Development of high performance micromechanical resonators for advanced sensing applications

Wang, Xiaowei

2005

Wang, X. (2005). Development of high performance micromechanical resonators for advanced sensing applications. Doctoral thesis, Nanyang Technological University, Singapore.

<https://hdl.handle.net/10356/5359>

<https://doi.org/10.32657/10356/5359>

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**DEVELOPMENT OF HIGH PERFORMANCE
MICROMECHANICAL RESONATORS FOR
ADVANCED SENSING APPLICATIONS**

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**SCHOOL OF MECHANICAL & AEROSPACE ENGINEERING
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2005

Development of High Performance Micromechanical Resonators for Advanced Sensing Applications

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

2005

ACKNOWLEDGEMENTS

I am sincerely grateful to my research supervisors, Assoc. Prof. Lin Rongming and Dr. Wang Zhe, for the support and guidance that they have provided throughout the research. With their constant help and encouragement, I have been offered the precious opportunities and experiences to fulfill this research.

Also many thanks and gratitudes are due to Dr. Jiang Ning, Ms. Jong Ming Ching, Dr. Feng Huanhua, Mr. Jia Guojun and Mr. Saxon Liw Sean Lian, from the MEMS Department of Institute of Microelectronics (IME), Singapore, for their sincere help and sharing of their valuable experiences in their respective fields.

I would like to thank all my friends who are working and studying in the Centre for Mechanics of Micro-Systems in the School of Mechanical and Production Engineering, Nanyang Technological University for giving and sharing their valuable thoughts and opinions during the period of research. Some of them are Dr. Wang Wei Jun, Dr. Zhang Wei Shan, Mr. Xu Guo Ming, Mr. Zhu Jun and Mr. Xu Jian Guo. Last but not least, appreciations are due to all friends, who gave so many encouragement and help during my research work in NTU and IME.

I take great pleasure in acknowledging the financial support from Nanyang Technology University and the Institute of Microelectronics.

Special thanks are due to my wife, Cai Lu, and my parents, for their eternal love and support in my life.

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ABSTRACT

This research focuses on the fundamental issues of microelectromechanical systems (MEMS) technology that is used to improve the performance of current microresonators, and seeks to develop new design methodology for desired optimal resonator characteristics of high frequency and high quality factor, and to realize advanced technologies in microfabrication and testing of improved prototype devices. Two types of resonator and relevant technologies have been investigated in this research, i.e., (i) micromechanical (or μ -mechanical) resonators, and (ii) thin film bulk acoustic resonators (TFBARs).

Researches on micromechanical resonator have been mainly focused on the investigation of possible approaches that can be used to improve present resonant frequencies and performances of micromechanical resonators. Through modeling and simulations, extensive studies on areas of the miniaturization of characteristic dimensions, the excitation of higher order harmonic frequencies as well as the reduction of effective mass, have been analyzed and discussed. Resonator structures with various geometrical configurations which are extensions of current designs for higher frequency applications have been designed and fabricated using conventional polysilicon based micromachining technology. Further research and development of such resonator devices have also been concentrated on using the state-of-the-art silicon-on-insulator (SOI) technology to improve the performance of devices, and the related fabrication processes have been successfully developed. Experimental studies on various resonator designs, fabrications and correlation with simulation results have been carried out. Alongside with these studies, an image measurement system has also been developed and applied as an

effective measurement tool needed during resonator batch fabrication. The results of the beam resonators have revealed such advantages of μ -resonators as wide applicable frequency range, orders of magnitude smaller size, batch fabrication capacity and integration with IC technology, while other anticipated important characteristics of possible large reduction in power consumption and potentially higher quality factor than other single-chip solutions have yet to be assessed.

The work on TFBAR devices begins with the improvement of quality factor Q of similar devices at frequencies up to GHzs. For this purpose, development and characterization of high performance AlN piezoelectric material have been carried out firstly by using our newly developed reactive sputtering method. Modeling and simulation of various influential factors on the performance of TFBARs have also been carried out and used to guide our designs. Two novel resonator structures have been proposed and analyzed in our work, i.e., electrode-isolation configuration that focuses on eliminating the metal electrode effects on the performance of TFBAR devices, and serial-resonator configuration that simplifies the device's processability. Researches on realization of these designs and optimization of deposition parameters of AlN film have been carried out in this part of the work.

During this research, some related technical achievements in design methodology, fabrication process, measurement method as well as material development have been successfully used in our resonator development and can be improved further for other MEMS applications. The good performances of the realized proposed μ -mechanical resonators and the potential design and core AlN material growth of TFBARs in our research have certainly provided one step closer to the ever increasing device performance requirements in high frequency or microwave communication applications.

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NOMENCLATURE

Symbol		Description
A	---	Cross-section area of beam resonator
C_0	---	Static or clamped capacitance
C_m	---	Motional capacitance
C_r	---	Capacitance ratio
c	---	Damping constant
D_n	---	Components of electric flux density vector
E	---	Young's modulus
E_n	---	Components of electric field intensity vector
F_{drive}	---	Induced electrostatic force in micromechanical resonator
f_a	---	Antiresonance frequency
f_r	---	Resonant frequency
g_0	---	Initial air gap spacing
h	---	Height of beam resonator
I	---	Moment of inertia
i_o	---	Output current
$J_n(x)$	---	Bessel function of the first kind of order n
k_{eff}	---	Effective stiffness of resonator
k_t	---	Electromechanical coupling constant in TE modes
L_d	---	Light diffusion intensity
L_e	---	Radiosity of light source
L_i	---	Irradiance on measured surface
L_m	---	Motional inductance
L	---	Length of beam resonator
M	---	Bending moment
m_{eff}	---	Effective mass of resonator
$p(x, t)$	---	Distributed external load
Q	---	Quality factor of oscillation system
q	---	Stored charge in capacitor
R	---	Radius of disc
R_L	---	Load resistance
R_m	---	Motional resistance
R_s	---	Source resistance
S_{11}	---	Forward reflection coefficient
S_{21}	---	Forward gain coefficient
S_m	---	Components of mechanical strain vector
s	---	Laplace operator

T_m	---	Components of mechanical stress vector
t	---	Thickness of piezoelectric layer
U	---	Potential energy of the electric field
V_p	---	DC bias voltage
V_{pull}	---	Pull-in voltage
v_a	---	Phase velocity of acoustic wave
v_i	---	Input voltage
W_e	---	Width of input electrode
W_r	---	Width of beam resonator
x, y, z	---	Rectangular coordinates
$y(x, t)$	---	Flexural displacement of beam resonator
Z	---	Total impedance of equivalent circuit
Z_0	---	Characteristic impedance of microwave transmission line
Z_L	---	Load impedance
Z_m	---	Motional impedance of equivalent circuit
Z_s	---	Source impedance
e_{eff}	---	Effective dielectric constant
ϵ_0	---	Dielectric constant in vacuum
ϵ_r	---	Relative dielectric constant
k	---	Electromechanical coupling coefficient
μ	---	Material Poisson's ratio
ρ	---	Material density
ω	---	Angular frequency
AES	---	Auger electron spectroscopy
AlN	---	Aluminum Nitride
BAW	---	Bulk acoustic wave
BOE	---	Buffered oxide etch
CAD	---	Computer aided design
CCD	---	Charge coupled device
CMOS	---	Complementary metal-oxide-semiconductor
CPW	---	Coplanar waveguide
CVD	---	Chemical vapor deposition
DRIE	---	Deep reactive ion etching
DUT	---	Device under test
FEA	---	Finite element analysis
HF	---	High frequency
IC	---	Integrated circuit
IF	---	Intermediate frequency
LPCVD	---	Low pressure chemical vapor deposition
MEMS	---	Microelectromechanical systems
MMIC	---	Monolithic microwave integrated circuit

PSG	---	Phosphosilicate glass
PVD	---	Physical vapor deposition
RF	---	Radio frequency
RIE	---	Reactive ion etch
SAW	---	Surface acoustic wave
SCS	---	Single crystal silicon
SEM	---	Scanning electron microscope
SiO ₂	---	Silicon dioxide
Si ₃ N ₄	---	Silicon nitride
SOI	---	Silicon-on-Insulator
STM	---	Scanning tunneling microscopy
TFBARs	---	Thin film bulk acoustic resonators
TE	---	Thickness excitation
TEOS	---	Tetraethoxysilane
UHF	---	Ultra high frequency
UV	---	Ultra violet
VHF	---	Very high frequency
VLSI	---	Very large scale integration
XRD	---	X-ray diffraction
ZnO	---	Zinc Oxide

Chapter 1

Introduction

1.1 Research Background

The rapid development of mobile communication, wireless local area networks, satellite communications, automotive electronics and radar detection has led to the increasing need for high performance components and their corresponding state-of-the-art technologies. As an enabling technology, the microelectromechanical system (MEMS) technology for wireless applications has been mainly in radio frequency (RF) device applications in recent decades. In this area, resonator is one of the key components as the fundamental sensing and actuating device in frequency selectors, tunable microwave filters, reconfigurable antenna arrays etc. Besides these, the basic principle of resonator applied to mechanical, acoustic, electromagnetic, electrothermal and other types of vibration sensing also makes the resonator applicable in other numerous areas, such as in frequency modulation, optical modulation, microfluidic measurement, medical imaging, nondestructive material testing, spectrum analyzer, precision positioning and so on. The potential commercial value of wireless and RF communication has also attracted many attentions to the research and development of high performance resonators. The miniaturization of RF filter array for frequency selection, LC resonator, tunable/switchable transmission line resonator and mechanical resonator have been in growing demand in wireless communication industry.

Currently, majority of communication transceivers rely heavily upon the high-Q quartz crystal and surface acoustic wave (SAW) resonators to achieve adequate frequency

selection in their RF selector stages and to realize the required low phase noise and stability in their local oscillators. However, these resonators are off-chip components, and so must interface with integrated electronics at the board level, often consuming a sizable portion of the total sub-systems area and more power. In this regard, they pose an important bottleneck against the ultimate miniaturization and portability of wireless transceivers. In addition to miniaturization, wireless communication applications also call for highly selective filter devices with high quality factor (Q on the order of 10,000), ultra-high frequency (UHF, from 300 MHz to 3 GHz) or even higher frequencies, and ultra-low-power consumption (on the order of 100-time reduction compared to current commercial counterparts). With such filters for front-end analog-frequency filtering, for example, all the specifications for the rest of transceiver circuit can be relaxed. That means lower sampling rates and power consumption in future digital elements.

As a rapidly developed enabling technology, MEMS technology has demonstrated its capabilities for the realizations of various IC-compatible micromechanical devices. One of the typical examples is the accelerometer fabricated by using surface micromachining technology. Development of MEMS resonators has been an active research area in recent years. There are basically two types of promising MEMS resonators, i.e., micromechanical vibrating resonators (or μ -mechanical resonators) and thin film bulk acoustic wave resonators (TFBARs).

