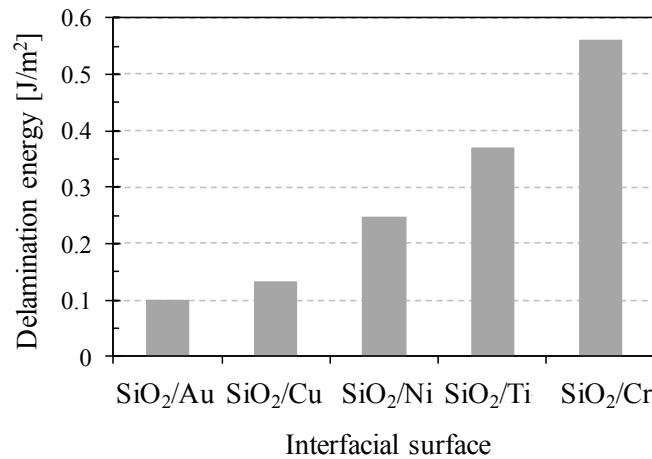


Figure 3.6 Calculated results of adhesive fracture energies between metal and SiO₂ films using molecular dynamics.

3.4.2 REMOVAL OF SiO₂ FROM ELECTRODES AND CONTACT AREAS

Figure 3.7 shows an SEM image of the Au contact area after the ultrasonic treatment. Figures 3.8 show EDX results on the contact area and the lower wiring.

As can be seen from Figure 3.7 and Figures 3.8, Au is only detected on the contact area but peaks related to the SiO₂ film deposited on the contact area are not detected, which means that the SiO₂ film can be removed by ultrasonic treatment. On the other hand, peaks of the SiO₂ film and the metals Ti, Pt and Au, with high adhesion to the insulating film, are detected on the lower wiring, which means that the SiO₂ film can be maintained on the lower wiring. Ti, Pt and Au were also detected on the lower wiring, since the EDX acceleration voltage was 20 kV, thus making possible detection of the metal elements under the insulating film. These results suggest that the SiO₂ film can be

selectively released on the contact areas produced by ultrasonic treatment when Au, with low adhesion to insulating film, is used for the contact areas.

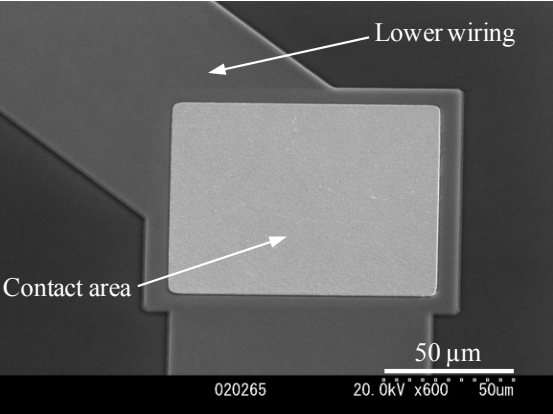
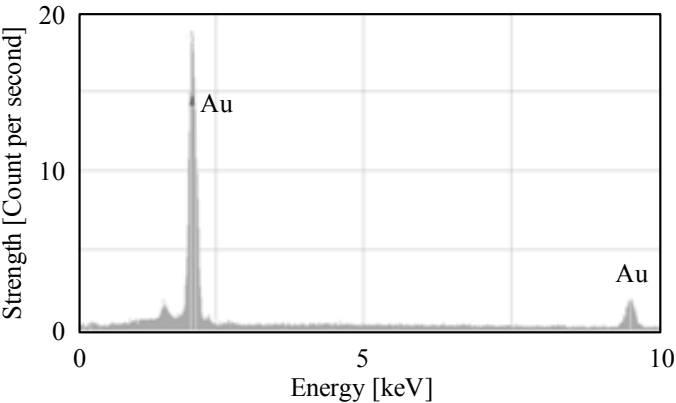
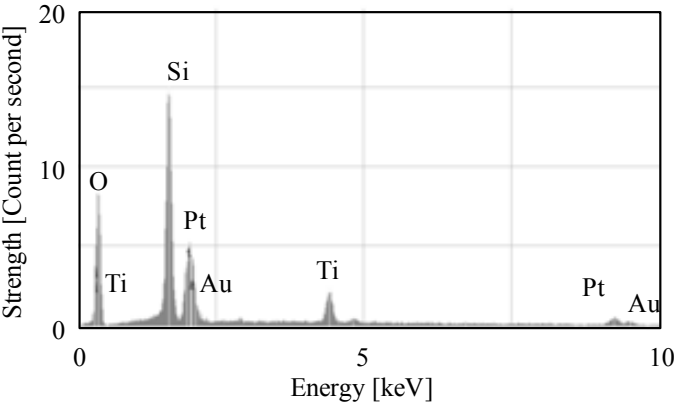


Figure 3.7 SEM image of Au contact area after ultrasonic treatment.



(a) Gold contact area

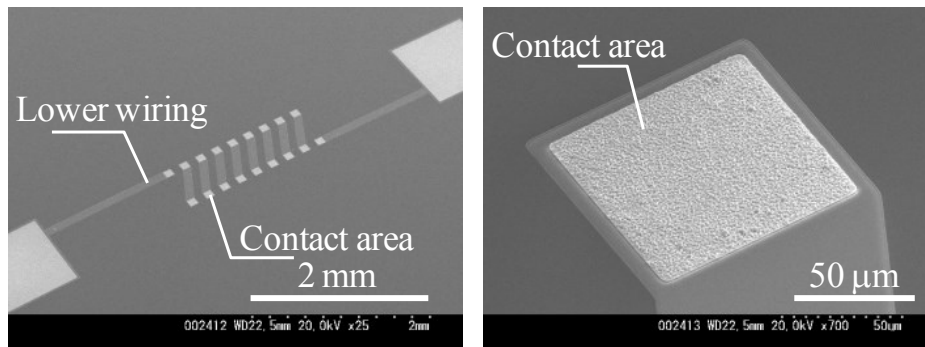


(b) Lower wiring

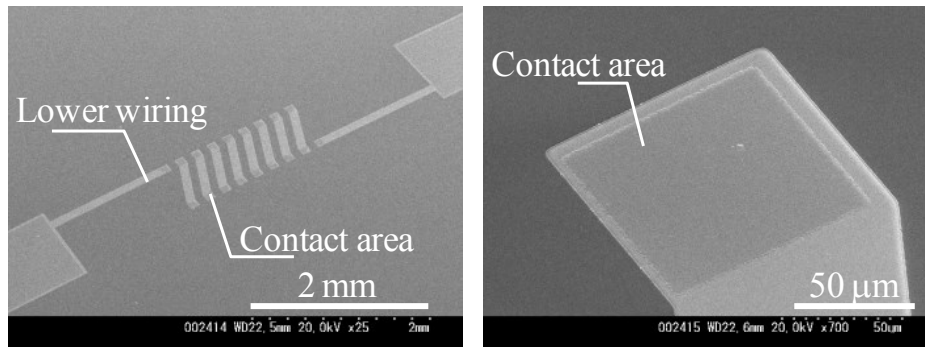
Figures 3.8 Chemical elements detecting results of contact area and lower wiring by EDX.

SEM images and EDX results for contact areas using Cu and Ni are shown in Figures 3.9 and Figures 3.10, respectively.

The results in Figures 3.9(a) and 3.10(a) confirm that when the contact areas are made up of Cu, the SiO₂ film can be removed from the contact areas by ultrasonic treatment, just as in the case of Au. On the other hand, as shown in Figures 3.9(b) and 3.10(b), peaks related to the SiO₂ film were detected on the contact areas; that is, the film was not removed by ultrasonic treatment. These results indicate that the SiO₂ film can be removed from the contact areas by providing a difference in adhesive fracture energy, when Cr, Ti and Ni with high adhesion to insulating film are used for the lower wiring, while Cu and Au, with low adhesion are used for the contact areas.

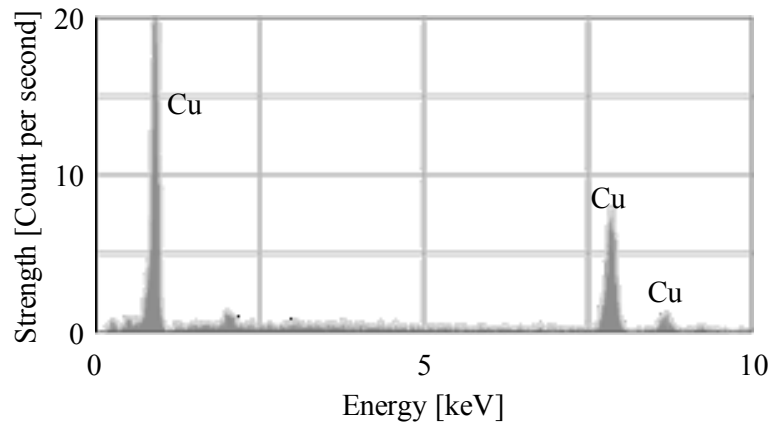


(a) Copper contact area

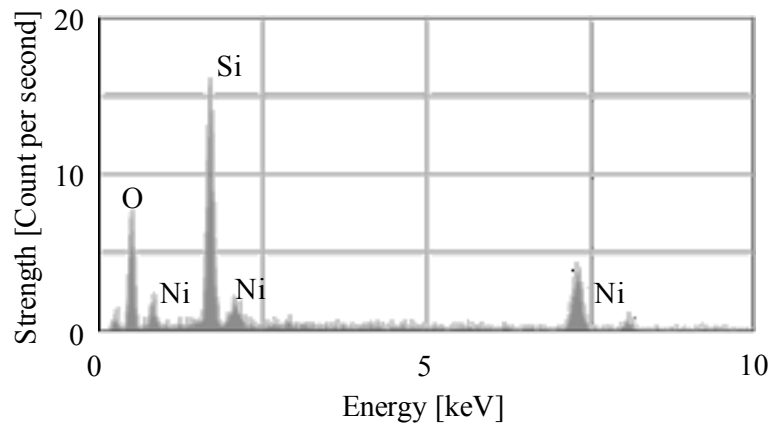


(b) Nickel contact area

Figures 3.9 SEM images of Cu and Ni contact areas.



(a) Copper contact area

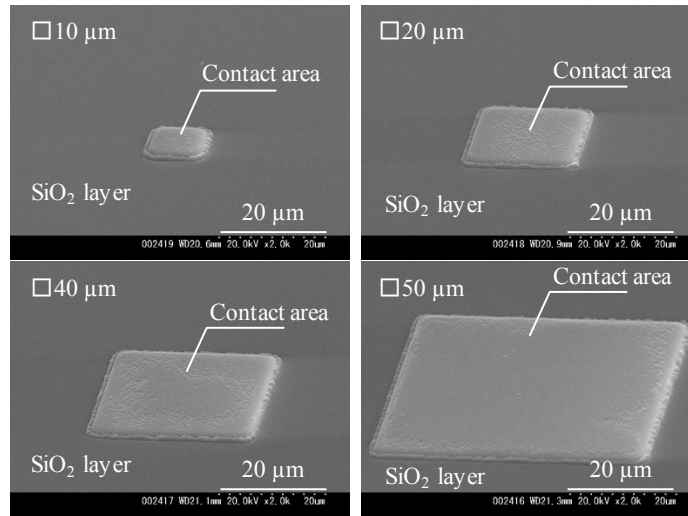


(b) Nickel contact area

Figures 3.10 Chemical elements detecting results of Cu and Ni contact areas by EDX.

3.4.3 SIZE EFFECT OF CONTACT AREA

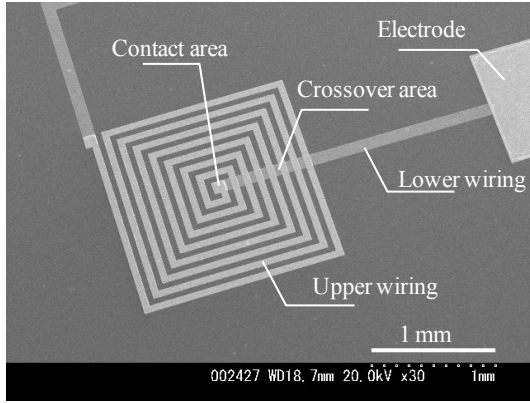
SEM images of Au contact areas ranged from 10×10 to $50 \times 50 \mu\text{m}$ after the ultrasonic treatment are shown in Figures 3.11. As can be seen in the SEM images, the SiO_2 film can be removed from the small patterns of 10×10 to $50 \times 50 \mu\text{m}$ by ultrasonic treatment. In the ultrasonic removal process, just as in the liftoff process, a thin film formed on a resist pattern is peeled gradually. The pattern size became the smaller, and the removal became the more difficult. This investigation confirmed that the SiO_2 film could be removed from the contact areas of larger than $10 \times 10 \mu\text{m}$ due to the use of metal (Au) with low adhesion to the insulating film.



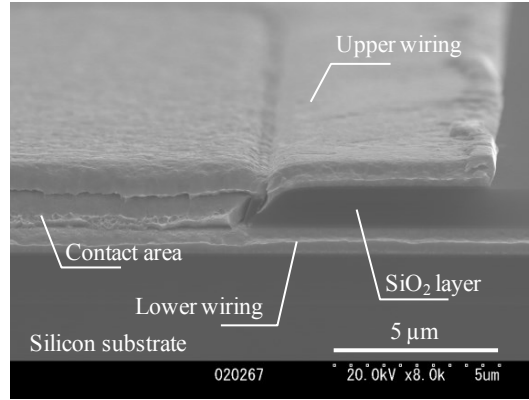
Figures 3.11 SEM images of contact area dependence on size of Au contact areas.

3.4.4 FABRICATING RESULTS OF MULTILEVEL INTERCONNECTION STRUCTURES

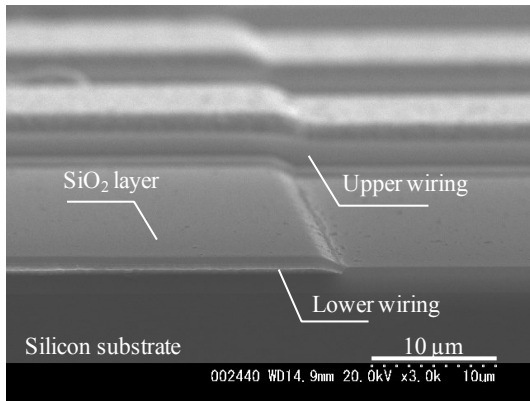
Figures 3.12 show SEM images of the multilevel interconnection structure with the configuration shown in Figure 3.4, fabricated by the process shown in Figure 3.5. In particular, Figure 3.12 shows the entire structure, Figure 3.12(b) a cross section of contact area, and Figure 3.12(c) the crossover part of the upper and the lower wirings. As showing in Figure 3.12(b), the SiO₂ film on the contact areas (Au) can be removed by ultrasonic treatment, thus assuring connection between the upper and the lower wirings. Figure 3.12(c) confirms that there are no peeling of the SiO₂ film in the crossover parts of the lower and the upper wirings, thus assuring insulation. Thus, with a structure proving a difference in adhesive fracture energy with respect to the SiO₂ film between lower wiring and contact areas, the insulating film can be removed from the contact areas by ultrasonic treatment, while remaining intact on the lower wiring. A multilevel interconnection structure can then be obtained by forming the upper wiring on top of this structure.



(a) Multilevel interconnection device



(b) Cross sectional view of the contact area



(c) Crossover area of the wiring

Figures 3.12 SEM images of multilevel interconnection structure.

3.5 CONCLUSIONS

In chapter 3, we considered a new process for multilevel interconnection structures suitable for MEMS devices with various metal materials, and reached the following conclusion. The adhesive fracture energy of metal films with respect to the SiO₂ film calculated by the molecular dynamics technique shows corresponds with the removability of insulating film from metal layer by ultrasonic treatment. We fabricated a multilevel interconnection structure with high adhesive fracture energy metals (Cr and Ti) used for the lower wiring and low adhesive fracture energy metals (Cu and Au) used for the contact areas. We found that the SiO₂ film could be removed selectively from the contact areas. By forming upper wiring to connect the contact areas and the electrodes, we realized a new process for fabricating multilevel interconnection structures.

REFERENCES

- [1] H. Jiang, Z. Li, and N. C. Tien, "REDUCING SILICON-SUBSTRATE PARASITICS OF ON-CHIP TRANSFORMERS", *MEMS2002*, pp. 649-652, 2002
- [2] J-B. Yoon, B-I. Kim, Y-S. Choi, and E. Yoon, "3-D LITHOGRAPHY AND METAL SURFACE MICROMACHINING FOR RF AND MICROWAVE MEMS", *TECHNICAL DIGEST MEMS2002*, pp. 673-676, 2002
- [3] J. K. John, E. Kim, H. Tu, J. Zhang, J. A. Loeb, and Y. Xu, "MULTIFUNCTIONAL CHRONIC 3D ELECTRODE ARRAYS BASED ON A SIMPLE FOLDING PROCESS", *TRANSDUCERS2013*, pp. 1476-1479, 2013
- [4] F. Xuan, X. Luo, and I-M. Hsing "A NEW SOLUTION-PHASE ELECTROCHEMICAL DNA DETECTION PLATFORM WITH TARGET RECYCLING-BASED SIGNAL AMPLIFICATION", *μ TAS2012*, pp. 761-763, 2012
- [5] T. Osaka, and M. Yoshino, "ELECTROCHEMICAL DEPOSITION PROCESS FOR ULSI INTERCONNECTION DEVICES", *Modern Electroplating, Fifth Edition*, pp. 369-382, 2010
- [6] P. T. Vianco, C. H. Sifford, and J. A. Romero, "Resistivity and Adhesive Strength of Thin Film Metallizations on Single Crystal Quartz", *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, 44, 2, pp. 237-249, 1997
- [7] F. Kuriyama, A. Fukunaga, A. Owatari, N. Saito, and M. Nagai, "Electroplating Copper Filling for 3-D Packaging", *Proc. of the ICEP2008*, pp. 489-492, 2008
- [8] T. Aono, Y. Yoshimura, Y. Nakayama and M. Kanamaru, "A method of Fabricating Electroplated Structures using Side-wall Electrical Contact", *IEEJ Trans. SM*, Vol. 134, No. 2, pp. 20-25, 2014
- [9] T. Iwasaki and H. Miura, "Analysis of adhesion strength of interfaces between thin films using molecular dynamics technique", *1999 Material Research Society Fall Meeting*, V8. 4, 1999
- [10] T. Iwasaki, "Application of Molecular-Dynamics Simulation to Interface Stabilization in Thin-Film Devices", *JSME International Journal Series B*, 47, 3, pp. 470-476, 2004

Chapter 4: Eutectic-based wafer-level-packaging technique for piezoresistive MEMS accelerometers and bond characterization using molecular dynamics simulations

4.1 INTRODUCTION

Capacitive [1], piezoresistive [2], and thermal [3] MEMS accelerometers have been developed for use in automobiles, mobile phones, gaming devices, and so on [4-7]. Piezoresistive MEMS accelerometers are especially appropriate to their miniature size since the driving circuit is relatively simple in comparison with that for capacitive and thermal accelerometers. Although the electrical wiring and packaging processes for tiny piezoresistive MEMS accelerometers are complicated, wafer-level-packaging (WLP) techniques have provided us some solutions.