The micromechanical resonators refer to those with micro-scale vibrating structures on Si substrates and fabricated by using IC compatible micromachining or MEMS technologies which provide the resonator with enormous Q values, wide applicable frequency ranges and seemingly simple and multiform designs. The vibrating structures

of the μ -mechanical resonators are normally actuated by electrostatic forces around their resonant frequencies which are determined by their material properties, geometric dimensions, boundary constraints and stress in the materials. The most obvious incentive for the development of μ -mechanical resonator can be seen from the comparison between a typical SAW resonator and a double-ends clamped beam micromechanical resonator with comparable frequency, as illustrated in Figure 1.1. Typical dimensions for a 100 MHz μ -mechanical resonator can be $L=13\mu\text{m}$, $W=2\mu\text{m}$ and $h=2\mu\text{m}$ (Clark *et al.*, 1999). With electrodes and anchors, the device occupies an area of only $420\mu\text{m}^2$. Compared with several square centimeters required for a typical very high frequency (VHF) range SAW resonator, this represents several orders of magnitude in size reduction. Another important incentive is the compatibility with integrated circuits in structure and process technology. In addition, the realization of high Q on-chip μ -mechanical resonators can lead to an evolution of the fundamental bases upon which communication systems are developed, giving rise to new system architecture with possible power and bandwidth efficiency advantages.

Figure 1.1: Comparison of typical dimensions of SAW and MEMS resonators

Owing to above attractive advantages, there have been many research and development activities focused on the micromechanical resonators in recent years. However, the development of a device capable of meeting both high frequency and high quality factor is still facing following obstacles and challenges:

- Limited choices in materials. The ideal material for constructing such a mechanical resonator needs to have very high Young's modulus (to provide enough stiffness) but very low mass-density. As required to be IC compatible, the materials reported so far are limited only to polysilicon, single crystal silicon (SCS) and some electroplated metals like Nickel;
- Limitations in dimension and process. To pursue higher frequency, resonator structures need normally to be designed as small in dimension as possible. The best μ -mechanical resonator reported so far is the radial contour-mode disk resonator with the dimensions shown in Figure 1.2. Even for such small feature sizes, the resonator can only achieve a frequency of about 150 MHz and a quality factor of about 9000. It is predicted that, if a 1.8 GHz resonant frequency is desired, the disk radius needs to be further reduced to 3 μ m. Precision control of such a small geometric dimension presents a major difficulty and challenge for current MEMS technology;
- Challenges in actuation and sensing. High frequency and high-Q structures normally have high stiffness and thus require strong actuation force to produce sufficient vibrating amplitudes. For the commonly used electrostatic drive and capacitive sensing scheme, this means that the driving voltage should be high enough and/or the electrode gap must be sufficiently small. For the resonator as shown in Figure 1.2, a DC bias voltage above 35V and a tiny gap of 1,000Å are

required to achieve the reported performance. The former conflicts with the low operational voltage as required by normal IC chips. The latter challenges the current capability of MEMS process technologies in feature patterning.

Figure 1.2: The radial contour-mode disk of micromechanical resonator with frequency of 156 MHz and quality factor of 9,400 (John R.Clark *et al.*, 2000).

Due to the above limitations and difficulties, it seems that the current development of μ -mechanical resonator still has certain distance away from becoming commercially viable for wireless communications.

Another type of MEMS resonator that can potentially meet the need for miniaturization is the TFBAR resonator, which is basically constructed by piezoelectric thin films (such as AlN, ZnO or PZT) sandwiched with metal electrodes. Unlike the SAW resonators where the acoustic waves only oscillate on the surface of the piezoelectric substrates, the TFBAR devices have acoustic waves resonating through the body of the piezoelectric films. Because of this, the TFBAR resonators have much smaller size, better power handling and higher operational frequencies (from 800MHz to more than 7.5 GHz) – ideal for wireless communications. However, the challenges in the TFBAR technology are the strict requirements of extremely precise and uniform thin film thickness for

frequency control, exact acoustic coupling and minimum residue stress level for good reliability. For this reason, a high volume production of the TFBAR resonators has not yet been realized though the technology has been researched for over 30 years.

1.2 Research Objectives

This research is initiated based on the micromechanical and TFBAR technologies to target at significant improvements of the MEMS resonator performance by directing the efforts towards the novel resonator designs that can be fabricated by the existing MEMS process technologies. The main objectives include:

- To develop new design methodologies for improved resonator characteristics such as high frequency $f > 1 \sim 2$ GHz (ultrahigh frequency bandwidth), high quality factor $Q > 10,000$, low energy dissipation and high stability;
- Detailed design, analysis, optimization and simulation to assess the effects of structural and geometrical parameter changes;
- Fabrication, testing and design improvement of prototype devices according to design objectives.

1.3 Dissertation Layout

This dissertation comprises three part of work around research and development of high performance resonator for RF applications. These are (i) μ -mechanical resonator design and fabrication using conventional polysilicon surface micromachining technology, (ii) improved resonator design and fabrication using the state-of-the-art SOI technology, and (iii) design and fabrication of high frequency, high Q-factor resonators using TFBAR technology. The whole content is organized as follows.

Chapter 2 seeks to present comprehensive review of recent research and development work on resonators for RF applications. Chapter 3 introduces the working and operating principles of micromechanical resonators, discusses possible factors that will affect the performance of such resonators, and presents simulation results of various resonator structures that have been designed and fabricated during this research, such as the clamped-clamped beam resonator with vertical flexural vibration mode and the disk-shape resonator with radial vibration mode. The realized 1st natural frequencies of these resonators range from several megahertz to hundreds of megahertz. In Chapter 4, research work on the design flows, the developed microfabrication processes, the off-chip test set-up and results, together with a novel image measurement method developed in this research work for the manufacture of μ -mechanical resonators are presented and discussed.

Using the newly developed SOI technologies, a different type of clamped-clamped beam resonators with improved performance of frequency response and quality factor has been fabricated and tested on-wafer. These results will be introduced in Chapter 5.

Chapter 6 introduces our research work on resonators using TFBARs technology. The working principle, simulation results and analysis are provided in this chapter. Two newly designed structures with good fabrication and operation capabilities are also presented in this chapter. Related work on preparation and characterization of high performance AlN piezoelectric material, fabrication and preliminary results will be presented and discussed in the following Chapter 7.

Finally, Chapter 8 summarizes the research work which has been accomplished and proposes some recommendations for future research effort.

This research involves collaboration with MEMS Department of Institute of Microelectronics (IME), Singapore. Preparations of AlN material, fabrication, test and analyses of the developed μ -mechanical resonators and TFBAR devices have all been carried out in IME.

Chapter 2

Literature Review

2.1 Introduction

Resonance is a common phenomenon in nature, and resonator is a kind of devices that use such phenomenon to work. As an ordinary sensing and actuating element, resonator has been extensively used in industry applications and in our everyday facilities for a long time. According to different resonance principles and application areas, resonator presents various classifications and structures, such as mechanical resonators, electrical or LC resonators, tunable/switchable transmission line resonators, chemical resonators, optical resonators etc (Clark *et al.*, 1998). Recently, the study on micromachined electromechanical devices (or MEMS devices) has led to the fabrication of a wide variety of components with micron to submicron dimensions. These MEMS devices potentially feature low cost, minimized size and high performance, e.g., high linearity for switches, quality factors superior to tens of thousands for resonators and low power dissipation for filters. Though MEMS devices have not yet been widely used in mass product applications due to cost issues and reproducibility of performance, intensive research is being performed worldwide nowadays to overcome these problems. With the rapid development of mobile personal communication market, resonator and other communication components using micromachined technologies are being studied and developed for RF/microwave wireless applications, and they are considered as a promising alternative approach to present electrical or piezoelectric components (Randy and H?ctor, 2001; K. Grenier *et al.*, 2001). Some of such devices are gradually emerging to be practicable. According to our research objectives, this chapter will give a brief

summary of the state-of-the-art of these micromachined resonators available for RF applications. The subsequent chapters will then introduce our research and development work on MEMS resonators.

2.2 Conventional Quartz, Ceramic and SAW Resonators

Quartz crystal is probably the most widely chosen resonator material because of its desired properties, such as its piezoelectricity, high hardness, small elastic hysteresis, good temperature stability and abundance in natural reserve (David Salt, 1987). A small quartz crystal is often accurately cut along certain axes so that it can be vibrated at a particular frequency by using its piezoelectric properties. The quartz resonator has been used for over 70 years and thus its growth, characterization and fabrication techniques are quite mature. As important and practicable resonant sensors, quartz resonators are used for extensive applications in RF and wireless systems nowadays. However, large volume size, large energy consumption and low integration compatibility with CMOS (Complementary Metal-Oxide-Semiconductor Transistor) fabrication are some of their unconquered problems.

In modern precision frequency sensing and control, another important resonator using material piezoelectricity is the ceramic resonator. Ceramic resonator uses the mechanical resonance of piezoelectric ceramics such as lead zirconium titanate (PZT), and its resonant frequency varies with the oscillation mode. By employing different vibration modes, a large variety of commercialized ceramic resonators have been developed and successfully deployed in extensive application areas for many years, such as in voltage controlled oscillator circuits in TVs, remote controls for TVs and VCRs, etc. Currently, micromachined ceramic oscillators have also been used in high volumes for

microprocessor clock generation and for intermediate frequency (IF) filters (Murata Report, 2003). Table 2.1 summarizes the general frequency application ranges of ceramic resonators and their corresponding vibration modes.

Table 2.1: Different Vibration Modes and Application
Ranges of Common Ceramic Resonators

Vibration mode		Frequency range (Hz)						
		1k	10k	100k	1M	10M	100M	1G
Flexural mode		■	■	■				
Torsional mode			■	■				
Longitudinal expansion & contraction				■				
Contour expansion & contraction					■			
Radial vibration					■			
Thickness excitation					■			
SAW						■	■	

With the improvement of microfabrication processes, more recent technology for realizing such ceramic resonators in high frequency applications has been concentrating on the use of surface acoustic waves (SAW) resonators. This development was initiated

in 1965 due to the requirements of pulse compression radar. However, SAW devices were later found to be very versatile and a variety of SAW devices have been developed for various professional and consumer applications, especially in communication systems. Although typical use of such devices is for filtering purposes especially in mobile phones, SAW devices are sometimes also used as resonators. The main attraction which had led to the more frequent use of SAW filters was their low losses (few dB) at high operation frequency (900MHz and higher). Quality factors of high performance SAW resonators can reach as high as 100,000 and the resonators have comparably long-term stability as their bulk quartz crystal counterparts (less than 1ppm/year). The fundamental frequency of SAW resonators ranges from 10MHz to 300MHz - higher than that for bulk quartz crystal resonators. Though for modest requirements, a SAW device can be made in a single lithographical step, SAW resonators are not as frequently used as bulk resonators due to problems associated with either electrode reflections in the transducers or manufacturing complexity especially when it comes to packaging. Further, SAW oscillator can also be made from a delay line, but the Q value of such SAW oscillator is relatively low at about few 100s level. This area has already been studied in depth, and references that give more information on the history of SAW and ceramic devices used in electronics can be found in the discussions of David's (1998) and Satoru's (2000) respectively.

Lead-Zirconate-Titanate (PZT) is an extensively used piezoelectric material which can be vibrated with extensive modes of flexural, longitudinal, radial, SAW and TE oscillations. Even though the piezoelectricity was first discovered in 1880, the development of PZT ceramic started in 1954 after the PZT replaced barium titanate ceramic devices that are still used today. PZT devices are widely used because of their high electro-mechanical coupling factor and good temperature characteristics. Such

resonators are also often used as bulk acoustic wave (BAW) resonators and filters (P. B. Kirby *et al.*, 2001), particularly as ladder-type filters due to their low cost, stability, robustness, and relatively low insertion losses. Though the characteristics of ceramic resonators such as PZT are good, quartz-crystal resonators are still superior and therefore more widely used as resonators and oscillators in communication systems where quality of resonator performance is vital. On the other hand, newly developed piezoelectric materials ZnO and AlN have drawn more and more attentions for their good piezoelectric properties and micromachining fabricability (C. Caliendo *et al.*, 1993; H. P. Löbl *et al.*, 2001). We will focus on the development of these piezoelectric materials for resonator applications as we discuss our work in this area in Chapter 7.

2.3 Advanced TFBARs Technology

Nowadays, an increasingly important requirement in military electronic and wireless communication system is for acoustic devices to be able to operate in the ultra high frequency (UHF, f_0 from 300MHz to 3GHz) to microwave frequency (f_0 above 3GHz) range that can be fabricated by traditional very large scale integration (VLSI) technologies. The integration of piezoelectric devices into monolithic chip structures would permit dramatic reductions in size, weight and cost. Unlike SAW resonators where the acoustic waves only oscillate on the surface of piezoelectric substrate and unlike flexural plate wave (FPW) resonators which have rectangular plates or diaphragms vibrating vertically or laterally, thin film bulk acoustic resonators (TFBARs) have bulk acoustic waves resonating through the body of the piezoelectric films. Because of this, the TFBAR devices will have much smaller size, better power handling and higher operational frequencies (from 800MHz to more than 7.5 GHz) – ideal for wireless communications (Ewald *et al.*, 1998). Recently, TFBAR resonators have been experimentally included into cell phones as duplexers and filters which are quite

technically challenging components of the cell phone design (Agilent report, 2004; ANT report, 2004). The requirement is that the resonator should be able to separate the weak received signal from the strong transmitted one (Henrik *et al.*, 1999). In addition, these devices can handle a few Watts of power.

The typical structures of TFBAR resonator are fabricated solely using MEMS fabrication techniques even though they were invented in the 1980's when MEMS micromachining was just being developed (Krishnaswamy *et al.*, 1990; R. Ruby and P. Merchant, 1994; Qing *et al.*, 2001). As shown in Figure 2.1, three main types of TFBAR have been researched and used in oscillator and wideband filter applications. Configuration (a) is a membrane structure, which is formed by etching an acoustic cavity in the substrate and supported by the edges of the substrate. The cavity is often made by using KOH or EDP (ethylene diamine pyrochatechol) solutions that are anisotropic silicon etchants and are incompatible with conventional CMOS technology. Configuration (b) involves fabricating an air gap under the resonator by removing the sacrificial layers between the bottom electrode and the substrate, and (c) is a multi-layer structure in which the piezoelectric layer is solidly mounted onto the substrate and isolated by a deliberately designed and fabricated reflector array (Z_1 , Z_2 , Z_3 ??). In general, the first two configurations are well known as the TFBAR resonators. The third is commonly called as SMR (solidly mounted resonator) and usually used as wideband filter.

(c) reflector array (Z_1, Z_2, Z_3 ???) isolated resonator

Figure 2.1: Common configurations of TFBARs

The TFBAR structure usually consists of a silicon-nitride or silicon-oxide membrane that lies over a bulk-etched cavity through a silicon wafer. Afterwards, a piezoelectric thin film is deposited on and patterned between two metal electrodes. According to Ruby's (1996) work, TFBARs with Q 's of 1,200-2,300 have been achieved with frequencies of 1.5-7.5GHz. Such Q values are still considered low when compared with those of quartz crystal resonators, but are good enough for filter applications. Giwan *et al.* (2000) researched a two-step RF magnetron sputtering technique for ZnO piezoelectric film deposition and for fabrication of the TFBAR devices. The Q -factor was found to be as high as 7000 at resonance frequency of 1.48GHz, and a large return loss of 35~50 dB was also achieved. More detailed discussions on the application of TFBAR resonators can be found in (Richard Ruby *et al.*, 2001; M. Stickel *et al.*, 2001; K.M. Lakin, 2001; ANT technical report, 2004). In these researches, the challenges in the TFBAR technology lie in the optimal preparation of high performance piezoelectric material, extremely precise and uniform film thickness for frequency control, exact acoustic coupling and minimum residue stress for good reliability. For this reason, a high volume production of the TFBAR resonators has not yet been realized though the technology has been researched for over 30 years.

According to reports of Agilent (William, 2002) and Unaxis (Philippe *et al.*, 2002), Table 2.2 summarizes the performance of ceramic, SAW and FBAR filters in personal-communications-services (PCS) applications.

Table 2.2: Comparison of Filter Performance at PCS Frequencies

Parameters	Ceramic	SAW	FBAR
Q	~200	~200	800-1200
Temperature coefficient [PPM / °C]	0 to -5	-35 to -40	-25 to -30
Frequency margin to fit in 20 MHz (MHz)	2 to 4	> 20	3 to 6
Power handling (dBm)	>35@2GHz	~31@900MHz	>32@2GHz
Insertion loss (dB)	1 ~ 2	2.5 ~ 4	1 ~ 1.5
ESD robustness	Excellent	Fair	Good
Size (mm ³)	675	140(cellular band)	126~42
Frequency range	Cellular/PCS	IF/Cellular/PCS	Cellular/PCS/MW (500M ~ 10GHz)
Possibility for MMIC	No	only Multi-chip Module	Now MCM Future full integration
Manufacturability	Mature	Mature	In progress

2.4 Micromechanical Resonators

The gravity pendulum is probably the first mechanical oscillator that was used to regulate the rate of a clock about 4 hundred years ago. However, mechanical resonators, for applications in precision frequency generation and control, have been used only as

far back as the late 1940's. As reported by Gregory (2000), machined metal components with a variety of mechanical-to-electrical transducers were typically used in early versions of such devices, and their primary application was as IF filters for heterodyne radios. A large variety of resonant devices operating with both torsional and flexural vibration modes were also developed and successfully employed for many years.

With the advancement and development of MEMS technologies, micromechanical resonators and filters with characteristic dimensions in micron or even submicron scales have been fabricated firstly in single crystal silicon (SCS) as well as polysilicon in the form of tuning fork and torsional structure which provide better performance than macro-mechanical counterparts. For example, a 1MHz surface micromachined oscillator with double-ended tuning fork structure was described in Trey's (1998) paper. It exhibits a noise floor of -88dBc/Hz with 500Hz offset from the carrier. The resonator and the integrated oscillation circuit are approximately $200\mu\text{m} \times 100\mu\text{m}$ in size, in which the resonant structure is only $2\mu\text{m}$ thick. Mattila *et al.*, (2002) demonstrates a silicon micromechanical resonator with longitudinal vibration mode. The natural frequency of this resonator is 12MHz and its quality factor is about 180000. Nevertheless, in order to excite such vibration mode, as high as 100V dc voltage must be applied. Using another high order vibration mode of 2-D plate expansion with original square shape, Ville *et al.* (2003) realized a silicon resonator with high quality factor of 130000 at about 13MHz resonant frequency and $160\mu\text{A}$ current output, at the cost of more complicated layout design and fabrication processes.

Since Clark invented the first interdigital resonant structure at the beginning of 1990's, resonators with similar configurations have been used extensively as resonant sensing and actuation elements. Continuous efforts were being made by Clark's group from the

points of view of design and fabrication. For instance, Kun *et al.* (1997) improved the performance of this resonator by using localized filament annealing technique with frequency trims of over 2.7% and Q improvement of up to 600%. A beam structure resonator with flexural vibration modes and simpler configuration has also been developed by using a rectangular piece of polysilicon that vibrates perpendicular to the substrate, and been fabricated using surface micromachining technology. Another creative idea of using non-intrusive supports made of the quarter-wavelength torsional beams was employed to achieve operating frequencies up to 90MHz with relatively high Q values of 8400. This resonator is just approximately 20 μ m x 30 μ m in size (Kun *et al.*, 1999). In reference (John R.Clark *et al.*, 2000), an innovative invention, a disk-shape μ -mechanical resonator, is described, which exhibits an operation frequency of 156MHz and a Q-factor of about 9,400. This resonator has a diameter of 34 μ m. Furthermore, John *et al.* (1997) used their clamped-clamped beam resonators to assemble two-resonator filters that have achieved passbands centered around 68 MHz, passband rejections in excess of 25 dB, and insertion losses less than 5 dB. Improved by using a new ratioed-folded beam resonator design, a three-resonator, spring-coupled micromechanical filter was also achieved, which has an operating natural frequency of 340kHz with a percent bandwidth of 0.09%, insertion loss less than 0.6 dB, and passband rejection more than 64 dB. More detailed discussions and researches of micromechanical resonators can be found from a serial of work of Clark's group (Kun *et al.*, 2000; Wan *et al.*, 2001). In general, all these devices were developed based on mechanical vibration principle, by utilizing the relatively sophisticated fabrication processes and rigorous measurement conditions. Operated in very high frequency (VHF, f_0 from 30MHz to 300MHz) range, the resonant frequency, the quality factor and the volume of these micromachined devices have been demonstrated to be very satisfactory. However, the applications of such devices from that particular research group were not originally intended for hand-

helds or related communication devices, but for fundamental science studies of charge detection and thermal transport.

A new area of interest in the research of μ -mechanical resonator nowadays is the potential application of the state-of-the-art silicon-on-insulator (SOI) technology and the corresponding material for the fabrication of micro-resonators. This type of wafers was originally developed for high speed CMOS circuits, but has subsequently been adapted for sensor micromachining. Working with SOI wafers offers several advantages over bulk Si wafers: fewer process steps are needed for feature isolation, parasitic capacitance is reduced, and power consumption is lowered. In addition, total electrical isolation of individual transistors results in complete latch-up immunity leading to smaller device size and higher packing densities. T. Lamminmäki *et al.* (2000) fabricated SOI beam resonator with laterally flexural vibration modes and managed to have obtained 1.6 MHz resonant frequency with Q-value of 30000. Using a so-called HARPSS fabrication process, Siavash and Farrokh (2003) fabricated another SCS disk-shape resonator with 3 μ m in thickness and 30 μ m in diameter, which had the resonant frequency of 148MHz and exhibited a high Q-factor of 40000 in vacuum. SOI has also demonstrated high temperature capability with CMOS circuits. Its high temperature performance will allow the fabrication of signal conditioning circuits on the same chip and near the sensing element. Sensors are often located in harsh environments where high-temperature operation can be important. It is believed optimistically that the marriage between the SOI's mechanical properties and its high temperature circuit operation would provide device performance which is unobtainable with other technologies.

Micromechanical resonators have also been fabricated using the most advanced microfabrication processes. Some researchers used unconventional materials for CMOS

technology on a single chip and used the state-of-the-art nanoelectromechanical systems (NEMS) technology (A. N. Cleland *et al.*, 1996). In Roukes's (2000) work, a nanomechanical resonator was realized with a feature size of $0.1 \times 0.01 \times 0.01 \mu\text{m}$ in dimension, owing to the help of advanced electron beam lithography and high precision etching. This nanomechanical resonator has an operating natural frequency of 12GHz and a Q-factor of several tens. It is believed that nanoresonators of even smaller size are attainable, leading to resonant frequencies in the THz range, which is typically the characteristics of molecular vibrations. In addition to MEMS, NEMS provides yet another potential and more powerful way to realize RF devices with higher frequencies and smaller volumes, even though NEMS resonator remains very much at its early research phase.