There are several types of WLP techniques [8] such as direct bonding [9, 10], anodic bonding [11-13], and eutectic bonding [14-16]. Direct bonding based on the chemical reaction of dehydration is one of simple WLP techniques for piezoresistive MEMS accelerometers. The direct bonding requires a high temperature above 400 °C to reach a large bonding strength. However, the dopant used as a piezoresistive element may diffuse into silicon at the temperature. The anodic bonding between silicon and glass substrates at a high bias voltage of more than 400 V is an appropriate technique for sealing a piezoresistive MEMS accelerometer in atmospheric pressure because it is a low temperature process done at around 250 °C. However, we have to avoid sticking a movable element of the device to the glass substrate at the high bias voltage. In addition, the process liberates oxygen into the sealed cavities in variable quantities across the wafer [8, 17]. In comparison, the eutectic-bonding-based WLP technique is a lot simpler and is a low temperature process done at around 300 °C, and no applied voltage is needed. Thus, it has the advantage of minimizing the risk of sticking and the diffusion of dopant. The remaining problems to be solved for eutectic-based WLP are realizing a large adhesive strength between a device and lid substrates without the diffusion of solder materials into the adhesive layer at a high bonding temperature and reducing the number of short circuits due to solder leakage during the bonding process.

The objective of this paper is to find a reasonable eutectic-bonding condition for establishing a reliable eutectic-based WLP accelerometer hermetically sealed in atmospheric pressure on the basis of the molecular dynamics (MD) diffusion simulations. The MD simulations are able to assist us in reducing the number of trial and error in the experiment, which can lead to a lower process cost. The bonding conditions for WLP were considered from MD simulations and shear tests of WLP

accelerometers followed by energy dispersive X-ray (EDX) spectrometry analysis. Classical MD simulations were carried out to clarify the effect of temperature on the diffusion behavior of solder material atoms. We also experimentally evaluated the effect of the bonding temperature on the shear strength between a device and top-side lid substrates. The relationship between the diffusion behavior of solder materials to the adhesion layer and the shear strength will be discussed through EDX spectrometry analysis and scanning electron microscopy (SEM) observation of the fracture surface after the shear tests. Finally, we will demonstrate the performance of eutectic-based WL packaged MEMS accelerometers.

4.2 DESIGN AND EXPERIMENTAL PROCEDURES

4.2.1 WLP STRUCTURE FOR SEALING PIEZORESISTIVE ACCELEROMETER

A piezoresistive MEMS accelerometer is hermetically sealed from the top and bottom sides. Figure 4.1 shows a layout design of the WLP for the piezoresistive accelerometer. The accelerometer is fabricated on a silicon-on-insulator (SOI) wafer with 6- μm -thick silicon (Si) and 1- μm -thick silicon dioxide (SiO_2) on a 400- μm -thick Si substrate by a conventional MEMS process. The nominal dimensions of the accelerometer are 1.32 mm in the x-direction, 1.18 mm in the y-direction, and 0.607 mm in the z-direction. The accelerometer has piezoresistive gauges fabricated on four beams from which a clover-shaped mass is suspended. The device substrate is sealed by top- and bottom-side lids of 400- μm -thick Si substrates with solder materials, cavities, and grooves. The cavities are prepared for creating a narrow vertical gap at the top and bottom of the accelerometer in order to generate large air-damping. The grooves can prevent solder materials from spreading across the device region. The top- and bottom-side lids are polished to a thickness of 100 μm after WLP in order to reduce the overall device thickness.

Figures 4.2(a) to 4.2(f) depict the process flow of the accelerometer. The starting substrate is an SOI wafer with a 6- μm -thick active layer and 1- μm -thick buried oxide layer on 400- μm -thick handle silicon. P-type piezoresistive gauges are fabricated on the active layer by a boron doping process [see Fig. 4.2(a)], and the active layer is covered by a SiO_2 layer with a thickness of 0.6 μm during the drive-in process [see Fig. 4.2(b)]. Electrical connection patterns of aluminum (Al) film are formed on the SiO_2 layer [see Fig. 4.2(c)] and sandwiched between the SiO_2 and a 0.17- μm -thick Si_3N_4 layer for use as lateral-through-electrodes [see Fig. 4.2(d)]. Chromium (Cr), nickel (Ni), and gold (Au) thin films used as adhesion layers are deposited on the top- and bottom-sides of the device substrate [see Fig. 4.2(e)]. The beam and the mass of the accelerometer are

finally fabricated on the top and the bottom sides with deep-reactive ion etching (DRIE), respectively [see Fig. 4.2(f)]. SEM image of the piezoresistive accelerometer is shown in Figs. 4.2(g).

Figures 4.3(a) to 4.3(g) depict the process flow of a (100)-oriented Si substrate used as a top-side lid. First, cavities are fabricated on the substrate by anisotropic etching in an alkali solution [see Fig. 4.3(a)]. Grooves with a width of 12 μm and depth of 9 μm are also fabricated around each cavity with DRIE [see Fig. 4.3(b)]. After a thermal oxidation process for the SiO_2 layer, 0.05- μm -thick Cr, 0.4- μm -thick Ni, and 0.2- μm -thick Au thin films are deposited as seed metals to electroplate solder material [see Figs. 4.3(c) and 4.3(d)]. Five- μm -thick gold-tin (Au-Sn) alloy used as solder material is electroplated [see Fig. 4.3(e)], and then, the Au, Ni, and Cr films are removed by an ion milling process [see Fig. 4.3(f)]. The process flow of the bottom-side lid is the same as that of the top-side lid till Fig. 4.3(f), although their groove and solder patterns at the edge of each device are different from those of the top-side lid. In the process for the top-side lid, a large step with a depth of 150 μm is etched at the edge of the chip by DRIE in order to expose the electrode pads using a polishing process after the WLP process [see Fig. 4.3(g)]. SEM images of the top- and bottom-side lids are shown in Figs. 4.3(h) and 4.3(i), respectively.

In Fig. 4.3(a), the depth of the cavity is an important factor for the high-speed response of the accelerometer. If the accelerometer receives a large vibration at or around its resonance frequency, the amplitude of the accelerometer rapidly attenuates because of the air-damping of the oscillating accelerometer. Thus, to achieve a large attenuation by air-damping, the accelerometer should be sealed at atmospheric pressure in a small space. The attenuation coefficient C of the accelerometer is expressed as the following equation [18].

$$C \propto \frac{S^2}{d^3} \mu, \quad (4.1)$$

where S , d , and μ are the area of the mass, the gap distance between the mass and its opposite wall, and the viscosity of the sealing gas, respectively. We controlled the gap distance d by changing the cavity depth. We prepared cavities with depths of 0 μm to 8 μm on the top- and bottom-side lids.

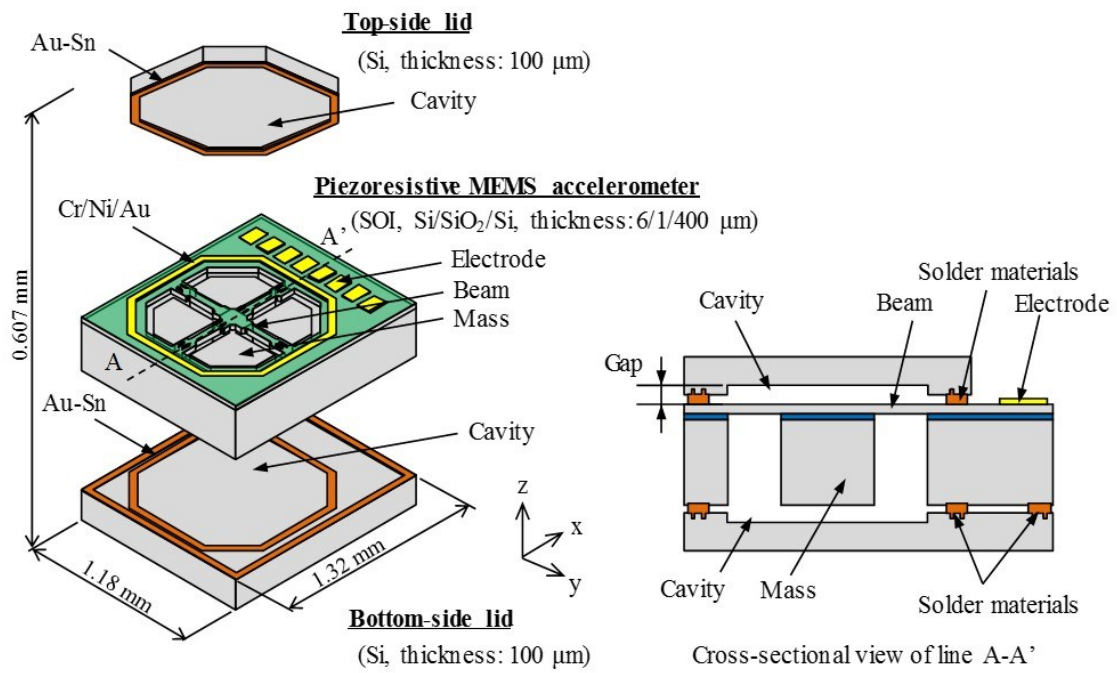
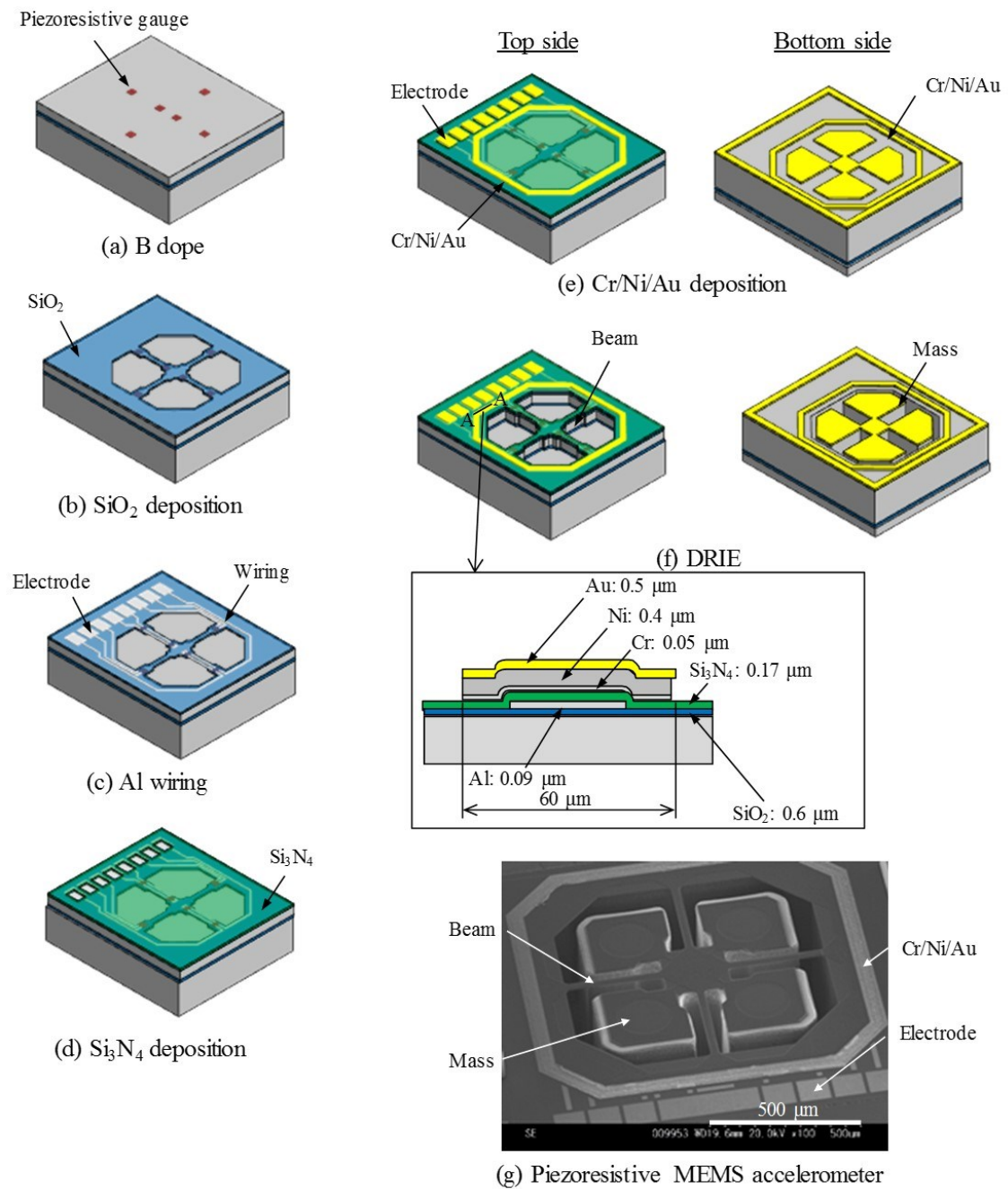
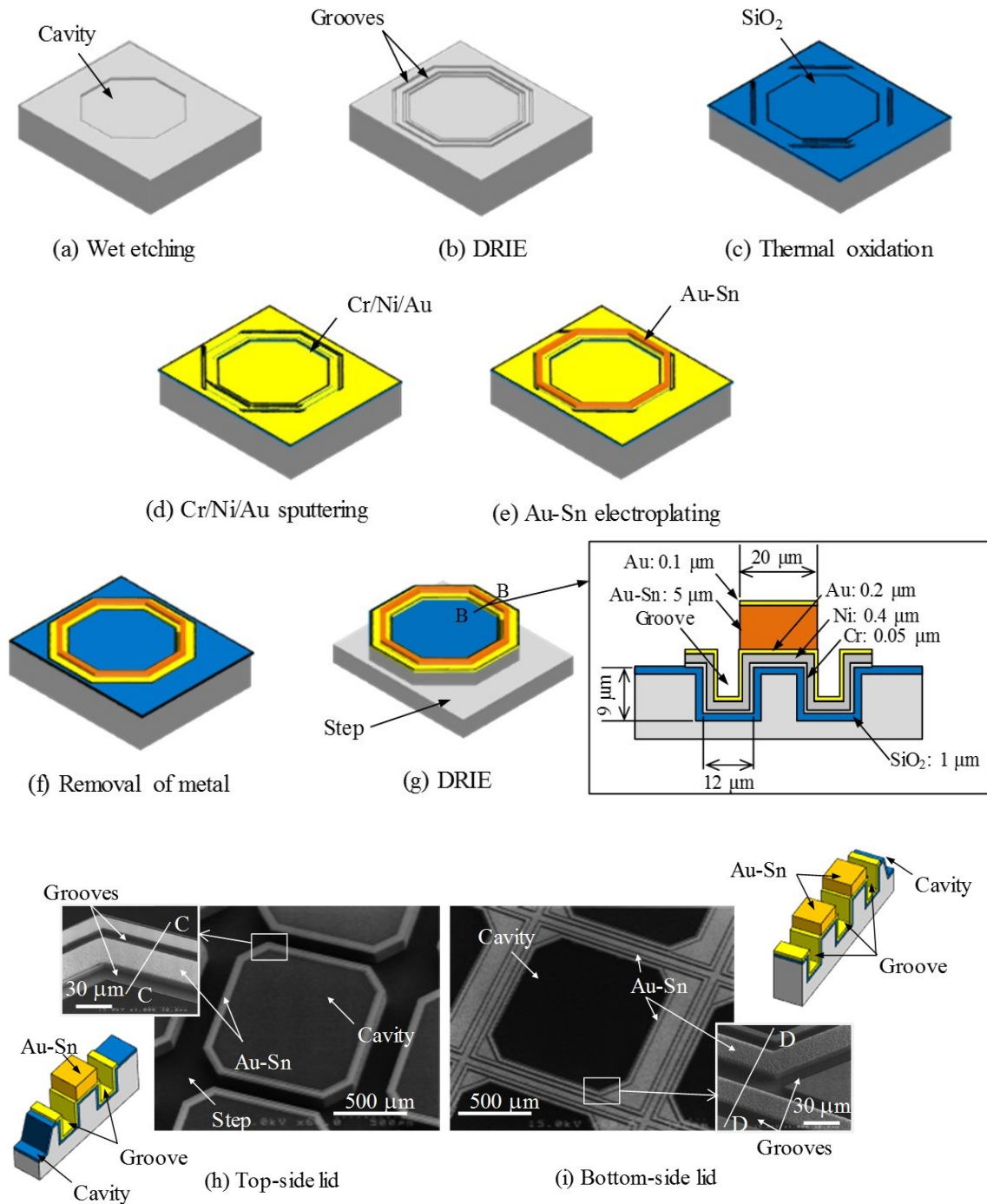


Figure 4.1 Design layout of eutectic bonding-based WLP for piezoresistive MEMS accelerometer.



Figures 4.2 Process flow and SEM image of device substrate.

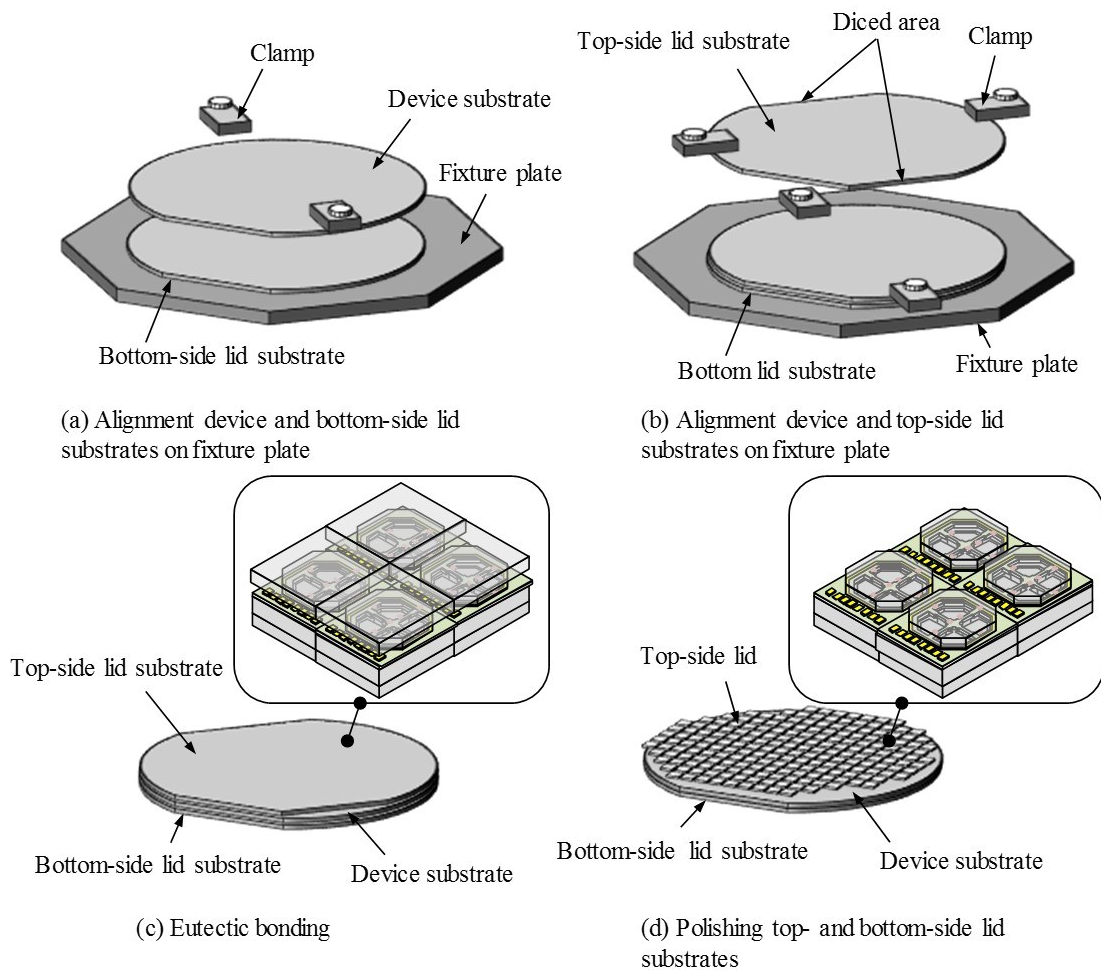


Figures 4.3 Process flow and SEM images of lid substrates.

4.2.2 WLP PROCESS OF PIEZORESISTIVE ACCELEROMETER

A schematic of the WLP process for the accelerometer is shown in Figs. 4.4(a) to 4.4(d). A device substrate is placed on the bottom-side lid substrate by aligning the sealing position with an infrared microscope on an aligner, and both substrates are

clamped on a fixture plate [see Fig. 4.4(a)]. The top-side lid substrate remains set on the device substrate, and it is clamped on a fixture plate at a point diagonal to the previous clamping position [see Fig. 4.4(b)]. The three substrates on the fixture are set inside a bond chamber and simultaneously bonded in nitrogen gas at atmospheric pressure under a contact load of 9.8 kN (4.0 MPa per accelerometer) [see Fig. 4.4(c)]. The bonding temperature is changed from 300 °C to 340 °C in the experiment. Finally, each lid substrate is polished to achieve a thickness of 100 μm [see Fig. 4.4(d)]. After the polishing process, the top-side lid substrate is separated into device pieces because of the 150- μm -deep step on the top-side lid substrate. The electrode pads for the accelerometer also appear outside.



Figures 4.4 Process flow of eutectic bonding-based WLP for piezoresistive accelerometers.

4.2.3 MOLECULAR DYNAMICS SIMULATIONS FOR DIFFUSION MECHANISM OF SOLDER MATERIALS

To investigate the diffusion mechanism of solder materials and their fracture behavior, classical molecular dynamics (MD) simulations were carried out. Figure 4.5 shows an MD model of solder materials in the WLP process. The model is comprised of films of 0.4-nm-thick Ni, 0.4-nm-thick Au, 3.5-nm-thick Au-Sn alloy, 0.4-nm-thick Au, 0.4-nm-thick Ni, and 2-nm-thick Cr on a 1.5-nm-thick SiO₂ film. The area of the films is $4 \times 4 \text{ nm}^2$. The total energy in the model is assumed to be described by the universal force field function [19]:

$$E = E_R + E_\theta + E_\phi + E_\omega + E_{vdw} + E_{el}, \quad (4.2)$$

where E_R is the bond stretching term, E_θ the bond angle bending term, E_ϕ the dihedral angle torsion term, E_ω the inversion term, E_{vdw} the van der Waals term, and E_{el} the electrostatic term. All specific details on each term in the universal force field can be referenced in [19].

The atomic diffusion of solder materials in MD simulations was observed by energy relaxation calculation under the following temperature condition: the model was raised from 20 °C to 300 °C and 340 °C, held for 100 ps., returned to 20 °C again, and kept for 1 ns.. The temperature in MD simulations was controlled by the Nose-Hoover method [20, 21]. Here, the MD simulations have been focused on clarifying the influence of only temperature on the diffusion mechanism of solder materials, except to conditions of the loading and the holding time. We defined these calculations as the 1st relaxation calculation. To understand the fracture behavior of solder materials, creep tensile MD simulations of the models after the 1st relaxation calculation were also carried out under a stress of $1.6 \times 10^{-7} \text{ N}$ added to the top and bottom atoms in the free boundary condition. The fracture behavior was discussed in terms of the local potential energy E_{local} , which was calculated from the difference in potential energy between the material-connected state, $E_{connected}$, and the material-separated state, $E_{separated}$, expressed by Eq. 4.3 [22].

$$-E_{local} = E_{connected} - E_{separated}, \quad (4.3)$$

$E_{connected}$ was equivalent to the total potential energy after the 1st relaxation calculation.

$E_{separated}$ is defined as the sum of potential energies obtained from the 2nd relaxation calculation for MD models separated at the center of one atomic layer or at one interface between the layers after the 1st relaxation calculation. E_{local} is in accordance with the interaction energy between separated atomic segments.

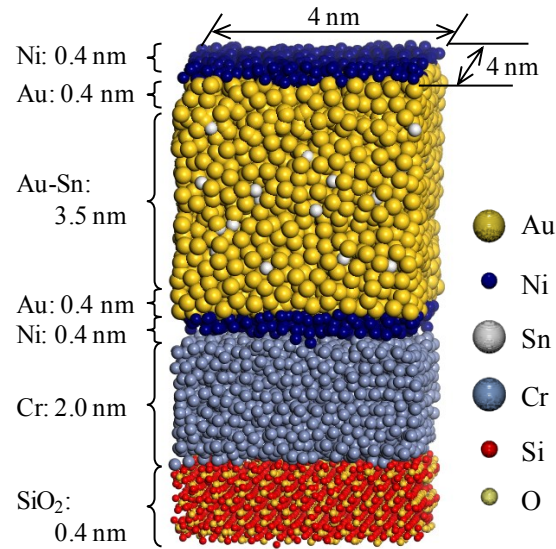


Figure 4.5 Molecular dynamics simulation model for solder materials.

4.2.4 SHEAR STRENGTH TESTS OF BONDING STRENGTH FOR WLP

We evaluated the effect of bonding temperature on shear strength between the device and the top-side lid substrates in a room temperature. Figure 4.6 shows a schematic of a shear strength test of WLP accelerometers. WLP accelerometers were prepared by changing the bonding temperatures from 300 °C to 340 °C under a constant bonding load of 9.8 kN. We used a bondtester (Series 4000, Nordson Advanced Technology K. K.) for the tests, where only the top-side lid was torn off from the device substrate using a scratching tool. The shear strength test of WLP was carried out for 16 samples bonded at each temperature. After the tests, energy dispersive X-ray (EDX) spectrometry analysis and SEM observation were carried out on the fracture surface in order to discuss the correlation between the shear strength, the fracture behavior, and the diffusion of solder material.

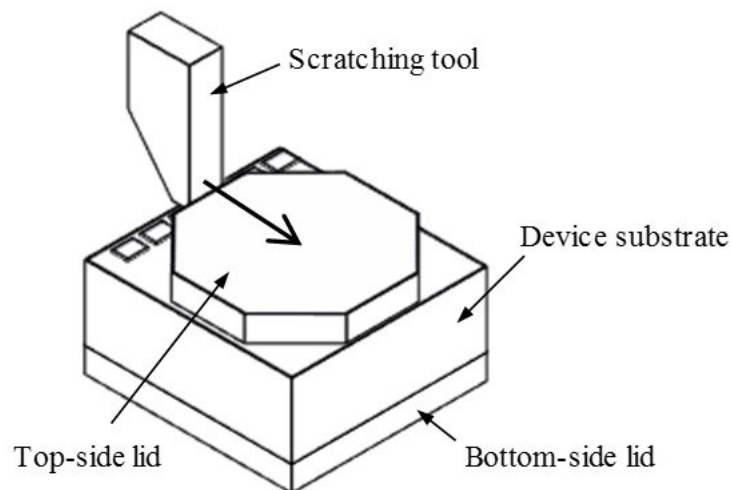
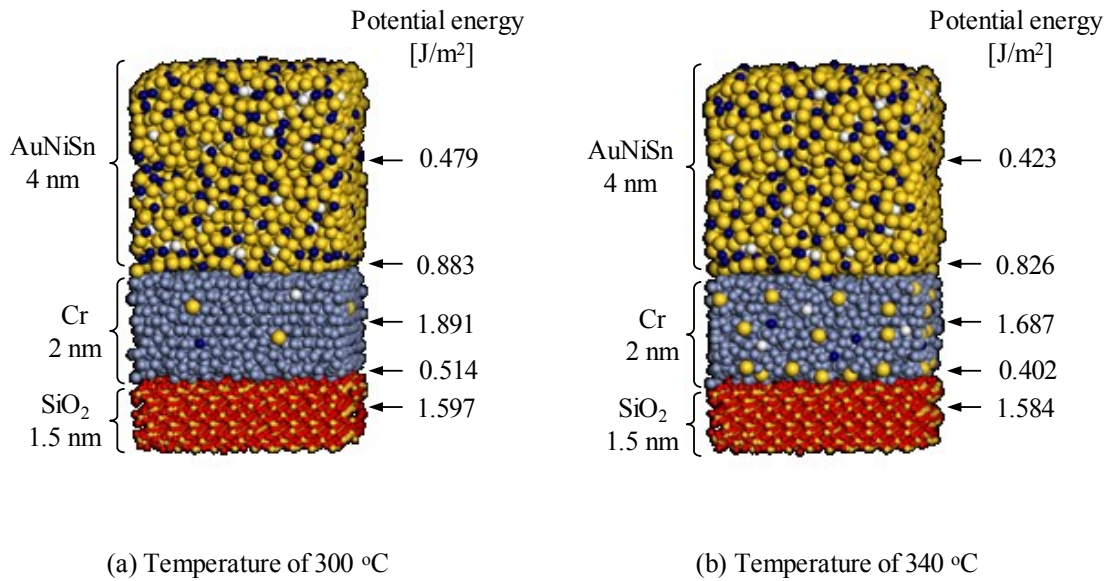


Figure 4.6 Schematic of shear test for WLP accelerometer.

4.3 RESULTS AND DISCUSSIONS

4.3.1 MD SIMULATIONS FOR ATOMIC DIFFUSION MECHANISM OF SOLDER MATERIALS

Figures 4.7(a) and 4.7(b) are snapshots of the diffusion behavior of solder material atoms after energy relaxation calculations at 300 °C and 340 °C, respectively. The potential energies of each layer and each interface, calculated by Eq. 4.3, are indicated in the figures. The Ni atoms at the top surface migrated to the Au-Sn layer, and those between the Au-Sn and Cr layers diffused into the respective layers at both temperatures. Thus, the Au-Sn layer changed to an AuSnNi alloy layer. The diffusion of the Au and Sn atoms into the Cr layer was much more extensive at 340 °C than at 300 °C. The position of potential energy minimum moved from within the AuSnNi layer at 300 °C to the Cr-SiO₂ interface at 340 °C. Although a small necking at the left side wall of the AuSnNi layer is observed in Figs. 4.7(a) and 4.7(b), any precipitations and grain boundary were not confirmed at the vicinity of necking.

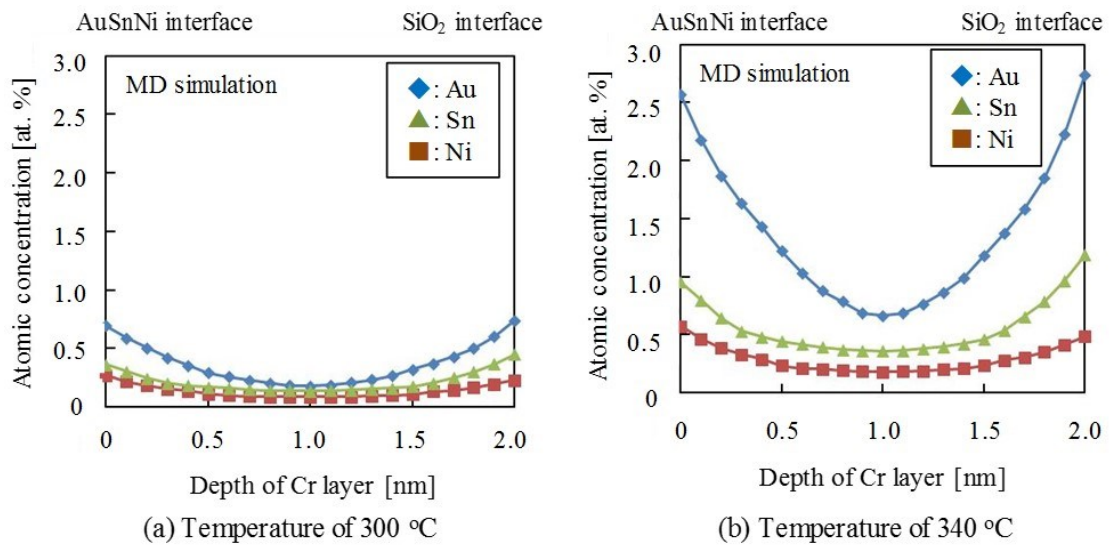


Figures 4.7 Snapshots of MD model for solder materials after energy relaxation calculations at (a) 300 °C and (b) 340 °C.

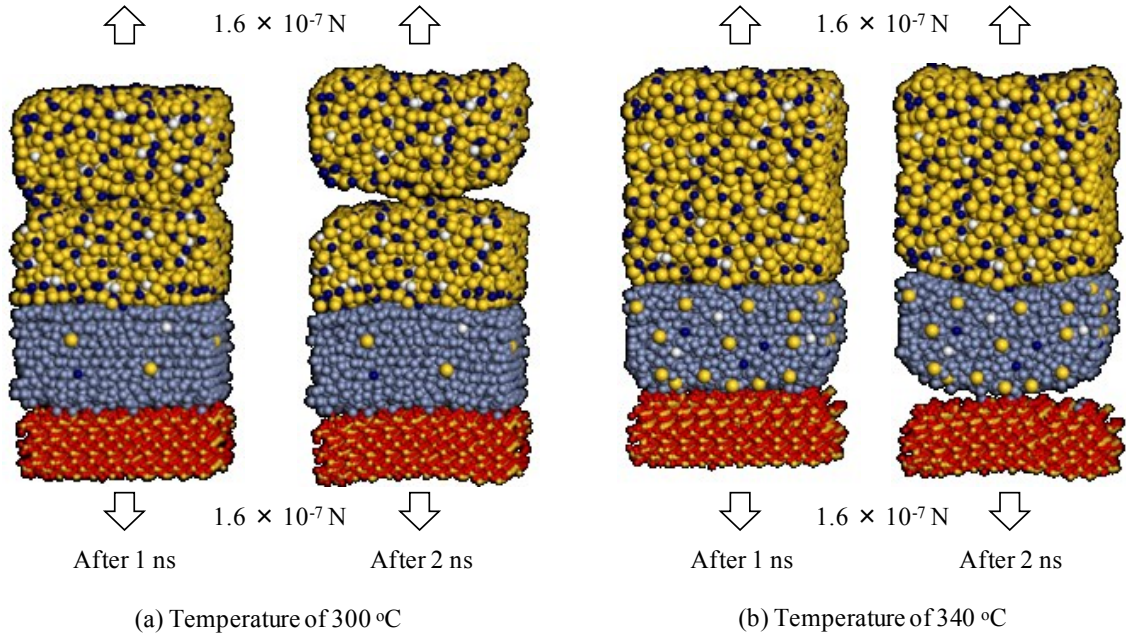
Figures 4.8(a) and 4.8(b) show the atomic concentrations of Au, Sn, and Ni atoms in MD simulations, which diffused into the Cr layer, against the depth of the Cr layer at 300 °C and 340 °C, respectively. The atomic concentrations at the middle of the Cr layer were small regardless of the temperature and the kind of atom, while the diffused atoms gathered at the upper and the lower regions of the layer since the potential

energies at the upper and lower boundaries of the layer were lower than the total potential energy of the layer. The atomic concentrations of Au, Sn, and Ni increased as the temperature increased because of wide diffusion at an elevated temperature; in particular, the number of Au atoms that diffused into the Cr layer increased, as shown in Fig. 4.7(b).