2.5 Other Relevant Resonators

LC oscillating circuit is a well-known resonant application in electrical engineering. When the frequency of an input excitation signal is equal or very close to the natural frequency of the electric resonant system, which is defined as $f_0 = \frac{1}{2\pi\sqrt{LC}}$ (L stands for inductance, C for capacitance of the oscillation system), the system output will reach maximum. In conventional IC systems, the oscillators employ discrete inductors and varactor diodes for frequency tuning. These off-chip devices rely on processes and materials that differ substantially from those of the standard IC fabrication and are consequently not suitable for monolithic integration, thereby increasing cost, size, and packaging complexity. It is also difficult to precisely control and minimize the inductance value to ensure accurate and adequate frequency to be obtained. With micromachining technologies, an oscillation system can integrate a complete monolithic

low-noise RF voltage controlled oscillators (VCOs) using on-chip, IC-compatible, high-Q variable capacitor and inductor. Attempts to use MEMS technologies have been made to fabricate the two on-chip transducers for VCOs in Young's *et al.* (1997) work. Figure 2.2 is an example of this type. With the help of on-chip inductors and capacitors, high performance VCOs become possible. But to date, resonant frequency and Q-factor for these devices are still too low, and existing relaxation and ring oscillators are mostly used for experimental purpose.

(a) 3D four-turn inductor

(b) variable capacitor

(c) VCOs system

Figure 2.2: Components of Voltage Controlled Oscillators using MEMS Technology (D. J. Young, 1998)

Table 2.3 summarizes the major characteristics needed to compare different resonator and oscillator technologies. It seems that the size advantage and the process compatibility of MEMS resonators and oscillators with the integrated circuitry make this technology a possibility for future applications, especially for hand-held communications devices.

Table 2.3: Comparison of Resonators Fabricated Using Different Technologies

	LC Tank	μ -mechanical Resonator	TFBARs	Ceramic	Quartz
Resonant frequency f_0	MHz ~ GHz	=156MHz	1~10GHz	=70MHz	=500MHz
Quality factor Q	10 ~ 100s	=9,400	1,300~2,500	500 ~ 1,000	=17,000
Typical size of device with this f_0 (μ m)	mm range	p x 17 ² x 2	10 x 100 x 1	2 x 2.5 x 1.2	10.7 x 4.6 x 17

2.6 Summary

Compared with conventional quartz or ceramic resonators, MEMS counterparts exhibit good performances in compatibility with ICs, small volume, low power consumption, batch processability and so on. As summarized previously, although many researches on various microresonators have been carried out, most of these works were done in laboratory and for experimental purpose. Our research is concentrated on the design and development of high frequency (several megahertz to gigahertz) with high Q-factor microresonators for RF applications, which can be potentially commercialized for industrial applications. Building on these objectives, the key focuses of this project are on the research and development of innovative solutions in the device design,

fabrication, materials development, test and other relevant engineering approaches that directly or indirectly address the performance issues of high-Q MEMS resonators or resonator arrays for UHF bandwidth or higher frequency range applications. Based on existing data and research achievements, three subprojects involving different types of resonators and relevant microfabrication methods have been carried out. They include:

- research on development of micromechanical resonator using conventional polysilicon surface micromachining technologies developed, analysis of the factors which influence the performance of resonators and the fabrications of prototype devices designed with higher operating frequencies than those of current devices;
- research on the state-of-the-art SOI technologies and its relevant fabrication processes, to improve the Q-factor and noise level of the former micromechanical resonators;
- and research on thin film bulk acoustic resonators (TFBARs) using bulk acoustic wave technologies and newly developed piezoelectric materials, to improve the operating frequencies of the former micromechanical resonators as well to enhance the Q-factor of existing devices using our newly proposed designs.

Around each subproject, relevant methods, designs, fabrication processes and experiments have been or are being developed and carried out. In the following chapters, we will present and discuss them one by one.

Chapter 3

Design and Simulation of Micromechanical Resonators

3.1 Introduction

Over the years, many concepts and structures of micromachined RF components, such as capacitors, inductors, switches and filters, have been researched and developed. This chapter will introduce the design and working principles of the micromechanical resonators with high frequency and high Q-factor developed in our research. The design theories are similar to those used for macro-mechanical and electrical resonators. But with MEMS technologies, the performances of resonator, such as its natural frequencies and quality factors, can be improved greatly. In this chapter, we would discuss some typical structures, including clamped-clamped beam resonator and disk-shape resonator. Based on the operation frequency range and simulation results, we can determine the structural parameters and its corresponding electric features, which are subsequently used as the reference of fabrication and test. Other related issues to the designs of micromechanical resonators are also presented and discussed in this chapter.

3.2 Design Approach

Structured and parallel design methods for MEMS promise to shorten the development cycle of a typical device to days, and to enable design of more complex systems comprised of hundreds to thousands of micromechanical elements. Furthermore, as Mukherjee (1997) pointed out, with the help of various existing CAD (Computer Aided Design) tools, the rapid exploration, analysis and renewal of components will become a reality. Through the complete and regular design environment, designers and engineers

can rapidly understand each other and iterate on ideas for MEMS designs. At the beginning of this chapter, we would like to introduce the design and process flow adopted in our research, which is shown below in Figure 3.1.

Figure 3.1: General flow for our MEMS development

The above development flow can roughly be divided into five parts, these are, (i) definition and evaluation of the problem, (ii) product design and simulation, (iii) devices fabrication and test, (iv) device packaging and (v) system test. The whole design process and subprocesses are inherently iterative. Hence, like most projects, this project will also revisit the different stages several times before the project is successfully completed. In order to reduce the cost and design periods, simulations with CAD tools are used extensively. Simulation, other than some of the expensive and slow fabricate-test-redesign development process, allows one to start designing devices several generations ahead of production, without requiring the development or purchase of expensive new fabrication equipment. The following is a brief introduction to some CAD tools involved in our work:

- ANSYS/Multiphysics, is a finite element analysis (FEA) software and is evolved into a multi-physics analysis environment that is capable of simulating a broad range of physics, such as structural, thermal, fluid, acoustics, electromagnetic, and electronic circuits (ANSYS user manual, 2002). In related work, it is mainly used to carry out the modal and harmonic response analysis for mechanical and electroacoustic resonant structures, as well as for electrostatic field and electrostatic force analysis.
- MATLAB & SIMULINK toolkit, is used as the simulation and programming tools for circuit and system response analysis, and for calculation and simulation of the electrical behaviors of the μ -mechanical resonators and TFBARs.
- CADENCE, is used to design and check the layouts of designed devices.
- CoventorWare (or the former MEMCAD), provides fully integrated computer aided design and analysis tools for MEMS design, system simulation, process analysis and packaging in our work.

3.3 Design and Operation of Clamped-Clamped Beam Resonators

The advantage of a clamped-clamped beam resonator lies in its high stiffness and simple fabrication process compared with other more sophisticated designs. Most importantly, micromachining technology originated from the IC industry, can be used to fabricate the device and hence results in complete on-chip system and very low unit cost. In our studies, the resonators are driven by electrostatic load, and we only consider compliant mechanical structures and restrict ourselves to model them as linear structures under small deformations as it is usually the case in practice.

3.3.1 Flexural Resonant Vibration Characteristics of Beam Structures

Figure 3.2: Flexural vibration model of clamped-clamped beam and effective loads on beam element

Figure 3.2 shows the schematic drawings of a double-ends clamped beam whose geometries and loading configurations are illustrated. We assume the mass of the beam is uniformly distributed and so is its cross-section. In detail, the length, width and thickness of the beam are expressed as l , w_b and h respectively. The beam has a cross-

sectional area A , flexural rigidity EI and material density ρ . The symbol $y(x, t)$ is assumed to be the displacement of the section which is of distance x from the origin at time t . Considering moments and forces acting on the element of the beam shown in Figure 3.2, M and Q are bending moment and shear force respectively. $\rho A dx \frac{\partial^2 y}{\partial t^2}$ is the inertial force on the segment. For element dx , neglecting its rotary inertia and shear deformation (assumed to be Bernoulli-Euler Beam), the moment equilibrium to center point C can be written as (C. F. Beards, 1981),

$$M + Q \frac{dx}{2} + (Q + \frac{\partial Q}{\partial x} dx) \frac{dx}{2} = M + \frac{\partial M}{\partial x} dx \quad (3-1)$$

Neglecting higher order terms, (3-1) can be simplified to become,

$$Q = \frac{\partial M}{\partial x} \quad (3-2)$$

Force equilibrium in y direction is,

$$\frac{\partial Q}{\partial x} dx = \rho A dx \frac{\partial^2 y}{\partial t^2} \quad (3-3)$$

Upon combining (3-2) and (3-3), one can have,

$$\frac{\partial^2 M}{\partial x^2} = \rho A \frac{\partial^2 y}{\partial t^2} \quad (3-4)$$

According to the relationship of bending moment and deflection of beam,

$$M = -EI \frac{\partial^2 y}{\partial x^2} \text{ and } \frac{\partial^2 M}{\partial x^2} = -EI \frac{\partial^4 y}{\partial x^4} \quad (3-5)$$

Substitute (3-5) into (3-4), one can get,

$$\frac{\partial^2}{\partial x^2} (EI \frac{\partial^2 y}{\partial x^2}) + \rho A \frac{\partial^2 y}{\partial t^2} = 0 \quad (3-6)$$

Since EI is constant for a uniform beam, (3-6) can be rewritten as,

$$EI \frac{\partial^4 y}{\partial x^4} + \rho A \frac{\partial^2 y}{\partial t^2} = 0 \quad (3-7)$$

This is the differential equation for the free flexural vibration of a uniform beam. When a beam performs a normal mode of vibration, the deflection at any point of the beam vibrates harmonically with time. The normal vibration mode $y(x, t)$ can be assumed as,

$$y(x, t) = Y(x)b \sin(\omega t + \mathbf{j}) \quad (3-8)$$

where $Y(x)$ defines the beam mode shape of the normal mode of vibration, ω is the angular frequency of vibration, b and f are constants determined by initial vibrating conditions. Substitute this expression into (3-7), we get,

$$\frac{d^4 Y}{dx^4} - \mathbf{b}^4 Y = 0 \quad (3-9)$$

where $\mathbf{b}$ is defined as,

$$\mathbf{b}^4 \equiv \frac{rA}{EI} \omega^2 \quad (3-10)$$

Then the natural frequency can be derived from (3-10),

$$\omega = \mathbf{b}^2 \sqrt{\frac{EI}{rA}} \quad (3-11)$$

The general solution of equation (3-9) is (Ni, 1989),

$$Y(x) = C_1 \cos \mathbf{b}x + C_2 \sin \mathbf{b}x + C_3 \cosh \mathbf{b}x + C_4 \sinh \mathbf{b}x \quad (3-12)$$

Substitute (3-12) into (3-8), $y(x, t)$ can be rewritten as,

$$y(x, t) = (C_1 \cos \mathbf{b}x + C_2 \sin \mathbf{b}x + C_3 \cosh \mathbf{b}x + C_4 \sinh \mathbf{b}x)b \sin(\omega t + \mathbf{j}) \quad (3-13)$$

where the constants C_1 , C_2 , C_3 and C_4 are determined by the given boundary conditions of the vibrating beam structure.