Figures 4.9(a) and 4.9(b) are snapshots of the fracture behavior of the solder material models at 300 °C and 340 °C, respectively. Both models fractured at each layer having the lowest potential energy: the AuSnNi layer at 300 °C and the Cr-SiO₂ interface at 340 °C. The potential energy after the diffusion of the solder material atoms had a large influence on the fracture point.



Figures 4.8 Atomic concentration of Au, Sn, and Ni atoms diffused into Cr layer at (a) 300 °C and (b) 340 °C in MD simulations.



Figures 4.9 Snapshots of fracture behavior for solder material models at (a) 300 °C and (b) 340 °C in creep tensile MD simulations.

4.3.2 SHEAR STRENGTH TEST RESULTS FOR WLP

Figure 4.10 shows the effect of the bonding temperature on the shear strength between the top-side lid and the device substrate of the WLP accelerometers. All results are plotted in the figure. The average of shear strength is connected by the solid line with the indication of standard deviation, σ , at each bonding condition. The averaged strength gradually decreases with an increase of the bonding temperature beyond 320 °C, although the decreasing trend line is buried within the data scatter band because the number of samples is small. This decreasing trend has been qualitatively suggested by the MD simulations. That is, the minimum potential energy in the MD simulation at 300 °C showed 0.479 J/m² in the AuSnNi layer, whereas it was 0.409 J/m² at the Cr-SiO₂ interface in the MD simulation at 340 °C; the small difference in the minimum energy between both bonding temperatures has corresponded to the slight reduction of the shear strength in the experiment.

The averaged strength shows 80 MPa at 300 °C under a load of 4 MPa in the figure, while it is 42.7 MPa in Ref. [23] at a bonding temperature of 310 °C under a load of 0.9 MPa and is 45.53 MPa in Ref. [24] at a bonding temperature of 310 °C under a load of 7 MPa. Therefore, the bonding condition extracted from the MD simulations has been greatly improved in the shear strength.

Considering the above MD simulations, this behavior would be caused by the

thermal diffusion of the solder materials. The fracture surface after the shear strength tests was observed by an SEM (S-4300, Hitachi High-Technologies Co.) followed by an EDX (EMAX-7000, Horiba Ltd.), as shown in Figs. 4.11(a) to 4.11(d). The WLP accelerometers bonded at 300° C in Fig. 4.11(a) exhibited a rough surface in both the electroplated and grooved areas. The EDX analysis clarified that the rough surface was composed of about 20 wt% of Ni, 40 wt% of Au, 40 wt% of Sn, which confirms that Ni atoms diffused to the Au-Sn layer. The fracture surfaces at 320 °C and 330 °C on the electroplated area were rough, similar to those at 300 °C, but the solder materials buried in the grooves fell out partially and formed a smooth surface, as shown in Figs. 4.11(b) and 4.11(c). The EDX detected peaks of Cr on only the smooth surface in the grooved area. The smooth surface spread to the electroplated area at 340 °C in Fig. 4.11(d). Cr was detected on the smooth surface by the EDX, whereas the Au and Sn decreased extremely, and the Ni increased on the surface. Considering the smooth surfaces that appeared and the order of deposition layers in the solder materials, the fracture would have been produced at the Cr-SiO₂ interface at 340 °C.

The reasonable bonding condition extracted from the MD simulations is qualitatively consistent with that in experiments; therefore, a bonding temperature range of 300 °C to 320 °C is considered to be suitable for eutectic bonding with the solder materials in this research. This fact suggests that even if other solder materials are used, we can reduce the number of trial and error which can lead to a lower process cost.

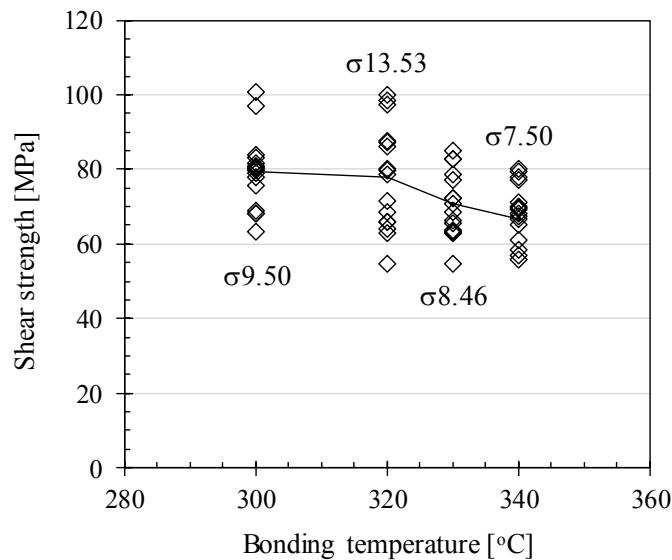
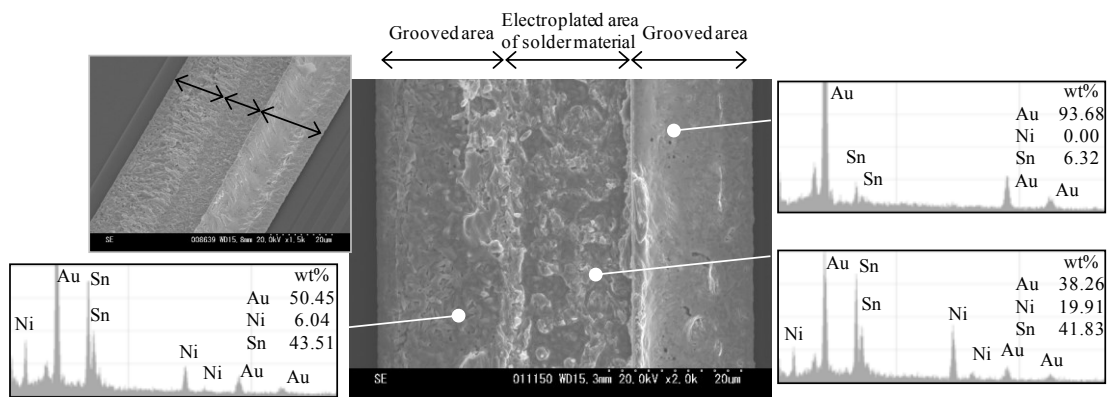
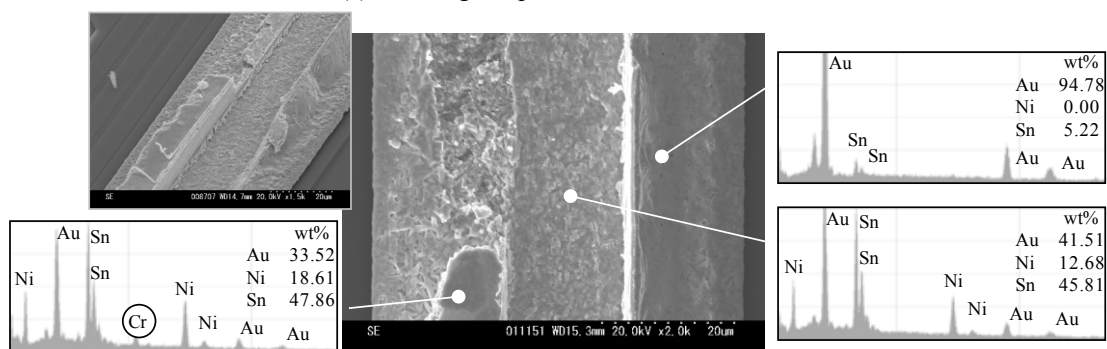


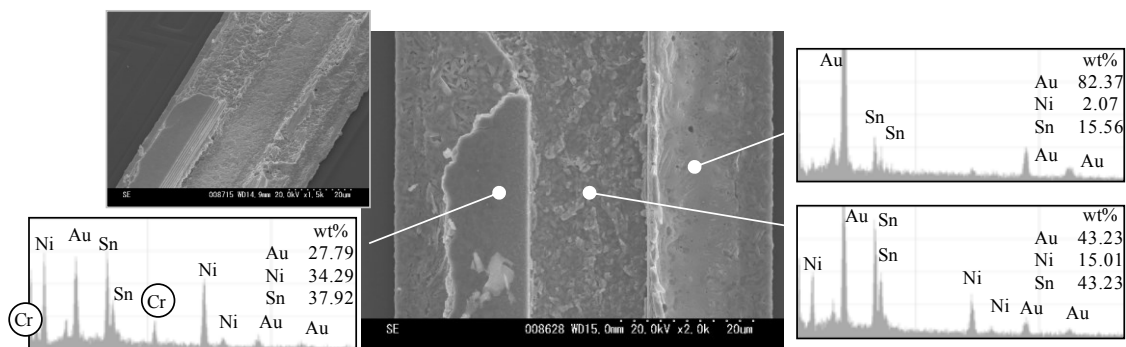
Figure 4.10 Correlation of shear bonding strength with bonding temperature.



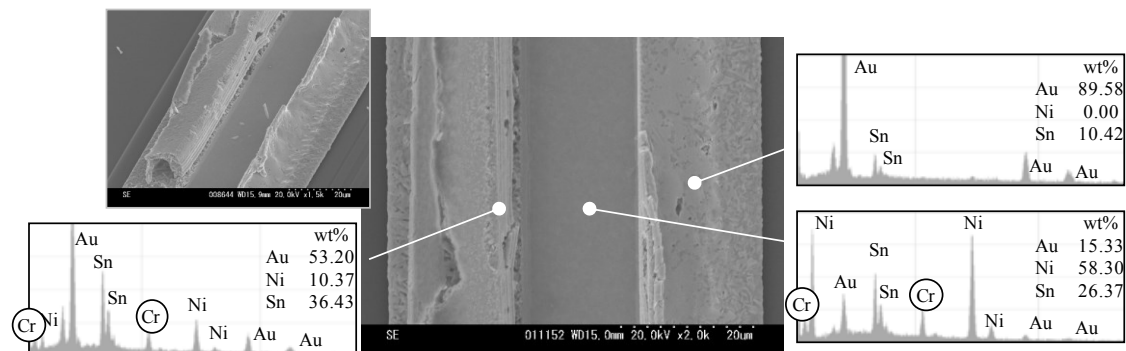
(a) Bonding temperature of 300°C



(b) Bonding temperature of 320°C



(c) Bonding temperature of 330°C

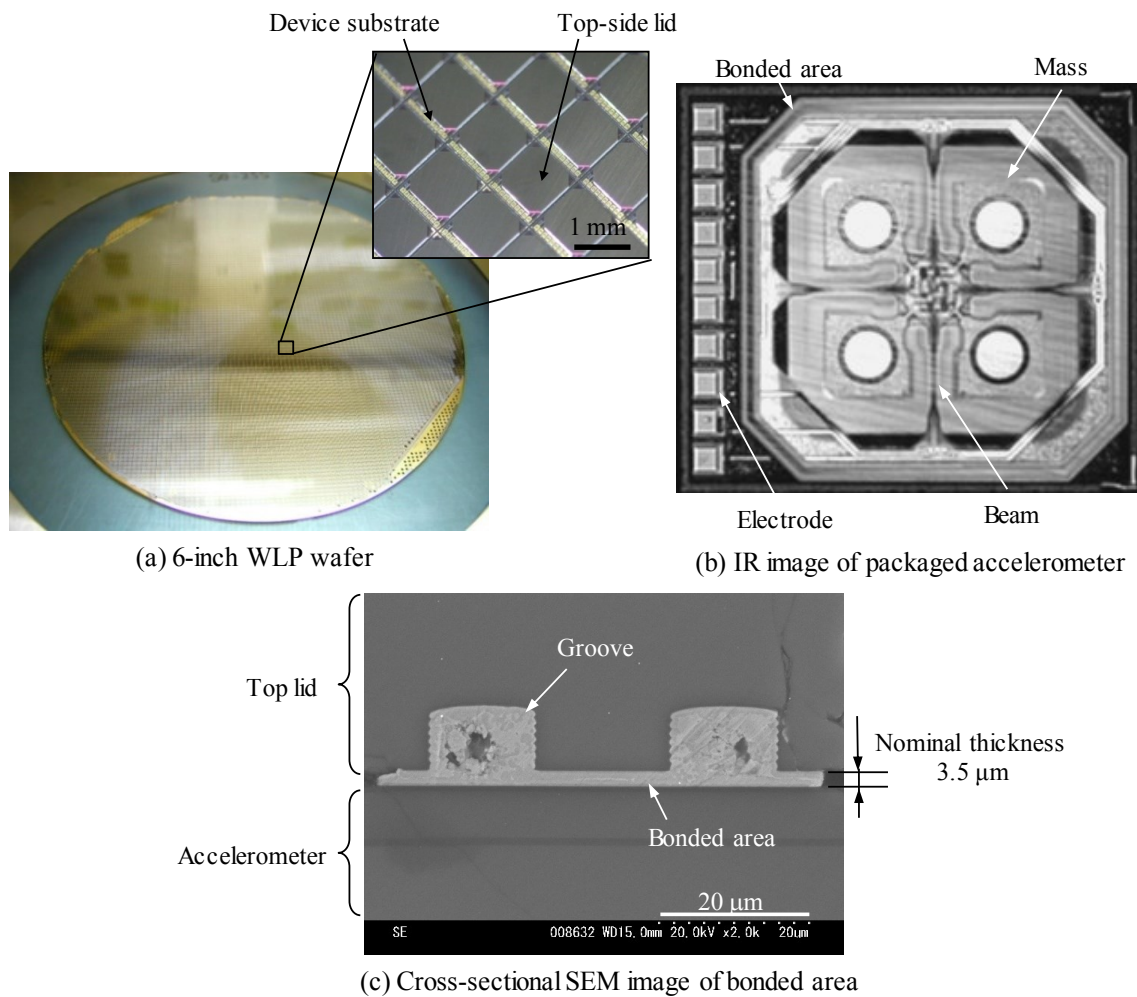


(d) Bonding temperature of 340°C

Figures 4.11 SEM images and EDX results of fracture surface WLP accelerometers: (a) bonding temperatures of 300 °C, (b) 320 °C, (c) 330 °C, and (d) 340 °C.

4.3.3 CHARACTERISTICS OF ACCELEROMETER AFTER WLP

Figure 4.12(a) show photographs of a 6-inch wafer after WLP at 300 °C under a contact load of 9.8 kN (4.0 MPa per accelerometer) followed by the polishing process. Since the all top-side lids separated after the polishing are completely held on the device substrate in the figure, the bonding strength achieved under the WLP condition is enough large compared with a mechanical load produced in the polishing process. There was also no leakage of the solder materials from the bonding area on the WLP accelerometer, since the solder materials were spread into the grooves during the bonding process (see Figs. 4.12(b) and 4.12(c)). Although the initial total thickness of solder materials and adhesion layers is 6.7 μm on the device substrate in Fig. 4.2 and the lid substrate in Fig. 4.3, the thickness after the WLP becomes 3.5 μm in nominal dimension, due to the compression of solder materials followed by its leak and expansion into the grooves during the process.



Figures 4.12 Optical, infrared microscopy and SEM images of WLP accelerometer.

The sensitivity of WLP accelerometer has already been examined in the previous report [25], but the hermeticity and the damping effect of WLP accelerometers have not been discussed at all. Although it is short-time reliability test, we examined the hermeticity of WLP accelerometers by a helium bombing test. In this test, after the WLP accelerometers set into a chamber pressurized to 0.6 MPa with helium for 24 hours, transferred to a vacuum chamber and the amount of helium leaking from WLP was measured with a helium detector. As the result of helium bombing test, the hermetically sealing of WLP was able to reach the leak rate of less than 10^{-9} Pa m³/s.

To evaluate the damping effect of the WLP accelerometers, we have measured their signal gain by changing the cavity depth of lid substrate from 0 μm to 8 μm . Since the total thickness of the solder materials was 3.5 μm , the gap distance between the accelerometer and the lid on one side was 3.5 μm to 11.5 μm in nominal values. Figures 4.13(a) and 4.13(b) show variations of the signal gain of the accelerometers with an increase in the oscillating frequency in the x- and z-directions. The signal gain of the accelerometer with a gap distance of 11.5 μm rose sharply at resonance frequencies of 2100 Hz and 3200 Hz in the x- and z-directions, respectively. The peaks of the gain were caused by the accelerometer being vibrated without air-damping. The peaks at each resonance frequency decreased as the gap distance reduced, and the attenuation of peaks was due to air-damping. The accelerometer with the 3.5 μm -gap did not have clear peaks in the x- and z-directions, which was attributed to air-damping, so their vibrations could be suppressed even at the resonance frequency.