The boundary conditions of a clamped-clamped beam resonator can be assumed as,

$$Y(x=0) = Y(x=l) = 0,$$

and

$$Y'(x=0) = Y'(x=l) = 0$$

i.e., at two ends of the beam, both the displacements and rotations are zero. Substitute these parameters into (3-13), following frequency equation can be formed,

$$\cos bl \cosh bl = 1 \quad (3-14)$$

Solve the equations of (3-14) and (3-11), the natural frequencies of the clamped-clamped beam resonator can be derived as,

$$w_i = \frac{a_i}{l^2} \sqrt{\frac{EI}{rA}} \quad \text{or} \quad f_i = \frac{w_i}{2p} = \frac{a_i}{2pl^2} \sqrt{\frac{EI}{rA}} \quad (i=1,2,\dots) \quad (3-15)$$

Some familiar forms of frequency equation and relative coefficients a_i s which are the roots of equation (3-14) and depend on the boundary conditions and the desired mode shapes are listed in Table 3.1. According to this table, the coefficient a_i of the clamped-clamped beam is 22.4 for the 1st vibration mode, which is much higher than those with other boundary conditions for the same beam geometry.

Table 3.1: Boundary Conditions and Frequency Equations of Flexure Vibration Beam*

Boundary conditions	Frequency equation	Values of relative coefficients a_i			
		1 st mode	2 nd	3 rd	4 th
Clamped-Free	$\cos bl \cosh bl = -1$	3.52	22.4	61.7	121.0
Pinned-Pinned	$\sin bl = 0$	9.87	39.5	88.9	157.9
Clamped –Pinned	$\tan bl = \tanh bl$	15.4	50.0	104.0	178.3
Clamped-Clamped	$\cos bl \cosh bl = 1$	22.4	61.7	121.0	199.9

(* Referred to C. F. Beards's (1981) works)

In order to solve the dynamic response of such Bernoulli-Euler beam, we presume the structure is exerted by external load $p(x, t)$, and the model of loads on the beam element is shown in Figure 3.3, which is a case of electrostatic loading in our work.

Figure 3.3: External loads on beam element shown in Fig. 3.2

Assume $p(x, t)$ is a harmonic load,

$$p(x, t) = p(x) \sin \omega t \quad (3-16)$$

The differential equation governing the motion of the element becomes,

$$\frac{\partial^2}{\partial x^2} \left(EI \frac{\partial^2 y(x, t)}{\partial x^2} \right) + rA \frac{\partial^2 y(x, t)}{\partial t^2} = p(x) \sin \omega t \quad (3-17)$$

Assume steady-state response of the beam is,

$$y(x, t) = w(x) \sin \omega t \quad (3-18)$$

Substitute (3-18) into (3-17), one has,

$$\frac{d^4 w(x)}{dx^4} - b^4 w(x) = \frac{1}{EI} p(x) \quad (3-19)$$

The general solution to this differential equation is (Ni, 1989),

$$w(x) = C_1 \cos bx + C_2 \sin bx + C_3 \cosh bx + C_4 \sinh bx + \frac{1}{2EIb^3} \int_0^x p(\mathbf{x}) [\sinh b(x-\mathbf{x}) - \sin b(x-\mathbf{x})] d\mathbf{x} \quad (3-20)$$

The four constants C_1, C_2, C_3, C_4 are also determined by the boundary conditions.

Finally, substitute $w(x)$, which is solved from (3-20), into (3-18), we can get a general expression for the steady-state response of the beam under the loading $p(x, t)$. As for the complete solution to this steady-state response, it is determined by the detailed conditions (such as loading conditions, initial conditions, boundary constraints, interested mode shapes etc.), and has been discussed in many reference books. We did not seek to establish this complicated derivation in this thesis.

When the rotary inertia and shear deformation of the beam element need to be considered, the vibration model of the beam becomes that of the Timoshenko Beam. Furthermore, when the ratio of the width of the beam to its length becomes substantial and hence cannot be neglected, using the plane or solid model will lead to more accurate results than the beam model discussed. In such a case, the theoretical formulas about frequency function, natural frequency, mode shape function, vibration amplitude etc. will be different from above derivations and they may appear in more complex forms. In our work, FEA software ANSYS, is used to analyze and simulate the performance of resonator structures designed. The simulation results of the structural static analysis and dynamic response analysis will be used to derive the optimal parameters in our designs of various micromechanical resonators.

3.3.2 Operation of Resonator Under Electrostatic Field

Among the various approaches currently employed, electrostatic method for excitation and detection is the most attractive and well developed for conductive microstructures because of its prominent advantages such as low power consumption, simplicity in fabrication and better sensing efficiency. This method employs the electrostatic attractive force between two oppositely charged plates and the elastic restoring force of the beam to excite the resonator into working state, and uses the change of electric field between the two plates to sense the output signal. Unlike other excitation methods, such as piezoelectric or electromagnetic excitations which require active film to be encapsulated in a sandwich of conducting and insulating films, using electrostatic excitation does not require a composite resonant structure incorporating electrode layers or diffusions. Furthermore, high electric field can be achievable at relatively low voltage, since micron or submicron electrode gap is readily fabricated using available surface micromachining techniques (Richard S. Muller, 1991). However, one inevitable

constraint applied on electrostatic actuation and sensing method is that the electric field intensity E must not exceed the atmospheric ionization breakdown voltage (the ionization breakdown field of air gap is typically around 3×10^7 V/m), otherwise an electric spark would be produced across the gap between the electrodes. In addition, the applied voltage should not exceed the pull-in voltage, or else it will make the moving part stick to the fixed electrode in an electrostatic MEMS and cause the instability problem (Y. He, 1999; Dimitri, 2003). Both constraints are also the main reasons why electrostatic actuation is only useful in the micro-domain (and less likely in nano-domain) and in low power application.

Considering the advantages and fabricability, electrostatic excitation and sensing method has been adopted in our resonator design. According to the model of flexural beam resonator as shown in Figure 3.4, a capacitor is formed between the beam structure and the fixed underlying electrode. To actuate the given beam resonator, an input voltage

Figure 3.4: Electrostatic field and force model between bottom electrode and beam structure

that consists of a dc-bias potential V_p and a small sinusoidal signal v_i (assume $v_i = V_i \sin(? t)$, V_i is the amplitude and $?$ is the angular frequency of the input signal) is applied across the electrode-to-resonator transducer. V_p is applied to the beam structure to

provide excitation power, and v_i is applied to the bottom input electrode to provide excitation frequencies. In common IC applications, V_p should be less than 40V and V_i is always less than 1V. In such a configuration, there is no dc current induced and hence no dc power consumption. This combination of voltages establishes an electrostatic field and resultantly generates an electrostatic force between the input electrode and the resonator structure. The induced electrostatic force F_{drive} is defined as the 1st derivative of the potential energy with respect to position,

$$F_{drive} = -\frac{\partial U}{\partial y} \quad (3-21)$$

Here the potential energy U of the electric field is defined as,

$$U = \frac{1}{2}CV^2 \quad (3-22)$$

where C is the working capacitance of the electrode-to-resonator capacitor. Applying this equation to above capacitive transducer where the structure is biased with V_p and the input electrode is supplied with v_i , the electrostatic force can be written as,

$$\begin{aligned} F_{drive} &= -\frac{\partial U}{\partial y} = -\frac{\partial}{\partial y} \left(\frac{1}{2}CV^2 \right) = -\frac{1}{2}V^2 \frac{\partial C}{\partial y} \\ &= -\frac{1}{2}(V_p + V_i \sin(\omega t))^2 \frac{\partial C}{\partial y} \\ &= -\frac{1}{2}[V_p^2 + \frac{1}{2}V_i^2 - \frac{1}{2}V_i^2 \cos(2\omega t) + 2V_p V_i \sin(\omega t)] \frac{\partial C}{\partial y} \end{aligned} \quad (3-23)$$

From (3-23), it is obvious that the relationship between the electrostatic force induced and the input voltage applied is nonlinear. In general, the amplitude of ac signal is much less than that of dc bias voltage. Therefore, after collecting terms of the same frequency as the drive input, the equivalent static load F_y and the dynamic load F_r can be respectively written as,

$$F_y = -\frac{1}{2}(V_p^2 + V_i^2) \frac{\partial C}{\partial y} \cong -\frac{1}{2}V_p^2 \frac{\partial C}{\partial y} \quad (3-24a)$$

$$F_r = -V_p \frac{\partial C}{\partial y} V_i \quad (3-24b)$$

where $\partial C / \partial y$ is the change in electrode-to-resonator capacitance per unit displacement of the resonator, and is approximately given by,

$$\frac{\partial C}{\partial y} = \frac{\partial}{\partial y} \left(\frac{e W_r W_e}{g_0 - y} \right) \quad (3-25)$$

where g_0 is the initial air gap spacing under static conditions and e is the dielectric constant of the electrode-to-resonator capacitor, W_r and W_e are widths of the beam resonator and the input electrode respectively. Neglecting the small energy loss resulted from fringing fields and surface leakage, and the small static bending of beam caused by V_p , and assuming the deflection y is much less than the nominal gap distance g_0 , equation (3-25) can be rewritten as,

$$\frac{\partial C}{\partial y} = \frac{e W_r W_e}{(g_0 - y)^2} \cong \frac{e W_r W_e}{g_0^2} \quad (3-26)$$

When the frequency of the input signal ν_i matches or approaches the natural frequency of the system, the beam begins to vibrate with zero-to-peak displacement amplitude, which is approximately given by (A. P. French, 1971),

$$|y(x)| = \frac{F_r Q}{k_{eff}} \cong \frac{Q V_p V_i}{k_{eff}} \frac{\partial C}{\partial y} \quad (3-27)$$

where k_{eff} is the effective stiffness of the system and Q is the quality factor. Then the output signal, often taken as current i_o , at the resonator's sensing pad is,

$$i_o = \frac{dq}{dt} = \frac{\partial(VC)}{\partial t} \approx V_p \frac{\partial C}{\partial t} = V_p \frac{\partial C}{\partial y} \frac{\partial y}{\partial t} \quad (3-28)$$

in which q is the charge stored in the capacitor.

3.3.3 Calculation of Equivalent Electrical Parameters of Micromechanical Resonators

Since a micromechanical resonator is a highly integrated electromechanical system, using the equivalent electric model is an effective way to design and match the mechanical and electric parts of the system as a whole, and consequently to achieve a better performance. From the point of view of system, any resonating transducer can be modeled either as a mass(m)-spring(k)-damper(c) vibration system or as a resistor(R)-inductor(L)-capacitor(C) oscillation system (as illustrated in Figure 3.5), both of them can be described with the well-known second-order differential equations (Grover, 1977),

$$m \frac{d^2 y}{dt^2} + c \frac{dy}{dt} + ky = F_{drive} \quad (3-29)$$

or

$$L \frac{d^2 q}{dt^2} + R \frac{dq}{dt} + \frac{1}{C} q = u_i \quad (3-30)$$

(a) mass-spring-damper oscillation system

(b) resistor-inductor-capacitor oscillation system

Figure 3.5: Typical second-order oscillation systems

If expressed in the form of transfer function $H(s)$, both transfer functions of equations (3-29) and (3-30) can be written in the following form,

$$H(s) = K \cdot \frac{1}{s^2 + \frac{w_0}{Q} s + w_0^2} \quad (3-31)$$

where K is a system constant. Therefore, there exist equivalent relationships among the parameters of the mechanical and electrical oscillation systems. Table 3.2 summarizes such relations.

Table 3.2: Some Equivalent Relations between Parameters of Mechanical and Electrical Oscillation Systems

Mechanical Oscillation System		Electrical Oscillation System	
F	Force (N)	V	Voltage (V)
m	Mass (kg)	L	Inductance (H)
c	Damping coefficient (Ns/m)	R	Resistance (Ω)
k	Spring stiffness (N/m)	$1/C$	1/Capacitance (1/F)
ω	Angular Frequency (rad/sec)	ω_e	Angular Frequency (rad/sec)

In our work, to ensure the equivalent electric parameters of the μ -mechanical resonators designed match well with the mechanical parameters when carrying out design and electric measurement, we will establish the relationships between the mechanical and electrical parameters, and analyze the electromechanical properties of the μ -mechanical resonator by using lumped circuit models. As shown in Figure 3.6, a micromechanical resonator can be represented by an LCR equivalent circuit model, which is also called Butterworth-Van Dyke or BVD model.

(a) physical model of μ -mechanical resonator with mechanical energy storage, inertial and damping. The lower plate is fixed, while the upper plate can move. Energy can be stored in the spring k (potential energy) or in the movements of the plate m (kinetic energy), and dissipated by the damper c .

(b) equivalent circuit model and corresponding electrical parameters of μ -mechanical resonator

Figure 3.6: Physical and equivalent electrical representation of a μ -mechanical resonator

In Figure 3.6(b), C_0 is the static capacitance of the electrode-to-resonator capacitor. The equivalent motional inductance L_m and capacitance C_m will determine the resonant frequency of the oscillation system. The motional resistance R_m is an equivalent mechanical loss factor in vibrating structure (Karl. S, 1925), and the resistance R represents the total electrical loss in signal line and substrate which can be roughly calculated as $R = \frac{\rho l}{A}$ (here, ρ is the resistivity of metal electrodes, l and A are the length and cross-section area of signal line). After determining the resonant frequency of a μ -mechanical resonator, its equivalent motional inductance L_m , capacitance C_m and resistance R_m can be derived as well.

We will present procedures for the calculations of these equivalent electrical parameters based on the derivations in Section 3.3.2. For convenience, the output current i_o in (3-28) is expressed in its phasor form, that is,

$$|i_o| = V_p \frac{\partial C}{\partial y} w Y \quad (3-32)$$

Substituting Y in equation (3-27) into (3-32) and upon collecting the terms, the amplitude of the output current I_o can be derived to become,

$$I_o = \frac{V_p^2 V_i Q}{k_{eff}} w \left(\frac{\partial C}{\partial y} \right)^2 \quad (3-33)$$

Here, the effective stiffness k_{eff} depends on the material constants, the geometric parameters and the boundary conditions of the resonator. According to the basic formula for fundamental natural frequency $f_0 = \frac{1}{2p} \sqrt{\frac{k_{eff}}{m_{eff}}}$, the effective stiffness and corresponding effective mass of such beam resonator with flexural vibration mode under uniform load can be calculated as (Senturia, 2001),

$$\begin{aligned} k_{eff} &= 32E \frac{W_r h^3}{l^3} \\ m_{eff} &= \frac{k_{eff}}{(2pf_0)^2} \end{aligned} \quad (3-34)$$

To find the equivalent motional resistance of the resonator, one can take the ratio of the drive voltage to the sensing current at resonance frequency f_0 to obtain,

$$R_m = \frac{V_i}{I_o} = \frac{k_{eff}}{w_0 V_p^2 Q \left(\frac{\partial C}{\partial y} \right)^2} \quad (3-35)$$

Upon combining (3-34) and (3-35) and substituting (3-26) for $\frac{\partial C}{\partial y}$, one has,

$$R_m = 4.95 \cdot \frac{\sqrt{Er}}{V_p^2 Q e^2} \cdot \frac{h^2 g_0^4}{l W_r W_e^2} \quad (3-36)$$

According to (3-36), R_m increases as the resonator's length l is decreased and thickness h is increased. A higher R_m will lead to a higher level of system noise and a larger loss of power (John and Yoonkee, 1999). For given dimensions of the resonator and its material constants, the relationship among R_m , g_0 , V_p and Q-factor can be established as,

$$R_m \propto \frac{g_0^4}{V_p^2 Q} \quad (3-37)$$

After R_m is determined, the derivations for L_m and C_m are as follows,

$$L_m = \frac{QR_m}{w_0} = \frac{k_{eff}}{w_0^2 (V_p \frac{\partial C}{\partial y})^2} = \frac{k_{eff}}{w_0^2 V_p^2 e^2} \frac{g_0^4}{W_r^2 W_e^2} \quad (3-38)$$

and

$$C_m = \frac{1}{QR_m w_0} = \frac{(V_p \frac{\partial C}{\partial y})^2}{k_{eff}} = \frac{V_p^2 e^2}{k_{eff}} \frac{W_r^2 W_e^2}{g_0^4} \quad (3-39)$$

If one defines the electromechanical coupling coefficient as $h = V_p \frac{\partial C}{\partial y}$, (3-35), (3-38)

and (3-39) can be rewritten as,

$$R_m = \frac{\sqrt{k_{eff} m_{eff}}}{Qh^2} \quad (3-40)$$

$$L_m = \frac{m_{eff}}{h^2} \text{ and } C_m = \frac{h^2}{k_{eff}} \quad (3-41)$$

It is obvious that to improve the coupling efficient and to decrease R_m without affecting resonant frequency, one should seek to decrease the air gap spacing g_0 , or increase the V_p or the Q-factor. In our design of μ -mechanical resonators, it is most desirable and necessary to increase the Q-factor by improving machining process and packaging technology to decrease the motional resistance. But the scopes of changes on values of g_0 and V_p are limited by the feasible micromachining process, the voltage requirement of the electronic circuit or the critical pull-in voltage. As discussed before, the pull-in voltage corresponds to the voltage at the instability point (i.e., 2/3 of initial air gap) and it is a common voltage constraint during the design and operation of electrostatic MEMS. The pull-in voltage can be calculated with (Y. He, 1999; Dimitri, 2003),

$$V_{pull} = \sqrt{\frac{8k_{eff}}{27e_r e_0 A}} g_0^3 \text{ at } y = \frac{2}{3} g_0 \quad (3-42)$$

From above deduction, we have established the links between the mechanical and electrical parameters of a micromechanical resonator. The formulas of (3-40) and (3-41)

will also be used to calculate the equivalent electrical parameters of the designed resonators for subsequent RF measurement. The results calculated with formula (3-42) will be used as a reference for the choice of the maximum voltage applied.

3.3.4 Proposal for Eliminating the Antiresonance Effect

In the oscillator circuit design, antiresonance is a noteworthy effect where the peak impedance happens and dampens the oscillations of such circuit. The existence of antiresonance will cause such a circuit to be subject to variations with the stray capacitance and resultantly cause filter frequency shift or big change of decay constant in resonator. In one of our MEMS resonator-based ASIC (application specific integrated circuit) application, this effect has caused the instability problem of modulator circuit (X. Wang *et al*, 2003). It is necessary to eliminate the antiresonance effect for this specific application. The accurate derivation for determining antiresonance is complex, while based on BVD model, approximate expression can be derived, and a proposal has been made in this section to eliminate the antiresonance effect possibly occurred in the μ -mechanical resonator.

After obtaining the equivalent electrical parameters of a μ -mechanical resonator, its complex impedance of the motional arm in the BVD model can be calculated based on Ohm's law,

$$Z_m(j\omega) = R_m + j\omega L_m + \frac{1}{j\omega C_m} \quad (3-43)$$

The total impedance of the equivalent circuit including the static conductance can then be written as,

$$\begin{aligned}
Z(j\omega) &= \frac{1}{j\omega C_0 + \frac{1}{Z_m(j\omega)}} \\
&= \frac{\frac{L_m}{C_0}(j\omega)^2 + \frac{R_m}{C_0}(j\omega) + \frac{1}{C_0 C_m}}{L_m(j\omega)^3 + R_m(j\omega)^2 + \left(\frac{C_0 + C_m}{C_0 C_m}\right)j\omega} \quad (3-44)
\end{aligned}$$

The modulus of the total impedance can be written as,

$$Z = \frac{1}{\omega} \cdot \sqrt{\frac{L_m^2 C_m^2 \omega^4 + (R_m^2 C_m^2 - 2L_m C_m) \omega^2 + 1}{C_0^2 L_m^2 C_m^2 \omega^4 + (C_0^2 R_m^2 C_m^2 - 2L_m C_0 C_m^2 - 2L_m C_0^2 C_m) \omega^2 + (C_0 + C_m)^2}} \quad (3-45)$$

To simplify the expression of impedance, the high order item $R_m C_m$ is neglected (the value of R_m ranges from few Os to few MOs and the value of C_m is in the range of tens to thousands of femto-farads), and the approximate impedance of the system becomes,

$$Z \cong \frac{1}{\omega} \cdot \frac{\omega^2 L_m C_m - 1}{\omega^2 L_m C_m C_0 - (C_0 + C_m)} \quad (3-46)$$

When the numerator of (3-46) is zero, Z is also zero and the output current will be maximum. This means that the serial resonance, or the so-called resonance, occurs at a resonant frequency as follows,

$$\omega_r = \frac{1}{\sqrt{L_m C_m}} \quad (3-47)$$

If the denominator is zero, Z is infinity and the output current will be minimum. In this case, parallel resonance or antiresonance occurs with the antiresonant frequency as,

$$\omega_a = \omega_r \cdot \sqrt{1 + \frac{C_m}{C_0}} \quad (3-48)$$

It shows besides the serial resonance, an undesirable antiresonance with a higher frequency value occurs. In this case, most of the input energy will be trapped into the resonant network, and the oscillator circuits or systems combined with μ -mechanical resonators will be subject to stability problems (Elwenspoek and Wiegerink, 2001; X. Wang *et al*, 2003). According to (3-48), the difference between ω_r and ω_a is determined

by the ratio of the motional capacitance C_m to the shunt static capacitance C_0 . When C_0 becomes very large, ω_a will be brought closer to ω_r . Because C_0 is physically unavoidable and varies with different processes, another circuit model, as illustrated in Figure 3.7, is developed in our work to modify the impedance characteristics in (3-45) and consequently to eliminate the antiresonance by compensating the effect of C_0 present in oscillation circuit.