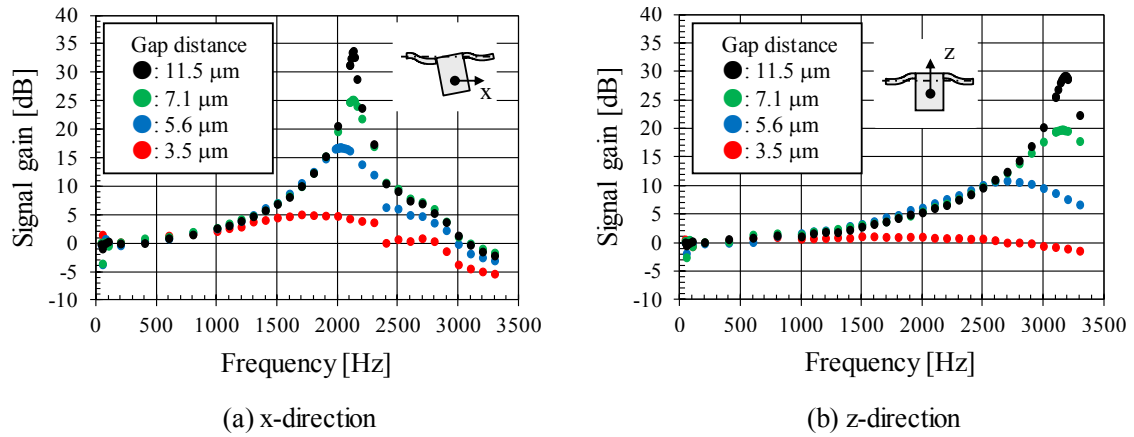
The signal gains at the resonance frequency for each accelerometer are plotted in Figure 4.14. The x- (SG_x) and z-axis signal gains (SG_z) are roughly proportional to the third power of the gap distance, d , in a semi-logarithmic diagram, as expressed by Eqs. 4.4 and 4.5.

$$SG_x = 20 \log_{10} d^{2.62} - 21.507, \quad (4.4)$$

$$SG_z = 20 \log_{10} d^{2.84} - 30.488, \quad (4.5)$$

These results mean that the gap distance had a larger influence on the attenuation of the z-axis acceleration than on that of the x-axis one. To achieve an accelerometer with a signal gain of less than 20 dB, the gap distance must be less than 6.2 μm in nominal value; in short, the depth of the cavity of the lid substrate should be less than 2.7 μm . Therefore, we decided not to use the cavities on the top- and bottom-side lid substrates

in the eutectic-bonding-based WLP process; consequently, the percentage of accelerometers with a signal gain of less than 20 dB having performances that satisfy design specifications to the total number of devices (9500) was larger than 95% on the 6-inch wafer.



Figures 4.13 Variations of signal gain of accelerometer with increase in oscillating frequency (a) in x-direction and (b) z-direction.

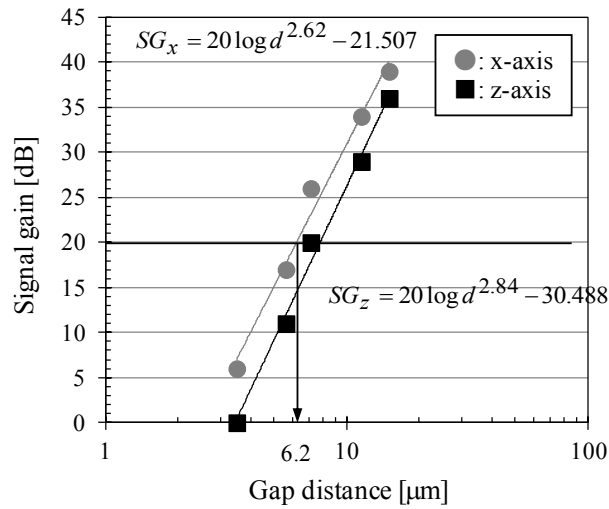


Figure 4.14 Effect of gap distance on signal gain at resonance frequency.

4.4 CONCLUSION

To realize eutectic bonding-based WLP accelerometers with a high shear strength, bonding conditions were analytically and experimentally investigated so that the solder material atoms did not diffuse to the adhesion layers too much.

MD simulations clarified the diffusion mechanism of solder material atoms at elevated temperatures. Ni atoms used as one adhesion layer easily migrated to an Au-Sn layer in temperature ranges of 300 °C to 340 °C, which created an AuSnNi alloy layer. Au and Sn atoms also diffused into a Cr adhesion layer at a high temperature of 340 °C. Tensile creep simulations showed that fractures in a solder model started from the lowest potential energy domain; the lowest potential energy at 300 °C was in the AuSnNi layer, and that at 340 °C was in the Cr-SiO₂ interface.

Shear tests of the WLP accelerometers followed by EDX analyses showed that a sample bonded at 300 °C had fractured at the AuSnNi layer and had a high shear strength, while that at 340 °C was exfoliated at the Cr-SiO₂ interface by the lower shear force. These experiments were qualitatively consistent with MD simulations. A 6-inch wafer after WLP at 300 °C under a contact load of 9.8 kN also completely bonded because there were no defects in the top-side lids on the wafer after the polishing process.

Eutectic bonding-based WLP was effective for controlling the attenuation of accelerometers by deciding the thickness of the electroplated solder materials that played the role of a cavity between the accelerometer and the lids. If the gap distance between the accelerometer and the lids was less than 6.2 μm, the signal gains for x- and z-axis acceleration was less than 20 dB even at the resonance frequency due to air-damping.

REFERENCES

- [1] S. Tez, U. Aykutlu, M. M. Torunbalci and T. Akin, "A Bulk-Micromachined Three-Axis Capacitive MEMS Accelerometer on a Single Die", *J. Microelectromech. Sys.*, Vol. 24, No. 5, pp. 1264-1274, 2015
- [2] F. Han, B. Sun, L. Li and Q. Wu, "Performance of a Sensitive Micromachined Accelerometer With Electrostatically Suspended Proof Mass", *IEEE SENSORS JOURNAL*, Vol. 15, No. 1, pp. 209-217, 2015
- [3] R. Hiratsuka, D. C. van Duyn, T. Otaredian, P. de Vries and P. M. Sarro, "Design consideration for thermal accelerometer", *Sens. Actuators A, Phys.*, Vol. 32, No. 1-3, pp. 380-385, 1992
- [4] A. C. Fischer, F. Forsberg, M. Lapisa, S. J. Bleiker, G. Stemme, N. Roxhed and F. Niklaus, "Integrating MEMS and ICs", *Microsystems & Nanoengineering*, 1, 15005, 2015
- [5] B. Vigna, "MEMS epiphany," *Proc. The 22nd IEEE International Conference on Micro Electro Mechanical Systems, MEMS2009*, pp. 1-6, 2009
- [6] G. Lammel, "THE FUTURE OF MEMS SENSORS IN OUR CONNECTED WORLD", *Proc. The 28th IEEE International Conference on Micro Electro Mechanical Systems, MEMS2015*, pp. 61-64, 2015
- [7] W. J. Fleming, "New Automotive Sensors – A Review", *IEEE SENSORS JOURNAL*, Vol. 8, No. 11, pp. 1900-1921, 2008
- [8] M. Esashi, "Wafer level packaging of MEMS", *J. Micromech. Microeng.*, Vol. 18, No. 7, 073001, 2008
- [9] X. Zhou, L. Che, J. Wu, X. Li and Y. Yang, "A novel sandwich capacitive accelerometer with a symmetrical structure fabricated from a D-SOI wafer", *J. Micromech. Microeng.*, 22, 085031, 2012
- [10] H. Moriceau, F. Rieutord, F. Fournel, Y. L. Tieg, L. D. Cioccio, C. Morales, A. M. Charvet and C. Deguet, "Overview of recent direct wafer bonding advances and applications", *Adv. Nat. Sci.: Nanosci. Nanotechnol.*, 1, 043004, 2010
- [11] D. B. Xiao, Q. S. Li, X. H. Wang, Z. H. Chen, D. W. Xia and X. Z. Wu, "A novel sandwich differential capacitive accelerometer with symmetrical double-sided serpentine beam-mass structure", *J. Micromech. Microeng.*, 26, 025005, 2016
- [12] S. Tez, U. Aykutlu, M. M. Torubalici and T. Akin, "A Bulk-Micromachined Three-Axis Capacitive MEMS Accelerometer on a Single Die", *J. Microelectromech. Syst.*, Vol. 24, No. 5, pp. 1264-1274, 2015
- [13] J. Zhang, W. Jiang, X. Wang, J. Zhou and H. Yang, "Design and fabrication of high performance wafer-level vacuum packaging based on glass-silicon-glass bonding

- techniques”, *J. Micromech. Microeng.*, 22, 125022, 2012
- [14] Z. Fang, X. Mao, J. Yang and F. Yang, “A wafer-level Sn-rich Au-Sn intermediate bonding technique with high strength”, *J. Micromech. Microeng.*, 22, 095008, 2010
- [15] Y. T. Cheng, L. Lin and K. Najafi, “Localized Silicon Fusion and Eutectic Bonding for MEMS Fabrication and Packaging”, *J. Microelectromech. Syst.*, Vol. 9, No. 1, pp. 3-8, 2000
- [16] D. Li, Z. Shang, Y. She and Z. Wen, “Investigation of Au/Si Eutectic Wafer Bonding for MEMS Accelerometers”, *Micromachines*, Vol. 8, No. 5, 158, 2017
- [17] S. Mack, H. Baumann, U. Gosele, H. Werner and R. Schlogl, “Analysis of Bonding-Related Gas Enclosure in Micromachined Cavities Sealed by Silicon Wafer Bonding”, *J. Electrochem. Soc.*, Vol. 144, No. 3, pp. 1106–1111, 1997
- [18] M. Andrews, I. Harris and G. Turner, “A Comparison of squeeze-film theory with measurements on a microstructure”, *Sens. Actuator A*, 36, pp. 79-87, 1993
- [19] A. K. Rappe, C. J. Casewit, K. S. Colwell, W. A. Goddard III and W. M. Skiff, “UFF, a Full Periodic Force Field for Molecular Mechanics and Molecular Dynamics Simulation”, *J. Am. Chem. Soc.*, 114, pp. 10024-10035, 1992
- [20] S. Nose, “A unified formulation of the constant temperature molecular dynamics methods”, *J. Chem. Phys.*, Vol. 81, No. 1, pp. 511-519, 1984
- [21] W. G. Hoover, “Canonical dynamics: Equilibrium phase-space distributions”, *Phys. Rev. A*, Vol. 31, No. 3, pp.1695-1697, 1985
- [22] T. Iwasaki, “Molecular dynamics study of adhesion strength and diffusion at interfaces between interconnect materials and under lay materials”, *Comput. Mech.*, 25, pp. 78-86, 2000
- [23] Y. S. Bang, J. M. Kim, Y. Kim, J. M. Kim and Y. K. Kim, “FABRICATION AND CHARACTERIZATION OF RF MEMS PACKAGE BASED ON LTCC LID SUBSTRATE AND GOLD-TIN EUTECTIC BONDING”, *TRANSDUCERS2007: 14th Int. Conf. Solid-State Sensors, Actuators and Microsystems*, pp. 2115-2118
- [24] J. Zhao, Q. Yuan, X. Kan, J. Yang and F. Yang, “A low feed-through 3D vacuum packaging technique with silicon vias for RF MEMS resonator”, *J. Micromech. Microeng.*, 27, 014003, 2017
- [25] A. Kazama, T. Aono and R. Okada, “Stress Relaxation Mechanism with a Ring-Shaped Beam for a Piezoresistive Three-Axis Accelerometer”, *J. Microelectromech. Syst.*, Vol. 22, No. 2, pp. 368-394, 2013

Chapter 5: Development of wafer-level-packaging technology for simultaneous sealing of accelerometer and gyroscope under different pressures

5.1 INTRODUCTION

The wafer-level packaging (WLP) technology is one of the significant post-assembly processes for improvement in reliability and reduction of production size and manufacturing cost of Micro Electro Mechanical Systems (MEMS) [1-3]. In particular, vibratory devices such as accelerometers, gyroscopes, scanning-mirrors and micro-resonators fabricated on one wafer should be packaged under the low pressure suitable for each device in order to fully exploit their performances [4-11]. Thus, WLP technology which enables pressure controlled packaging of plural devices individually is required not only for their reliability and reduction in size and cost, but also for their high performance and multi-function of MEMS products [12-14].

Until now a lot of sealing techniques, such as the glass frit sealing [15, 16], direct bonding [17, 18], plasma-activated bonding [19, 20], eutectic bonding [21, 22] and anodic bonding [23-27], have used as a WLP for MEMS devices. Although these bonding techniques have their own advantages, it is inappropriate to directly use them as an individual pressure-controlling WLP for plural devices. For example, the direct bonding based on a chemical reaction of dehydration cannot result in a high pressure sealing of MEMS devices, since it is usually carried out at a high temperature for achieving a large bonding strength. The plasma-activated bonding can effectively seal MEMS devices only in vacuum, because the bonding surfaces are inactivated by exposing the atmosphere. The eutectic bonding can be used as a simultaneously wafer-level sealing technique for plural MEMS devices under different pressures if it is possible to prepare a non-evaporable getter that is able to chemically adsorb active gases [21]. However, it is extremely difficult to control the pressure with accuracy on the eutectic bonding-based WLP because the pressure in the cavity is determined by various factors such as the adsorption capacity of the getter, the gas concentration and the size of cavity.

On the other hand, the anodic bonding-based WLP can directly bond between silicon and glass substrates by electrostatic force without any bonding materials. We can easily prepare the glass substrate with a suitable shape of cavities for hermetic packaging of vibratory MEMS devices such as gyroscope, accelerometer, and scanning mirror, which can seal devices under a wide range of pressure [23-26]. The anodic bonding is also superior in an electrical connection between MEMS devices and outside

output electrodes by feed-through structures fabricated by a conventional MEMS process technique [12, 27]. Furthermore, the anodic bonding is acceptable for many MEMS devices. However, we cannot achieve an individually pressure-controlling WLP for plural devices by using only the conventional anodic bonding technique. Thus, a new WLP technology is required for simultaneous sealing of couples of MEMS devices under different pressures.

This research proposes a two-stage anodic bonding-based WLP between silicon and glass substrates for simultaneous sealing of an accelerometer in the atmosphere and a gyroscope in vacuum. The key technique of the new WLP is to prepare tiny bumps on the glass substrate that are regarded as surface roughness. The bumps can partially make unsealed areas between silicon and glass substrates, so that sealed and unsealed areas are selectively formed at the interface. The 1st bonding step is done to seal the accelerometer in the atmosphere, and the 2nd bonding step is done to seal the gyroscope at a high temperature under a high contact load in vacuum. We also investigated the performance of the MEMS sensors after the WLP process.

5.2 DESIGN AND EXPERIMENTAL METHODOLOGY

Figure 5.1 shows the layout design of the WLP for sequentially sealing the accelerometer and gyroscope. The accelerometer and gyroscope are fabricated on a silicon-on-insulator (SOI) wafer with 40- μm -thick silicon (Si) film and 4- μm -thick silicon dioxide (SiO_2) film on a 400- μm -thick Si substrate, which are covered by a glass substrate made of Pyrex glass (Corning 7740). Since the Pyrex glass is no longer a popular glass wafer, other borosilicate glasses such as TEMPAX Float[®] (SCHOTT) can be applied to the anodic bonding-based WLP.

The nominal dimension of one unit of MEMS sensors is $3.4 \times 8.3 \times 0.84$ mm. The accelerometer and gyroscope are fabricated by using a conventional MEMS process [28, 29]. Grooves with a width of 100 μm and depth of 40 μm are also fabricated on the sensor substrate to control the pressure of the gyroscope during the WLP process. The width of the sealing region around all devices is 300 μm . The accelerometer is composed of two-axis differential capacitive displacement sensors. Since the damping oscillation of the accelerometer is required for its high-speed response, the accelerometer should be sealed in the atmosphere. If the accelerometer sealed in the atmosphere receives a large vibration at or around the resonant frequency, the amplitude of the accelerometer rapidly attenuates because of the air-damping of oscillating accelerometer. Thus, the accelerometer can immediately detect the vibration signal continuously produced. The gyroscope constitutes an electrostatic driven oscillator and

a differential capacitive displacement sensor on the sensor substrate. As the gyroscope with a large displacement at the resonant frequency without air-damping can achieve high sensitivity, the gyroscope must be sealed in vacuum.

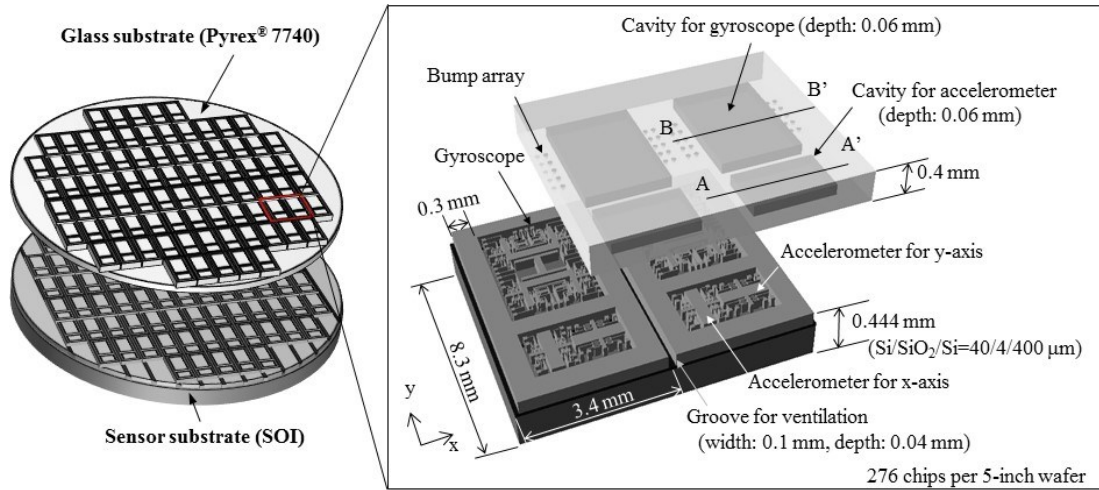


Figure 5.1 Layout design of WLP for simultaneously sealing accelerometer and gyroscope.