Figure 3.7: A tactic to eliminate the antiresonance in μ -mechanical oscillation system

In this new model, the currents flowing out from the real C_0 and the assumed $-C_0$ are equal in magnitude while opposite in sign. The total impedance of this model can then be approximately rewritten as,

$$Z(s) \cong \frac{s^2 L_m C_m + s C_m R_m + 1}{s C_m} \quad (3-49)$$

The above formula shows that this new model has removed the item which can lead the denominator to zero in the impedance expression of (3-45), and thus reduces the influence of static capacitance C_0 to the antiresonance response. Because the negative capacitance cannot be realized physically, this proposal can be achieved by using specific signal processing method. Results of simulation and off-chip measurement by using specific subtract circuit have verified the feasibility of this new idea in principle. By using discrete tunable capacitor and relevant processing circuits, X. Wang *et al.* (2003) has realized similar idea on Sigma-Delta modulator, even though further

accomplishment of system-on-chip (SOC) combined with MEMS resonator and conditioning circuit need to be further investigated.

3.4 Simulations and Analysis of Beam Resonator

In the following simulations, all resonant beams are assumed to be $10\mu\text{m}$ in width (W_r) and $2\mu\text{m}$ in thickness (h). The length l , which is also the characteristic dimension in our design, changes from $10\mu\text{m}$ to $90\mu\text{m}$, the minimum air gap spacing g_0 is set as $1000\text{\AA}$, and high Q value is modeled as in near vacuum condition. Finite element analysis is used to evaluate the accuracy of the beam vibration modes. Considering its attractive material properties and its traditionally excellent fabricability in conventional CMOS cleanroom (Kurt, 1991), we used polysilicon as structural material and used conventional polySi surface micromachining technology to fabricate the beam resonator, which will be introduced in Chapter 4. The main mechanical properties of surface micromachined polysilicon are set as (Marc Madou, 1997): Young's modulus $E = 160\text{GPa}$, density $\rho = 2330\text{ kg/m}^3$ and Poisson ratio $\mu = 0.22$. The model and the relevant parameter denotations used for simulations are illustrated in Figure 3.8.

Figure 3.8: FEA model and relevant parameters of a beam resonator

3.4.1 Frequency Simulations

Table 3.3 gives the simulation results of fundamental resonant frequency, and Figure 3.9 shows the corresponding 1st mode shape of one of the beam resonators. As the length decreases, the element types used in our simulation also vary from beam element to plane or solid element. However, when the length of the resonators designed reaches the limitation of fabrication capabilities in our cleanroom (i.e., the planar dimensions not less than 5 μm when using manual alignment method and ultra violet lithography), the maximum 1st natural frequency of μ -mechanical beam resonators developed can be achieved to be around 150MHz. This value of frequency is not high enough for many commercialized RF applications and it seems we need new design methodology other than only by reducing the characteristic dimensions to raise the operating frequency to a much higher bandwidth. For simplicity of discussions, we will use the Resonator No. to represent the corresponding resonator structure as shown in Table 3.3.

Table 3.3: Results of the 1st Natural Frequency of Beam Resonators

Resonator No.	l (μm)	W_r (μm)	h (μm)	Simulation value f_0 (MHz)	Theoretical value (MHz)	Difference (%)
B1	92.4	10	2	1.994	1.997	0.15
B2	58.4	10	2	4.991	5.001	0.20
B3	41.3	10	2	9.974	10.00	0.26
B4	16.6	10	2	57.88	59.37	2.51
B5	11.8	10	2	106.9	108.02	1.04
B6	9.7	10	2	149.4	154.81	3.49

Figure 3.9: The 1st mode shape of clamped-clamped beam resonator

3.4.2 Simulation of Electrostatic Field and Electrostatic Force

Using the ESSOLV macro provided by ANSYS, a coupled electrostatic-structural analysis and calculation of the electrostatic forces have been carried out. Based on the requirements in our IC design and the micromachining capability, we assumed that the bias voltage V_p does not exceed 40V which is for the requirement of IC voltage or pull-in voltage V_{pull} which can be calculated using formula (3-42). The width of the electrode W_e is equal to the length of the beam and the initial air gap of the electrode-to-resonator is 1000Å. We have simulated various beam resonators and the results for B3 are shown in Figure 3.10. Figure 3.10(a) shows the modeling for electrostatic analysis, Figure 3.10 (b) and (c) show the simulation results of values and distributions of electrostatic force F_y and electric field E_y in y direction along the beam resonator. We can notice that the distribution profiles of the electrostatic force and electrostatic field are alike and their distributions are not uniform along the length of the beam resonator. Upon integrating F_y , the total driving force becomes $-83.25\mu\text{ N}$, which is very close to the theoretical value of $-86.07\mu\text{ N}$ computed based on formulas (3-24) and (3-26). This shows the model is accurate for evaluating the effect of the electrostatic field.

(a) 2D model for electrostatic field and electrostatic force simulation

(b) distribution of electrostatic force F_y (c) distribution of electrostatic field E_y

Figure 3.10: Model and coupled electrostatic field/force simulation for B3 resonator

It's found out that the distribution of electrostatic field is similar to that of electrostatic force. The fringing field effect and its resultant force is small. Most of the electric energy is confined to the space formed between the beam resonator and the underlying electrode. Excited by this electrostatic force F_y , the beam resonator will be bent downwards to the bottom electrode and its maximum displacement has also been simulated as a reference for our choice of the applied voltage. Similar models and processes are also used to simulate and design other beam resonator structures. Table 3.4 tabulates the simulation results.

Table 3.4: Simulation Results of Static Force and Displacement

Resonator No.	Initial gap g_0 (μm)	Effective stiffness k_{eff} (N/m)	Pull-in voltage V_{pull} (V)	Static force F_y (μN)	Displacement under F_y y_0 (μm)
B1	0.1	5.19e2	4.3	7.69@ V_{pull}	4.48e-2
B2		2.06e3	10.9	30.52@ V_{pull}	4.34e-2
B3		5.81e3	21.7	86.07@ V_{pull}	4.93e-2
B4		8.95e4	134.4	117.53@40V	1.31e-3
B5		2.49e5	265.8	83.54@40V	3.35e-4
B6		4.49e5	393.7	68.67@40V	1.53e-4

From the simulation results, it is found out that the pull-in voltage of B1, B2 and B3 is less than 40V due to their relatively small stiffness, and the selection of dc bias for these devices must be very careful.

3.4.3 Simulation of 1st Harmonic Response

In order to estimate the range of vibration amplitude when resonance is provoked, we have carried out the stimulation of the dynamic response of the beam resonators. It's assumed that the input power is less than 2dbm. The maximum vibration displacement corresponding to the input voltage should not exceed 2/3 of the initial air gap, and in the case of 1000Å air gap, the total displacement should be less than 67nm. For simplicity, the loss due to squeeze film damping is not considered since all the resonators are assumed to be working under vacuum environment with mTorr or μ Torr pressure, and the Q-factor is set to be 8000 for such ideal vacuum environment. Table 3.5 lists the

simulation results of harmonic response analysis.

Table 3.5: Simulation of Amplitude in 1st Harmonic Response

Resonator No.	Max. dc bias V_p (V)	Assumed ac voltage V_i (mV)	Assumed conditions	Dynamic load F_r (μ N)	Displacement under F_r y (μ m)
B1	4.3	0.7	$Q = 8000$ $g_o = 0.1 \mu\text{m}$	3.42e-3	2.27e-2
B2	10.9	1.8		1.39e-2	2.41e-2
B3	21.7	3.5		3.82e-2	2.12e-2
B4	40	120		0.72	6.47e-2
B5	40	480		2.02	6.49e-2
B6	40	1100		3.79	6.75e-2

Combined with the simulation results in Table 3.4, the total displacements under the operation of our selected voltages and assumed conditions do not exceed 2/3 of initial air gap. However, the measured Q-factor as presented in Chapter4 is not as high as our expectation, the real operation voltages for B1, B2 and B3 can be higher than those shown in Table 3.5.

3.4.4 Determination of Equivalent RLC Parameters

Using the formulas (3-40) and (3-41), and referring to the equivalent BVD model shown as Figure 3.6(b), we can calculate the electric parameters of the equivalent circuits of the beam resonators designed. The computed results of C_0 , R_m , L_m and C_m are shown in Table 3.6. These values not only can help us understand the resonator characteristics from the electric point of view, but also can be used to derive the initial parameters of the following RF measurement.

Table 3.6: Equivalent RLC Parameters of Beam Resonators Designed

Resonator No.	k_{eff} (N/m)	m_{eff} (kg)	γ	C_0 (F)	R_m (Ohm)	L_m (H)	C_m (F)
B1	5.19e2	3.30e-12	2.04e-5	0.82e-13	12.37	7.88e-3	0.80e-12
B2	2.06e3	2.08e-12	1.29e-5	0.52e-13	48.50	1.25e-2	0.81e-13
B3	5.81e3	1.47e-12	9.14e-6	0.37e-13	138.54	1.76e-2	0.14e-13
B4	8.95e4	0.64e-12	3.67e-6	0.15e-13	2133.58	4.58e-2	0.16e-15
B5	2.49e5	0.54e-12	2.61e-6	0.10e-13	5940.02	7.00e-2	0.31e-16
B6	4.49e5	0.47e-12	2.14e-6	0.08e-13	10693.41	8.79e-2	0.12e-16

Figure 3.11: Equivalent circuit model of μ -mechanical resonator
for frequency response simulation using Simulink™

The equivalent circuit used in test is demonstrated in Figure 3.11. Based on this circuit model, we have simulated the electric performance of the designed resonators with amplitude-frequency response and phase-frequency response. One example of such performance for beam resonator B3 is shown in Figure 3.12. The simulation for the proposed model in Figure 3.7 is also verified as can be seen from the results shown in Figure 3.13, in which R_S and R_L are the source and load impedances respectively. It can be found that the antiresonance peak which is so obvious in Fig. 3.12(a) has been totally suppressed. Therefore, the new proposed model as shown in Fig. 3.13 is workable in eliminating the antiresonance effect.

From V0 Bode Diagrams

(a) amplitude-frequency plot

(b) phase-frequency plot

Figure 3.12: Simulation results of gain and phase response for B3 resonator using the model shown in Fig 3.11 and parameters listed in Table 3.6

(a) model for antiresonance elimination simulation. In the dash-lined box, $C_{01} = C_{02}$, then the subtraction of signals from the two capacitors will be suppressed.

From V0 Bode Diagrams

(b) amplitude response in model (a). The antiresonance in Fig. 3.12 has been mostly suppressed.

Figure 3.13: Modeling and simulation to eliminate the antiresonance effect in μ -mechanical resonator

3.4.5 Substrate Effect on the Performance of μ -Mechanical Resonators

For high frequency applications, if one would like to consider the electrical power loss from the source to the load, a typical and complete electrical circuit model including both the equivalent model of μ -mechanical resonator and the parasitic effect of substrate should be used. Such a model can be shown as Figure 3.14. In this model, the series resistance R_s accounts for contact and current spreading resistances caused by signal lines. For metal transmission line, R_s is about 50 Ω . R_L is the load resistance. $C_{p1,2}$ and $R_{s1,2}$ account for the parasitic capacitances and leakage current resistances related to the electrical characteristics of the substrate. $R_{1,2}$ is a resistance caused by spreading current through the substrate surface or body, and its value is difficult to obtain by analytical calculation but by experiment.