The glass substrate has two types of cavities with depth of 60 μm for the upper space of the accelerometer and gyroscope, as shown in Figure 5.2. There are also a number of bumps with height of 0.4 to 1.2 μm and diameter of 1 to 18 μm around the cavity of the gyroscope on the glass substrate. The bumps achieve the unsealing condition at the interface during the 1st bonding step. The cavities and the bumps are fabricated by a wet etching process with HF solution. The dimensions of the bumps will be determined in experiments.

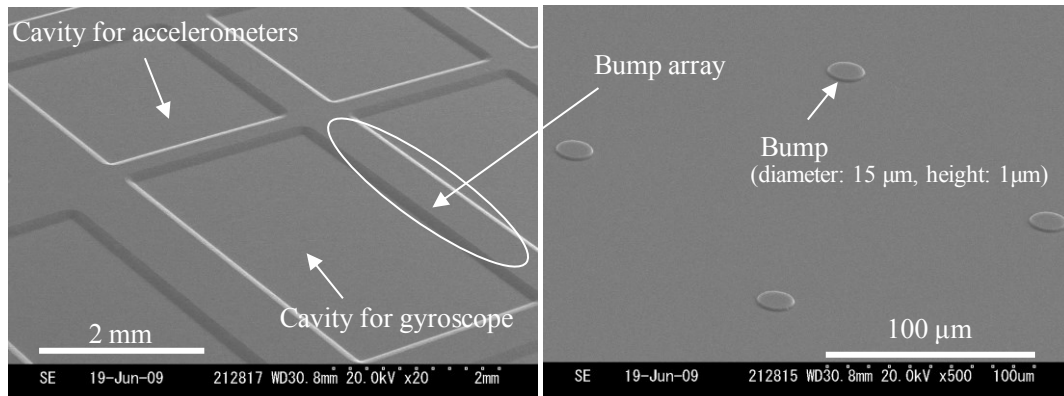
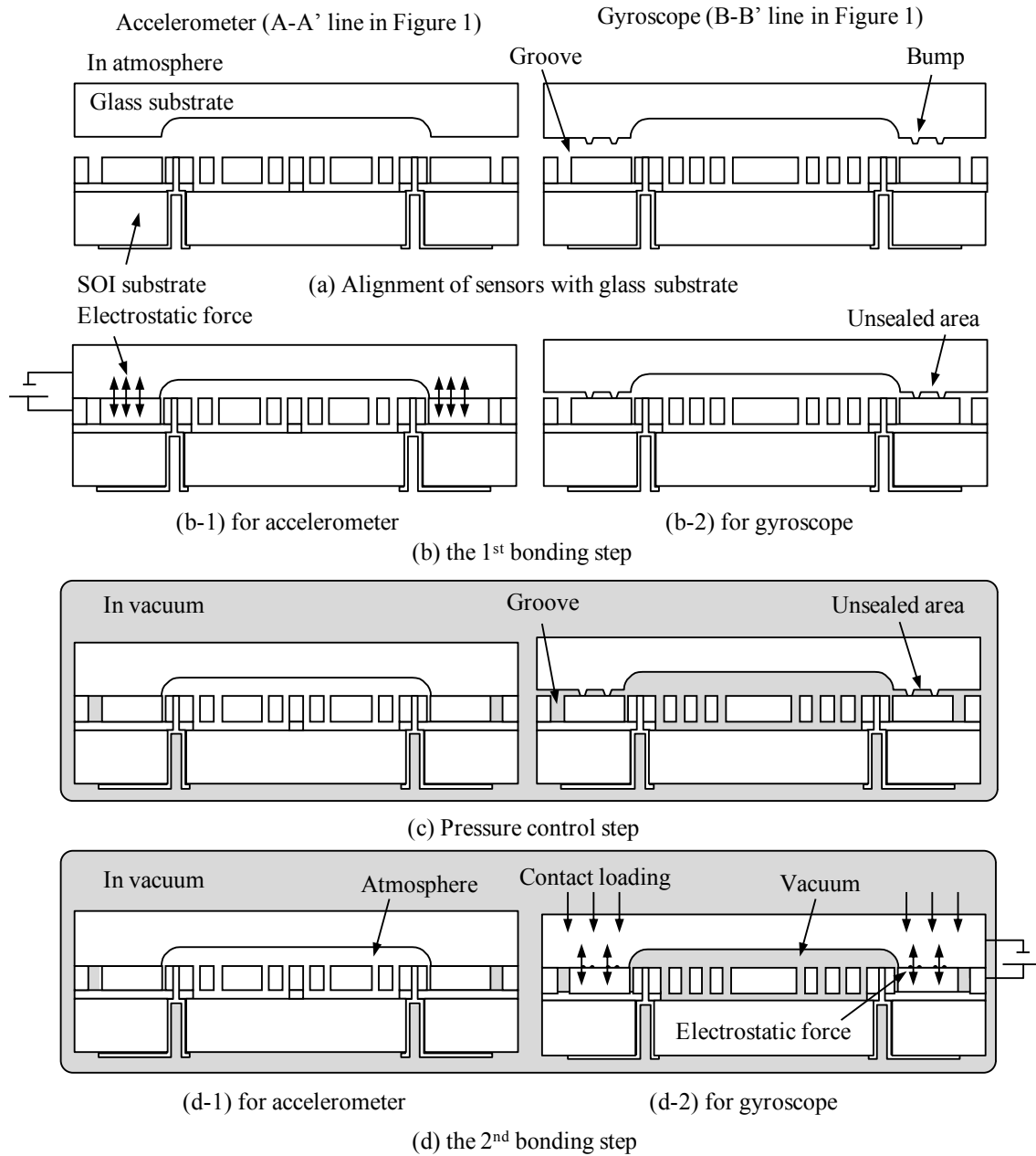


Figure 5.2 Photographs of glass substrate used in WLP process.

Figures 5.3(a) to 5.3(d) depicts the process flow of the WLP. The SOI and the glass substrates, where the sensors, the cavities and the bumps have already been fabricated, are prepared. These substrates are aligned by a bond aligner (BA6e, SUSS Microtec), and they are set into a bond chamber (SB6e, SUSS Microtec) in the atmosphere [see Fig. 5.3(a)]. In the 1st bonding step, the bonding area for the accelerometer is completely sealed with the glass substrate by the electrostatic force of anodic bonding in the atmosphere. At this time, the gyroscope is not sealed because of the bumps [see Fig. 5.3(b)]. The pressure of the bond chamber is controlled by a vacuum pump at a pressure lower than the atmospheric [see Fig. 5.3(c)]. Finally, the glass substrate is deformed in the 2nd bonding step by applying a higher contact load at a higher temperature [see Fig. 5.3(d)], and the gyroscope is completely sealed by the anodic bonding at a low pressure.

In the next sections, detailed experimental procedures, results and discussions will be explained in accordance with the process sequence in Figure 5.3 for a better understanding of the newly proposed WLP.



Figures 5.3 Process flow of WLP.

5.3 INVESTIGATION OF BONDING CONDITIONS

5.3.1 1st BONDING STEP FOR SEALING ACCELEROMETER

A high bonding strength strong enough not to reduce the airtightness of the accelerometer is necessary for the pressure control step. We examined the effect of the anodic bonding temperature on the shear strength between the Si on SOI and the glass in order to confirm the effectiveness of the 1st bonding condition. Figure 5.4 shows a schematic of the shear strength test of a glass chip bonded on an Si substrate and a

scanning electron microscopy (SEM) image of this test specimen. The glass chip has a length and width of 1.4 mm and a thickness of 400 μm . We used a Bondtester (Nordson Advanced Technology K. K., series 4000) as the test apparatus. The glass chip was bonded on the Si substrate by an electrostatic force generated at a voltage of 400 V under atmospheric pressure. The anodic bonding temperature was changed from 220 to 300 $^{\circ}\text{C}$ in preparation for the test specimens. The holding time of the electrostatic force was 30 min for all specimens.



Figure 5.4. Schematic of shear strength test and SEM image of test specimen.

Figure 5.5 shows the variation of the shear strength with increasing bonding temperature. The shear strength increased as the temperature increased, reaching 13 MPa at 250 $^{\circ}\text{C}$. The fracture mode was also observed after shear tests by SEM (Hitachi High-Technologies, S-4300), as shown in Figures 5.6(a)-5.6(c). An interfacial fracture was observed on the greater part of the bonding area at 220 and 240 $^{\circ}\text{C}$ [see Figs. 5.6(a) and 5.6(b)], whereas a base material fracture on the Si substrate was totally dominated at 250 $^{\circ}\text{C}$ [see Fig. 5.6(c)]. This fracture was observed at temperatures of 270 to 300 $^{\circ}\text{C}$, and these fractures are similar to that of 250 $^{\circ}\text{C}$. Thus, the bonding temperature in the 1st bonding step must be set above 250 $^{\circ}\text{C}$ under atmospheric pressure for the accelerometer.

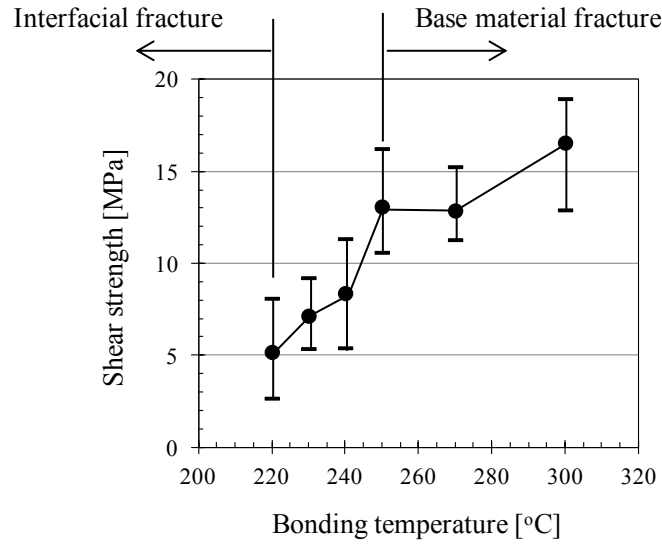
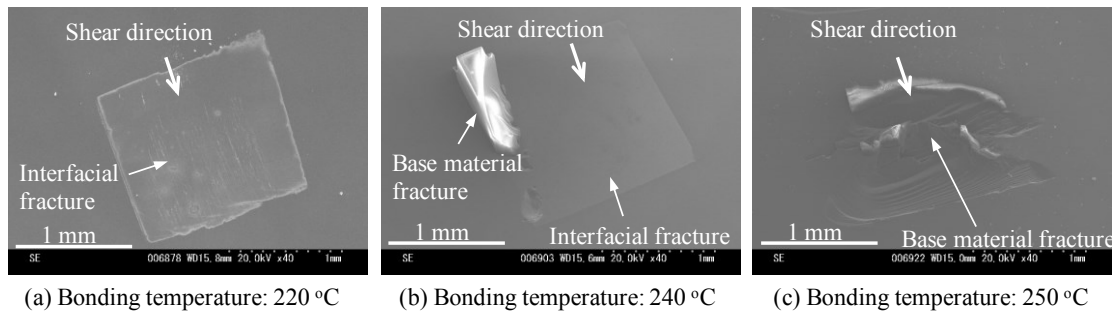


Figure 5.5 Variation of shear strength with increasing temperature in the 1st bonding step.



Figures 5.6. SEM images of fracture mode after shear strength tests.

5.3.2 1st BONDING STEP FOR UNSEALING GYROSCOPE

The gyroscope has to be unsealed by the bumps on the glass substrate even if the electrostatic force of the anodic bonding is applied in the 1st bonding step. To determine the suitable dimensions of the bumps in order to ensure the unsealed area around the gyroscope, trials of the 1st bonding step were carried out by changing the dimensions of the bumps: the heights used were from 0.4 to 1.2 μm and the diameters from 1 to 18 μm .

Figure 5.7 shows the relationship between the bump diameter and the ratio of the number of unsealed gyroscopes to the total number of gyroscopes fabricated on the 4-inch SOI wafer. Here, the ratio becomes 0 % when the bumps do not work rightly after the 1st bonding step. The unsealed gyroscopes were identified by the appearance of interference fringes on the glass observed using a microscope. The ratio was 0 % for the glass substrate with the 0.4- μm -high bumps regardless of the diameter of the bumps as

shown in Figure 5.7. This means that the glass substrate was completely bonded to the sensor substrate by only the electrostatic force in the 1st bonding step. However, the ratio increased as the diameter of bumps with heights of 0.8 μm and 1.2 μm increased. In particular, most of the gyroscopes were unsealed by the glass substrate having bumps with a diameter larger than 15 μm . Thus, bumps with a diameter larger than 15 μm and height larger than 0.8 μm are reasonable for forming an unsealed area around the gyroscope in the 1st bonding step.

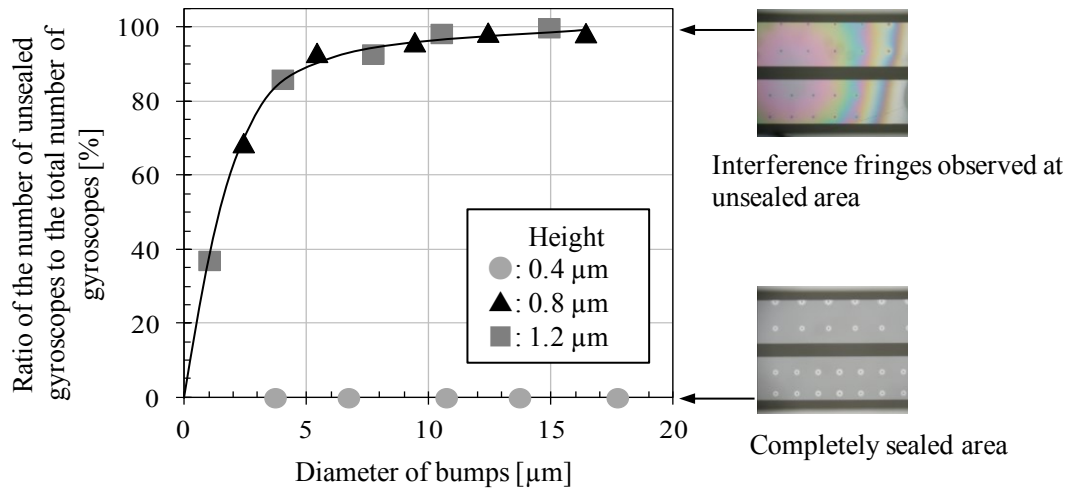


Figure 5.7 Relationship between bump diameter and ratio of the number of unsealed gyroscopes to the total number of gyroscopes fabricated on 4-inch SOI wafer.

Figure 5.8 shows the effect of the bonding temperature on the ratio defined above. Here, bumps with 15- μm -diameter and 1.2- μm of height were used. The ratio reduced to 25 % at 300 $^{\circ}\text{C}$ and to 22 % at 400 $^{\circ}\text{C}$. These results were caused by the deflection of the glass substrate at temperatures above 300 $^{\circ}\text{C}$, which could lead to contact between the glass and the Si substrates around the gyroscope by only the electrostatic force.

From the above results, the bumps with a diameter larger than 15 μm and a height larger than 0.8 μm should be prepared on the glass substrate for unsealing the gyroscope. The bonding temperature for sealing the accelerometers and unsealing the gyroscope in the same bonding step should be set at 250 $^{\circ}\text{C}$.

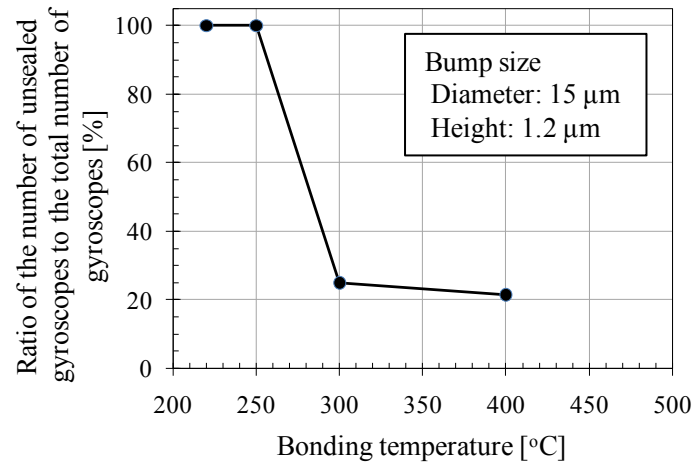


Figure 5.8 Effect of bonding temperature on ratio of the number of unsealed gyroscopes to the total number of gyroscopes fabricated on 4-inch SOI wafer.

5.3.3 PRESSURE CONTROL STEP FOR GYROSCOPE

Since a gyroscope under a low pressure increases the quality factor of the electrostatic driven oscillator, the gyroscope sealed in vacuum has a high sensitivity. We investigated the influence of pressure for sealing the gyroscope on its quality factor. Here, the gyroscope fabricated on the sensor substrate was set in a pressure-control chamber, and its quality factor was measured by using a laser doppler velocimeter (LDV) through the view port of the chamber. The pressure of the chamber was controlled at 0.1 to 10^5 Pa.

Figure 5.9 relates the quality factor of the gyroscope with the chamber pressure. The quality factor was about 500 above 1000 Pa. However, it gradually increased with the decrease in the chamber pressure from 1000 to 200 Pa and drastically increased up to more than 2000 below 200 Pa. Although the target of the quality factor is larger than 1000 in this research, we decided to reduce the chamber pressure to 0.1 Pa to perform the WLP process in safety.

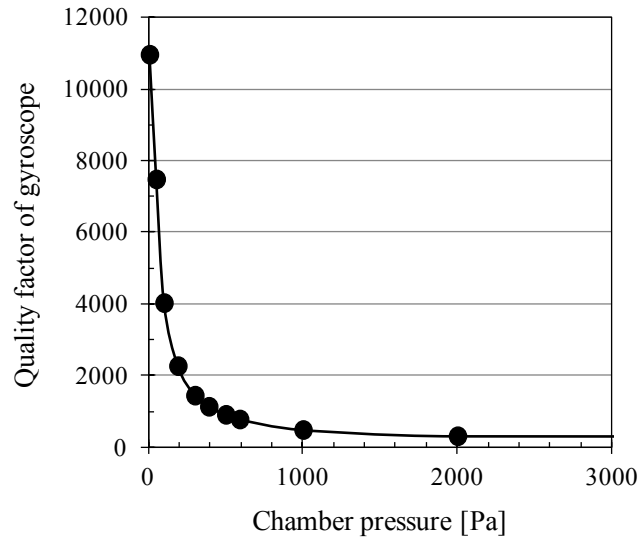


Figure 5.9 Variation of quality factor of gyroscope with increasing chamber pressure.

5.3.4 2nd BONDING STEP FOR SEALING GYROSCOPE

Since the glass substrate is easily deformed elastically at high temperatures under high loads, the glass substrate around the bumps comes into contact with the sensor substrate. To seal the gyroscope in the pressure-control chamber in the 2nd bonding step, we applied a high temperature and high contact load to the sensor and glass substrates. This process was to collapse the gap space between the sensor and glass substrates around the bumps. A reasonable condition for the 2nd bonding step was investigated by changing the contact load from 1.0 to 1.5 MPa at 500 and 520 °C under a pressure of 0.1 Pa. The applied voltage of the anodic bonding was 400 V, and the bonding time was kept for 30 min. The process temperature was gradually decreased at a rate of 4 °C/min to room temperature after the bonding to avoid a residual stress caused by the mismatch of coefficient of thermal expansion between the SOI and glass substrates.

Figure 5.10 shows the relationship between the contact load and the percentage of the sum of the residual unsealed area to the total designed sealing area around gyroscopes on the 4-inch SOI wafer. Here, the unsealed area was roughly estimated from widths of outer fringes in the interference patterns observed by a microscope, as listed in Table 5.1. The percentage of unsealed area reached 40 % in the bonding tests at 500 °C regardless of the weight of the contact load in Figure 10. However, in the bonding tests at 520 °C, the percentage of unsealed area decreased with an increase in the contact load, and it reached 0 % at a contact load of 1.5 MPa. At this time, the bumps fabricated on the glass substrate were clearly observed from the top without any

interference patterns as shown in Table 5.1, since the flat area of the glass substrate around and between the bumps completely touched the sensor substrate.

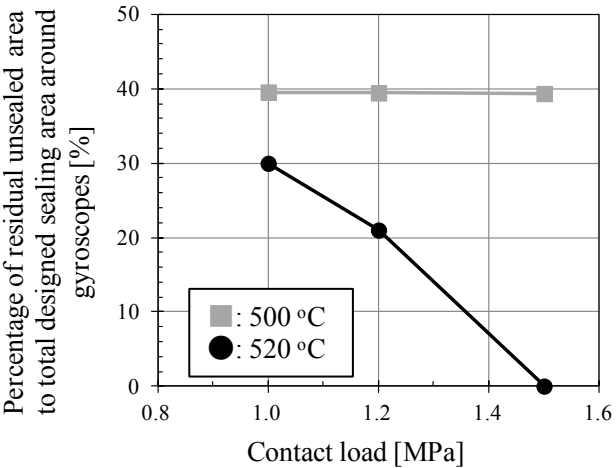


Figure 5.10 Relationship between contact load and percentage of the sum of residual unsealed area to total designed sealing area around gyroscopes on 4-inch SOI wafer.

Table 5.1 Optical microscopy images of bump area after the 2nd bonding step.

		Contact load		
		1.0 MPa	1.2 MPa	1.5 MPa
500°C				
520°C				

To confirm the residual stress of bonded wafer after the 1st and 2nd bonding steps, the bending curvature of the SOI substrate was measured by a stylus surface profiler (KLA-Tencor P14) in the y-direction shown in Figure 5.1. The height of curvature at the position of each device was less than 0.1 μm in average after the 1st bonding step, whereas it was between 0.6 and 0.7 μm in average after the 2nd bonding step. Thus, the

residual stress of bonded wafer produced at the 1st and 2nd bonding steps can be negligible.

To evaluate the shear strength after the 2nd bonding step, we again carried out a shear test on the packaged substrate by using the same technique in Figure 4. Here, glass chips with a length and width of 0.6 mm and a thickness of 400 μm were bonded to the Si substrate by changing the contact load from 0 to 1.5 MPa in the 2nd bonding step. There were no bumps fabricated on these specimens. The variation in shear strength with an increasing contact load is shown in Figure 5.11. The averaged shear strength was in the range of 14 to 17 MPa even with no loading condition, which was caused by the high bonding temperature. The fracture mode was also observed in shear tests in Figures 5.12(a)-(c). All specimens fractured from the base material of the Si substrate or glass chip without interfacial fracture. These results mean the shear strength at the interface after the 2nd bonding step has been larger than that of the base materials. Therefore, a bonding temperature of 520 $^{\circ}\text{C}$ and contact load of 1.5 MPa was concluded to be suitable for the 2nd bonding step when using a glass substrate with bumps.

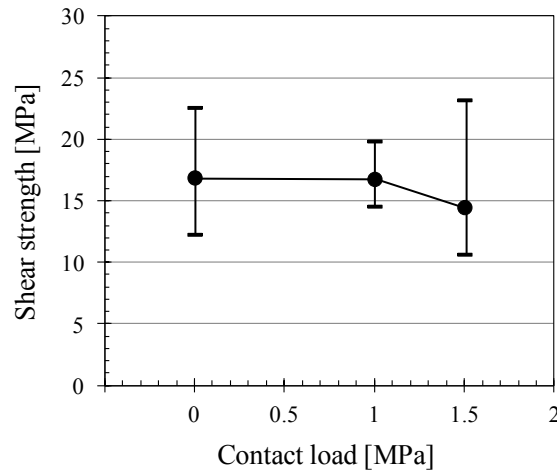
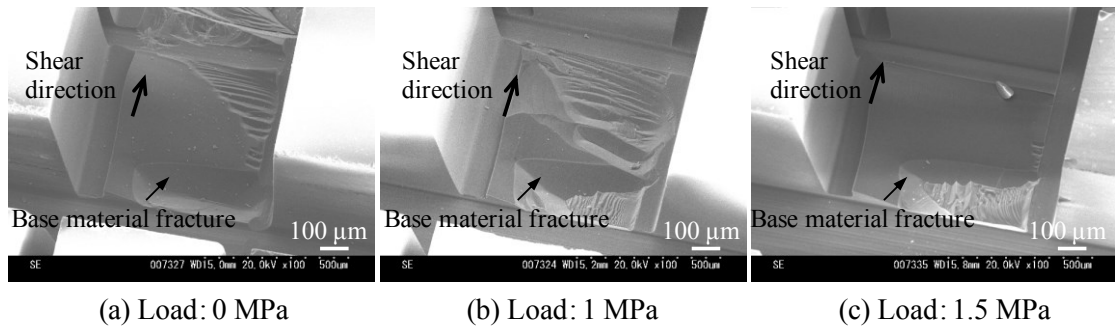


Figure 5.11 Variation in shear strength with increasing contact load at 520 $^{\circ}\text{C}$.

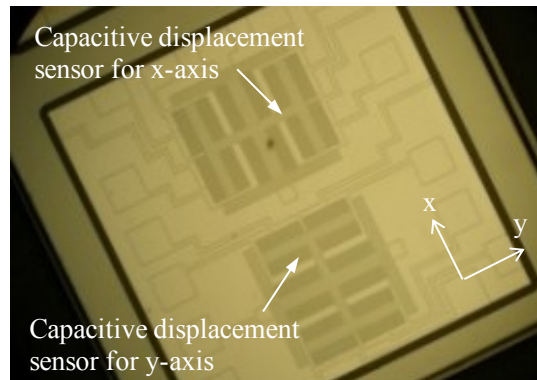


Figures 5.12 SEM images of fracture mode after shear strength tests.

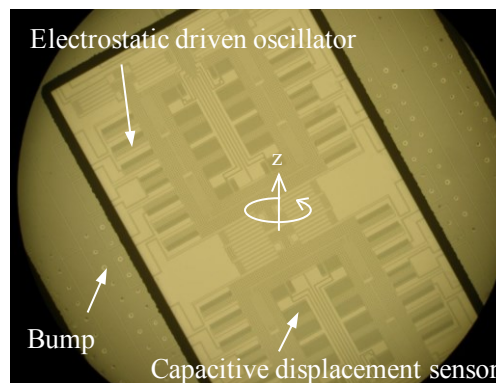
5.4 CHARACTERISTICS OF MEMS SENSORS

5.4.1 PERFORMANCE OF ACCELEROMETER AND GYROSCOPE AFTER WLP

Figures 5.13(a) and 5.13(b) show photographs of the accelerometer and the gyroscope completely sealed with the glass substrate in the 2nd bonding step. Interference fringes were not observed at the bumps around the gyroscopes. To ensure the sealing condition of the WLP, the performance of these devices was demonstrated by the amplitude ratio of the dynamic oscillation to the quasi-static driving, $|X|/X_{st}$ for each device. The X_{st} of the accelerometer was defined as the displacement produced at the capacitive displacement sensor when a D. C. voltage of 0.2 V was applied to the sensor, regarding the sensor as an electrostatic driven actuator. The $|X|$ was the amplitude of the accelerometer when an A. C. voltage of ± 0.2 V was applied to the sensor by changing its frequency. The X_{st} and the $|X|$ of the gyroscope were equivalent to the displacement produced at the electrostatic driven oscillator when we applied a D. C. voltage of 2.5 V and an A. C. voltage of ± 2.5 V to the electrostatic driven oscillator, respectively. The amplitude ratios for both sensors sealed in not only a vacuum but also an atmosphere were evaluated.



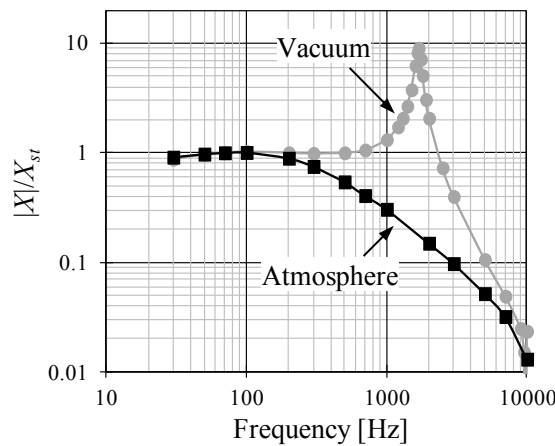
(a) Accelerometer



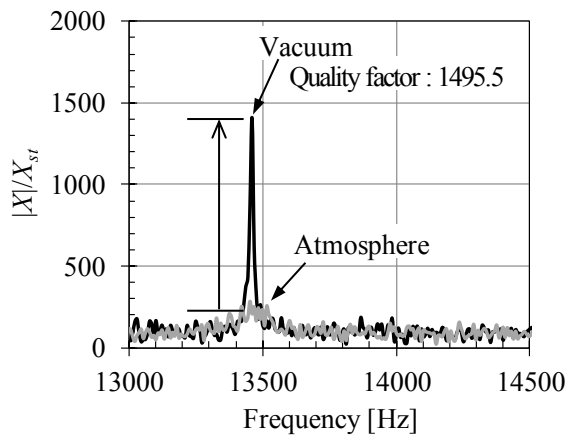
(b) Gyroscope

Figures 5.13 Photographs of accelerometers and gyroscope sealed with glass substrate.

Figures 5.14(a) and 5.14(b) show variations of the amplitude ratio with an increase in the driving frequency of the dynamic oscillation in the accelerometer and the gyroscope, respectively. The amplitude ratio of the accelerometer sealed in vacuum showed a sharp rise at a resonant frequency of 1800 Hz, as shown in Figure 5.14(a). This is caused by the capacitive displacement sensor being vibrated without air-damping. The accelerometer sealed in the atmosphere did not have any peaks owing to air-damping, so its vibration could be suppressed even at the resonant frequency.



(a) Accelerometer



(b) Gyroscope

Figures 5.14 Variation of amplitude ratio with increase in driving frequency of dynamic oscillation in accelerometer and gyroscope.

The gyroscope also showed a similar trend to the accelerometer as shown in Figure 5.14(b). The quality factor was estimated to be 1495.5 at the resonant frequency of 13460 Hz and FWHM of 9 Hz. The gyroscope sealed in vacuum had peak amplitude at

the resonant frequency of 13460 Hz, whereas the one sealed in the atmosphere had a small peak. The quality factor at the resonant frequency was estimated to be about 1495.5 from the half bandwidth of 3 dB at the peak, which was smaller than the one measured in the pressure-control chamber of Figure 5.9. The small value of quality factor would have been caused by the degassing from the SOI and glass substrates [30, 31], the O₂ gas generation in the 2nd anodic bonding step [12, 32] expressed as the following chemical reaction, and the effect of the small gap at the bumps on the pumping speed.



The degassing from the substrates and the O₂ gas generation could increase the pressure of the sealing space of the gyroscope. The small gap at the bumps would also produce a pressure loss during pumping, which probably caused an influx of gas in the sealing space. Thus, the quality factor would have reduced. However, the quality factor of the gyroscope after the 2nd bonding step was not lower than the target factor (>1000) in this research.

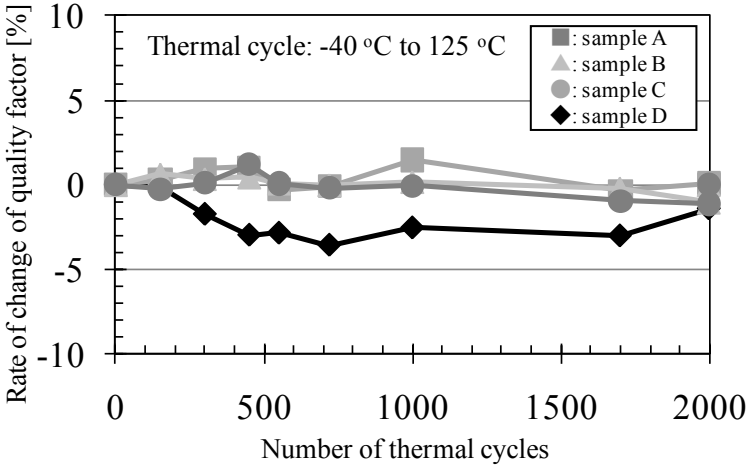
The percentage of MEMS devices having performances that satisfy design specifications to the total number of devices of 256 was larger than 85 % on 5-inch wafers.

5.4.2 RELIABILITY TESTS OF GYROSCOPE FOR AUTOMOTIVE APPLICATIONS

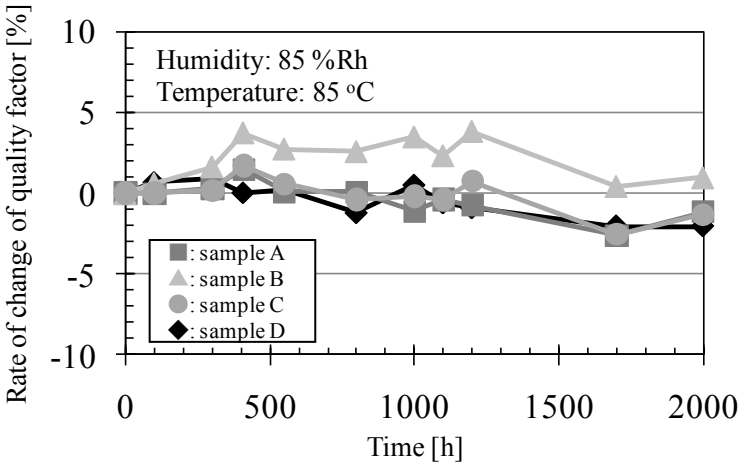
A thermal cyclic test and an endurance test in high humidity at high temperature were carried out for the gyroscope after WLP for automotive applications. We changed from -40 °C at minimum to 125 °C at maximum with a holding time of 30 min for the thermal cyclic test. The endurance test was carried out under humidity of 85 %Rh and at a temperature of 85 °C. The quality factor of the gyroscope was evaluated in these tests using the LDV.

Figure 5.15(a) shows the variation of the rate of change of the quality factor with an increasing number of cycles for the thermal cyclic test. The rate of change remained fairly stable in the range of ±5 % until 2000 cycles. The sealing of the gyroscope under a low pressure was able to withstand an abrupt change of temperature. Figure 5.15(b) shows the variation of the rate of change of the quality factor with an increasing operation time for the endurance test. This also indicated a trend similar to that in the

above figure. The rate of change was constant until 2000 hours in the test. The sealing in the 2nd bonding step fully endured a severe environment under high humidity and a high temperature for a long time. Therefore, we can conclude that the WLP process proposed in this research is effective for use in a simultaneous packaging process for low cost applications.



(a) Thermal cyclic test



(b) Endurance test

Figures 5.15 Reliability testing results of accelerometer and gyroscope sealed with glass substrate in WLP.

5.5 CONCLUSION

An anodic bonding-based wafer-level-packaging technique was developed for simultaneous sealing of a MEMS accelerometer and gyroscope under different pressures. Bumps with height larger than 0.8 μm and diameter larger than 15 μm fabricated on glass substrate around the gyroscope enabled a selective sealing of the accelerometer in the atmosphere in a 1st bonding step and the gyroscope in vacuum in a 2nd bonding step. The shear strength between the sensor and glass substrates sealed at 250 °C with a voltage of 400 V in the 1st bonding step reached 13 MPa. A pressure control of 0.1 Pa before the 2nd bonding step was able to keep the quality factor of the gyroscope at higher than 1000. Sealing the gyroscope in vacuum at 520 °C with a contact load of 1.5 MPa in the 2nd bonding step led to shear strength of 14 MPa, which was close to the value obtained in the 1st bonding step.

The vibration of the accelerometer after the WLP was suppressed even at the resonant frequency owing to the air-damping. The quality factor of the gyroscope after the WLP reached 1495 even when degassing, O₂ gas generation and pressure loss due to the small gap were not negligible. The quality factor of the gyroscope after WLP also remained fairly stable in the range of $\pm 5\%$ during the thermal cyclic test. From the performance and the reliability of the MEMS sensors, the anodic bonding based-WLP process was effective for simultaneous sealing of the accelerometer and gyroscope under different pressures.

REFERENCES

- [1] B. Vigna, "MEMS epiphany," in *Proc. IEEE Int. Conf. MEMS*, Jan. 2009, pp. 1–6.
- [2] G. Lammel, "THE FUTURE OF MEMS SENSORS IN OUR CONNECTED WORLD", *Proc. The 28th IEEE International Conference on Micro Electro Mechanical Systems, MEMS2015*, pp. 61–64, 2015
- [3] W. J. Fleming, "New Automotive Sensors—A Review", *IEEE SENSORS JOURNAL*, Vol. 8, No. 11, pp. 1900–1921, 2008
- [4] P. Merz, W. Pilz, F. Senger, K. Reimer, M. Grouchko, T. Pandhumsoporn, W. Bosch, A. Cofer and S. Lassig, "IMAPCT OF Si ON VIBRATORY MEMS GYROSCOPE PERFORMANCE", *The 14th International Conference on Solid-State Sensors, Actuators & Microsystems, Transducers 2007*, pp. 1187-1190, 2007
- [5] T. Akashi, Y. Omura, H. Funabashi, M. Fujiyoshi, Y. Nonomura and Y. Hata, "A Y-AXIS SOI-MEMS GYROSCOPE WITH A ZIGZAG-SHAPED Z-ELECTRODE SUPPORTED BY THREE-Dimensionally-INTERSECTED Z-BEAMS", *The 17th International Conference on Solid-State Sensors, Actuators & Microsystems, Transducers 2013*, pp. 1851-1854, 2013
- [6] C. T. Kou, T. Y. Chao, I. Ta. Chiang and Y. T. Cheng, "Wafer level fabrication of hermetically sealed microcavity with robust metal interconnects for chip cooling application", *Sens. Actuators. A*, 139, pp. 259-264, 2007
- [7] H. Okada, T. Itoh and T. Suga, "Wafer level sealing characterization method using Si micro cantilevers", *Sens. Actuators. A*, 147, pp. 359-364, 2008
- [8] V. A. Vitikkate, K. I. Chen, W. T. Park and T. W. Kenny, "Development of wafer scale encapsulation process for large displacement piezoresistive MEMS devices", *Sens. Actuators. A*, 156, pp. 275-283, 2009
- [9] J. Oberhammer, F. Niklaus and G. Stemme, "Sealing of adhesive bonded devices on wafer level", *Sens. Actuators. A*, 110, pp. 407-412, 2004
- [10] S. Marauska, R. Jahns, C. Kirchhof, M. Claus, E. Quandt, R. Knochel and B. Wagner, "Highly sensitive wafer-level packaged MEMS magnetic field sensor based on magnetoelectric components", *Sens. Actuators. A*, 189, pp. 321-327, 2013
- [11] R. Elfrink, M. Renaud, T. M. Kamel, C. de Nooijer, M. Jambunathan, M. Goedbloed, D. Hohlfeld, S. Motova, V. Pop, L. Caballero and R. van Schaijk, "Vacuum-packaged piezoelectric vibration energy harvesters: damping contribution and autonomy for a wireless sensor system", *J. Micromech. Microeng.*, 20, 104001, 2010
- [12] M. Esashi, "Wafer level packaging of MEMS", *J. Micromech. Microeng.*, 18, No. 7, 073001, 2008

- [13] S. Tanaka and M. Esashi, "Wafer-level MEMS Package and Its Reliability Issues", *MICROELECTRONICS RELIABILITY*, Vol. 54, pp. 875-881, 2014
- [14] S. J. Kang, Y. S. Moon, W. H. Son and S. Y. Choi, "Vacuum-controlled wafer-level packaging for micromechanical devices", *Jpn. J. Appl. Phys.*, Vol. 53, 066501, 2014
- [15] G. Wu, D. Xu, B. Xiong, Y. Wang, Y. Wang and Y. Ma, "Wafer-Level Vacuum Packaging for MEMS Resonators Using Glass Frit Bonding", *J. Microelectromech. Sys.*, Vol. 21, No. 6, pp. 1484-1491, 2012
- [16] K. Notzild, C. Dresbach, J. Graf and B. Bottge, "Temperature dependent fracture of glass frit bonding layer", *Microsyst. Technol.*, 16, pp. 1243-1249, 2010
- [17] R. Stengel, T. Tan and U. Gosele, "A Model for the Silicon Wafer Bonding Process", *Jpn. J. Appl. Phys.*, Vol. 28, No. 10, pp. 1735-1741, 1989
- [18] H. Moriceau, F. Rieutord, F. Fournel, Y. L. Tiec, L. D. Cioccio, C. Morales, A. M. Carvet and C. Deguet, "Overview of recent direct wafer bonding advances and applications", *Adv. Nat. Sci.: Nanosci. Nanotechnol.*, 1, 043004, 2010
- [19] S. Kuhne and C. Hierold, "Wafer-level packaging and direct interconnection technology based on hybrid bonding and through silicon vias", *J. Micromech. Microeng.*, 21, No.8, 085032, 2011
- [20] H. Takagi and R. Maeda, "Aligned room-temperature bonding of silicon wafers in vacuum by argon beam surface activation", *J. Micromech. Microeng.*, 15, No. 2, pp. 290-295, 2005
- [21] P. Merz, K. Reimer, M. Weis, O. Schwarzelbach, C. Schroder, A. Giambastiani, A. Rocchi, and M. Heller, "Combined MEMS Inertial Sensors for IMU Applications", *Proc. 23th IEEE International Conference on Micro Electro Mechanical Systems, MEMS2010*, pp. 488-491, 2010
- [22] J. S. Mitchell and K. Najafi, "A DETAILED OF YIELD AND RELIABILITY FOR VACUUM PACKAGES FABRICATED IN A WAFER-LEVEL AU-SI EUTECTIC BONDING PROCESS", *The 15th International Conference on Solid-State Sensors, Actuators & Microsystems, Transducers 2009*, pp. 841-844, 2009
- [23] U. Hofmann, H. J. Quenzer, C. Eisermann, J. Janes, C. Schroeder, B. Jensen, J. Hagge, F. Soerensen, F. Senger, D. Vick, O. Schhwarzelbach, L. Rantzmam, B. Wagner and W. Benecke, "A NOVEL VACUUM-PACKAGED LOW-POWER SCANNING MIRROR WITH INCLINED 3D-SHAPED WINDOW", *The 16th International Conference on Solid-State Sensors, Actuators & Microsystems, Transducers 2011*, pp. 1527-1530, 2011

- [24] S. Tez, U. Aykutlu, M. M. Torunbalci and T. Akin, "A Bulk-Micromachined Three-Axis Capacitive MEMS Accelerometer on a Single Die", *J. Microelectromech. Syst.*, Vol. 24, No. 5, pp. 1264-1274, 2015
- [25] H. Tachibana, K. Kawano, H. Ueda and H. Noge, "VACUUM WAFER LEVEL PACKAGED TWO-DIMENSIONAL OPTICAL SCANNER BY ANODIC BONDING", *Proc. 22th IEEE International Conference on Micro Electro Mechanical Systems, MEMS2009*, pp. 959–962, 2009
- [26] R. M. Haque and K. D. Wise, "A Glass-in-Silicon Reflow Process for Three-Dimensional Microsystems", *J. Microelectromech. Syst.*, Vol. 22, No. 6, pp. 1470-1477, 2013
- [27] J. Liu, J. Shang, J. Tang and Q. A. Hung, "Micromachining of Pyrex 7740 Glass by Silicon Molding and Vacuum Anodic Bonding", *J. Microelectromech. Syst.*, Vol. 20, No. 4, pp. 909-915, 2011
- [28] M. Degawa, H. Jeong, H. Sonobe, C. Takubo, K. Yamanaka and Y. Goto, "Laterally-Driven Deformation-Robust MEMS Gyroscopes with Three Sets of Symmetrically Arranged Folded-Beam Suspensions", *The 15th International Conference on Solid-State Sensors, Actuators & Microsystems, Transducers 2009*, pp. 664–667, 2009
- [29] H. Jeong, K. Yamanaka, Y. Goto, T. Aono and M. Hayashi, "Three-Axis MEMS Inertial Sensor for Automobile Applications", *Proc. IEEE Sensors 2011*, pp. 444–447, 2011
- [30] Y. Yuzi, M. Kobayashi and K. Asano, "Adsorption of Mixed Gases on a Pyrex Glass Surface at Very Low Pressures", *J. Vac. Sci. Technol.*, Vol. 9, No. 1, pp. 248-252, 1972
- [31] J. T. Law and E. E. Francois, "ADSORPTION OF GASES ON A SILICON SURFACE", *J. Phys. Chem.*, 60(3), pp. 353-358, 1956
- [32] S. Mack, H. Baumann, U. Gosele, H. Werner and R. Schlogl, "Analysis of Bonding-Related Gas Enclosure in Micromachined Cavities Sealed by Silicon Wafer Bonding", *J. Electrochem. Soc.*, Vol. 144, No. 3, pp. 1106–1111, 1997

Chapter 6: Conclusions

This thesis investigates the post-process for miniaturizing and integrating MEMS-based sensors. The MEM-based sensors are applied as various applications such as automobile, robot, smartphone, medical analysis etc. These sensors are required an endurance of temperature, humidity and shock, miniaturizing for mounting on small equipment and precise accuracy for detecting. Therefore, these MEMS-based sensors should be improved in reliability and reduction of production size and manufacturing cost. The conclusion of each chapter is summarized as below.

In chapter 3, we considered a new process for multilevel interconnection structures suitable for MEMS devices with various metal materials, and reached the following conclusion. The adhesive fracture energy of metal films with respect to the SiO_2 film calculated by the molecular dynamics technique shows corresponds with the removability of insulating film from metal layer by ultrasonic treatment. We fabricated a multilevel interconnection structure with high adhesive fracture energy metals (Cr and Ti) used for the lower wiring and low adhesive fracture energy metals (Cu and Au) used for the contact areas. We found that the SiO_2 film could be removed selectively from the contact areas. By forming upper wiring to connect the contact areas and the electrodes, we realized a new process for fabricating multilevel interconnection structures.

In chapter 4, to realize eutectic bonding-based WLP accelerometers with a high shear strength, bonding conditions were analytically and experimentally investigated so that the solder material atoms did not diffuse to the adhesion layers too much.

MD simulations clarified the diffusion mechanism of solder material atoms at elevated temperatures. Ni atoms used as one adhesion layer easily migrated to an Au-Sn layer in temperature ranges of 300 °C to 340 °C, which created an AuSnNi alloy layer. Au and Sn atoms also diffused into a Cr adhesion layer at a high temperature of 340 °C. Tensile creep simulations showed that fractures in a solder model started from the lowest potential energy domain; the lowest potential energy at 300 °C was in the AuSnNi layer, and that at 340 °C was in the Cr- SiO_2 interface.

Shear tests of the WLP accelerometers followed by EDX analyses showed that a sample bonded at 300 °C had fractured at the AuSnNi layer and had a high shear strength, while that at 340 °C was exfoliated at the Cr- SiO_2 interface by the lower shear force. These experiments were qualitatively consistent with MD simulations. A 6-inch wafer after WLP at 300 °C under a contact load of 9.8 kN also completely bonded because there were no defects in the top-side lids on the wafer after the polishing process.

Eutectic bonding-based WLP was effective for controlling the attenuation of

accelerometers by deciding the thickness of the electroplated solder materials that played the role of a cavity between the accelerometer and the lids. If the gap distance between the accelerometer and the lids was less than 6.2 μm , the signal gains for x- and z-axis acceleration was less than 20 dB even at the resonance frequency due to air-damping. It is possible to reduce the chip size of accelerometer with the developed WLP technique, and the cost was able to be reduced to 50 % or less.

In chapter 5, an anodic bonding-based wafer-level-packaging technique was developed for simultaneous sealing of a MEMS accelerometer and gyroscope under different pressures. Bumps with height larger than 0.8 μm and diameter larger than 15 μm fabricated on glass substrate around the gyroscope enabled a selective sealing of the accelerometer in the atmosphere in a 1st bonding step and the gyroscope in vacuum in a 2nd bonding step. The shear strength between the sensor and glass substrates sealed at 250 °C with a voltage of 400 V in the 1st bonding step reached 13 MPa. A pressure control of 0.1 Pa before the 2nd bonding step was able to keep the quality factor of the gyroscope at higher than 1000. Sealing the gyroscope in vacuum at 520 °C with a contact load of 1.5 MPa in the 2nd bonding step led to shear strength of 14 MPa, which was close to the value obtained in the 1st bonding step.

The vibration of the accelerometer after the WLP was suppressed even at the resonant frequency owing to the air-damping. The quality factor of the gyroscope after the WLP reached 1495 even when degassing, O₂ gas generation and pressure loss due to the small gap were not negligible. The quality factor of the gyroscope after WLP also remained fairly stable in the range of ± 5 % during the thermal cyclic test. From the performance and the reliability of the MEMS sensors, the anodic bonding based-WLP process was effective for simultaneous sealing of the accelerometer and gyroscope under different pressures.

Acknowledgements

The present author is sincerely grateful to Professor Yoshitada Isono for his kind direction and valuable discussions through this study.

I am very grateful to Professor Katsushi Tanaka, Professor Masatoshi Kitamura and Associate Professor Koji Sugano for their valuable discussions for my doctoral dissertation.

I would like to acknowledge Dr. Tomio Iwasaki for his valuable discussions through the study of post processes with molecular dynamics simulations in chapters 2 to 4 of this thesis.

I would like to acknowledge Dr. Ryoji Okada, Dr. Atsushi Kazama, Dr. Shohei Hata and Mr. Mitsuyasu Furusawa for their valuable discussions and encouragements through the study of wafer-level-packaging for piezoresistive MEMS-based accelerometers in chapter 4 of this thesis.

I would like to acknowledge Mr. Akira Koide, Mr. Kengo Suzuki and Mr. Masahide Hayashi for their valuable discussions and encouragements through the study of wafer-level-packaging for accelerometer and gyroscope under different pressures in chapter 5 of this thesis.

I am also very grateful to Dr. Yoshishige Endou, Mr. Yasuhiro Yoshimura, Mr. Masatoshi Kanamaru, Dr. Tatsuya Nagata, Mr. Teruhisa Akashi and Mr. Hitoyuki Tomotsune for their valuable discussions and encouragements through the study of fabricating and packaging techniques of MEMS-based sensors.

I also thank to all members of Hitachi, Ltd., Hitachi High-Technologies Corporation, Hitachi Metals, Ltd. and Hitachi Automotive Systems, Ltd. for their kind encouragements and helps.

Appendix

Articles related to this thesis

Technical Papers

1. T. Aono, T. Iwasaki, Y. Yoshimura and Y. Nakayama, “Method for Fabricating Multilevel Interconnection Structures Using Differential Delamination Energies between Metal and Silicon Oxide Thin Films”, Electronics and Communication in Japan, Vol. 99, No. 4, pp. 41-49, 2016
2. T. Aono, A. Kazama, R. Okada, T. Iwasaki and Y. Isono, “Eutectic-based wafer-level-packaging technique for piezoresistive MEMS accelerometers and bond characterization using molecular dynamics simulations”, Journal of Micromechanics and Microengineering, 28, 035004, 2018
3. T. Aono, K. Suzuki, M. Kanamaru, R. Okada, D. Maeda, M. Hayashi and Y. Isono, “Development of wafer-level-packaging technology for simultaneous sealing of accelerometer and gyroscope under different pressures”, Journal of Micromechanics and Microengineering, 26, 105007, 2016

International Conferences

1. T. Aono, A. Kazama, R. Okada, T. Iwasaki and Y. Isono, “BONDING STRENGTH CHARACTERIZATION OF EUTECTIC-BASED WLP USING MOLECULAR DYNAMICS AND WAFER LEVEL SHEAR TESTING”, Technical Digest of the 19th International Conference on Solid-State Sensor, Actuators and Microsystems (Transducers’17), pp. 1199-1202, 2017

Doctoral Dissertation, Kobe University

“Study on Wiring and Packaging Techniques for Miniaturizing and Integrating MEMS-Based Sensors”

(小型・集積化MEMSセンサの配線・パッケージング技術に関する研究), page 97

Submitted on January, 16, 2018

The date of publication is printed in cover of repository version published in Kobe University Repository Kernel.

© Takanori AONO
All right Reserved, 2018