Figure 3.14: Complete equivalent circuit of MEMS resonator for high frequency applications

In this simulation, we check the substrate effect on the performance of μ -mechanical resonator. 6" Si wafers about 650 μ m thick with normal resistivity (10 – 100 Ω -cm) and high resistivity (1000 – 10000 Ω -cm) are assumed during the simulations. Figure 3.15 shows an example of beam resonator B4, whose motional resistance R_m (as shown in Table 3.6) is as high as 2100 Ω . The interconnect from pad to resonator device typically introduces parasitic resistance with tens to hundreds of Ohms, which is in series with the device to be measured.

Figure 3.15: Electrical model and parameters with substrate effects of beam resonator B4

An example of such simulation results is shown in Figure 3.16, in which the forward gain coefficient S_{21} is adopted for the 2-port electrical network, and it can be calculated approximately as V_2/V_1 (V_2 is the output voltage at port2, V_1 is the input voltage at port1).

(a) normal substrate with 13 Ω -cm resistivity

(b) high resistivity substrate with 1000 Ω -cm resistivity

Figure 3.16: Substrate effect simulation of beam resonator B4

Another forward reflection coefficient S_{11} is defined as the ratio of the reflected voltage to the input voltage at port1. By comparing the simulation results shown in Fig. 3.16(a) and (b), it can be found out that the simulated Q-factor (measured approximately with $f_0/\Delta f_{-3dB}$, f_0 is the central frequency and Δf_{-3dB} is the 3dB degressive frequency bandwidth with center frequency f_0) increases from 680 to about 3000 after using high resistivity substrate, and its return loss (corresponding to the valley value of the S_{11} curve) keeps at about -1dB, while its insertion loss (corresponding to the peak value of the S_{21} curve) degrades from about -18.5dB to -23dB. Because the accurate parameters of the related parasitic and leakage effects in substrate are difficult to calculate, the simulation results of the substrate effect are not complete. To investigate the substrate effects on the performance of device and to optimize the design parameters, different substrates have been used in our fabrication and some actual measurement results will be presented in the next Chapter 4 and Chapter 5.

3.5 Other Simulations and Results

3.5.1 Characteristics of Disk-Shape Resonator with Radial Vibration Mode

In addition to beam resonators, typical disk-shape μ -mechanical resonators with radial vibration modes have also been researched, designed and fabricated using similar processes to those of the beam resonators. As illustrated in Figure 3.17, this type of μ -mechanical resonator is excited by radially distributed electrostatic field and electrostatic force. The working principle of such radial vibration resonator is the same as that of a beam resonator, even though the derivation and expression of its fundamental natural frequency are different.

Figure 3.17: Model of disk-shape μ -mechanical resonator

Neglecting the second order effects due to thickness and finite anchor dimensions, the resonant frequency can be determined by finding a numerical solution to the system equation, which can be expressed as the following (John *et al.*, 2000),

$$\frac{J_0(z/x)}{J_1(z/x)} = 1 - m \quad (3-50)$$

$$z = R \sqrt{\frac{r(2+2m)}{E}}, \quad x = \sqrt{\frac{2}{1-m}} \quad (3-51)$$

where R is the radius of the disk. E , μ and ρ are the Young's modulus, Poisson's ratio and density of the material, respectively. $J_n(x)$ is the Bessel function of the first kind of order n . Having searched for a suitable solution to the differential equations of transversal vibration of a thin circular plate, John (2000) has given a more direct expression for the natural frequency f , which satisfies (3-50) and (3-51), that is,

$$f_i = \frac{a_i}{R} \sqrt{\frac{E}{\rho}} \quad (i=1,2,\dots) \quad (3-52)$$

where a_i is a parameter dependent on Poisson's ratio as well as the desired mode shape. In the case of polysilicon and assuming the resonator vibrates at its 1st radial mode, a can be taken as 0.342. According to (3-52), the natural frequency for a disk-shape resonator with its 1st radial vibration mode is governed mainly by material properties and the radius of the disk.

Several disk-shape resonators with radial vibration modes have been simulated. The natural frequencies of the disk resonators designed change from 4MHz to 280MHz, corresponding to the radius R changing from 700 μ m to 10 μ m. Finite element analysis is used to evaluate the vibration modes of the disk resonators as well as their probable range of vibration amplitudes. The properties of the polysilicon material used are assumed to be the same as those discussed above. The thickness of all resonators is assumed to be 2 μ m, the applied voltage is 30V, the amplitude of input signal is 10mV and the Q value is 8,000. The simulation results of the natural frequency and the maximum displacement of the radial vibration disk-shape resonator are shown in Table 3.7. We also use the resonator No. to represent the corresponding structure for the convenience of subsequent discussions.

Table 3.7: Natural Frequency of Disk-Shape Resonator with Radial Vibration Mode

Resonator No.	Radius (μm)	Radial Vibration Frequency		Max. displacement δR (μm)
		Theoretical Values (MHz)	Simulation Values (MHz)	
D1	700	4.05	3.86	0.586 e-2
D2	280	10.12	9.74	0.238 e-2
D3	40	70.85	67.51	0.337 e-3
D4	26	109.04	102.44	0.201 e-3
D5	17	166.73	159.15	0.143 e-3

Figure 3.18 shows the corresponding mode shape of D3, which expands and contracts along its radial direction. All the nodes on the circumference have the same maximum displacement when the resonator is excited by symmetrically distributed electrostatic field and electrostatic force.

Figure 3.18: Expansion and contraction of a disk-shape resonator along its radial direction

One can see from Table 3.7 that theoretical predictions and simulation results agree very well. Further, when comparing Table 3.7 and Table 3.3, for example D4 and B2, one

should notice that given the same characteristic dimensions (the diameter of a disk in the case of disk resonator and the length of a beam in the case of beam resonator), the radial vibration resonator has much higher resonant frequency (102MHz) than that (5MHz) of the bending vibration beam resonator. Nevertheless, the vibration amplitude of disk resonator is much smaller than that of the beam resonator, consequently leading to smaller output signal under the same amplitude of driving voltage. How to effectively detect the tiny output signal of such disk resonator has not yet been resolved and further research effort towards this direction will be carried on in our future work.

3.5.2 Frequency Characteristics of Resonators with Longitudinal Vibration Mode

In our work, a bar-type resonator with longitudinal vibration mode has also been analyzed and designed. It is assumed in this study that the bar is of constant cross-sectional area A , the plane section keeps normal to the x axis during vibration, and its geometry and load configurations are as illustrated in Figure 3.19. After establishing the

Figure 3.19: Model of bar-type resonator with longitudinal vibration mode

dynamic equilibrium of the element dx and solving the subsequent differential equations as in the case of clamped-clamped beam resonator (Ni, 1989), the natural frequency for this μ -mechanical resonator with longitudinal vibration mode can be expressed as,

$$f_i = \frac{i}{2l} \sqrt{\frac{E}{\rho}} \quad (i=1,2,\dots) \quad (3-53)$$

where l is the length of the bar and $\sqrt{E/\rho}$ is the longitudinal velocity of elastic wave propagating along axis direction. This expression is similar to that of (3-52), which

characterizes an elastic wave propagating along radial direction. Thus, this kind of resonator also has higher resonant frequency than that of the beam resonator, given the same characteristic dimensions and properties of the material. In addition, the Q-factor of bar-type resonator is not so easily influenced by the air damping as compared with resonators with bending vibration modes.

Simulations for such type of μ -mechanical resonators have also been verified in this section. One of the resonators designed with longitudinal vibration mode is sketched as shown in Fig. 3.20. In this simulation, we have designed a bar-type resonator whose

Figure 3.20: Design I of a bar-type μ -mechanical resonator

characteristic parameters have been chosen similar to those of the disk-shape resonator developed by Clark *et al.* (2000). The body of the bar expands and contracts under the action of the symmetrically arranged electrodes. The dimensions of W , L and t are $17\mu\text{m}$, $106\mu\text{m}$ and $2\mu\text{m}$ respectively, and polysilicon is used as the structural material. The initial air gap g_0 is $1000\text{\AA}$, the bias voltage V_p is 35V , and the simulation results are shown in Table 3.8.

Table 3.8: Simulation Results of Bar Resonator with Longitudinal Vibration Mode

Natural frequency f_0 (MHz)	250
Parallel plate area A (m ²)	2.12e-10
Static capacitance C_0 (pF)	$C_0 = \frac{\epsilon_0 \epsilon_r A}{g_0} = 0.02 \quad (\epsilon_r = 1)$
Electrostatic force F (N)	$F = \frac{V_p^2 C_0}{2 g_0} = 1.2 \times 10^{-4}$
Displacement in x (m)	$\Delta W = \frac{F W}{AE} = 0.6 \times 10^{-10}$
Variation of Capacitance (pF)	$\Delta C = \frac{\epsilon_0 A}{g_0^2} \Delta g = \frac{\epsilon_0 A}{g_0^2} \Delta W = 11.32 \times 10^{-6}$
Output current I (A)	$ i = \left V_p \frac{C_0}{g_0} \frac{\partial W}{\partial t} \right = 0.4 \times 10^{-15}$

From the simulation results, one can see that only very small displacement and resultantly very weak output current can be acquired under the limitations of bias voltage and air gap spacing. As shown in Figure 3.21, another bar-type resonator has also been proposed, designed and simulated. In this model, two bars are arranged symmetrically on both sides of an anchor, and the interdigital electrodes are distributed evenly along the bar structure. Electrostatic field is applied across the electrodes. Excited by the electrostatic force, the resonator will vibrate along its axial direction. The dimensions of the bar are 40 μ m x 2 μ m x 2 μ m, the dimensions of each electrode are 2 μ m x 10 μ m x 2 μ m, the initial air gap g_0 is assumed to be 1000Å, and polysilicon is assumed to be used as the structural material. The simulated fundamental natural frequency with longitudinal vibration mode reaches as high as 78MHz. When voltages ($V_p=30$ V and $v_i=10$ mV) are applied to each electrode, the maximum displacement at end-point of each bar is found to be only 5Å, where a high Q-factor of 8000 is assumed.

Figure 3.21: Design II of another bar-type μ -mechanical resonator

Similar to the disk-shape resonators, although the bar-type resonators with longitudinal vibration mode have shown much higher fundamental frequencies than those of the beam resonators with bending vibration mode, one obvious problem arising here is that the vibration amplitude is too small, leading to very small change in capacitance and hence the difficulty in the detection of the tiny output signal, which is usually the output current as shown in Table 3.8. An ideal vibration detection method is presented in Matthew's *et al.* (2000) paper, which is based on optical laser vibrometer in which a light beam is impinged on a reflective resonator surface and then is compared with its reflected beam to detect the vibration amplitude. However, this method is not available for on-chip integration because of its relatively complicated designs of optical paths. In our consideration, STM (scanning tunneling microscopy) technology combined with MEMS technology will probably provide a more integrated solution not only to the on-chip detection of the tiny vibration amplitude of μ -mechanical resonators with higher order vibration modes, but also to other MEMS devices which have difficulties in sensing the weak output signals with current sensing methods.

3.5.3 Simulation of I-Beam Resonator

Because the natural frequency is known to be inversely proportional to the effective mass of a resonator, a lower mass of a resonator can possibly lead to higher natural frequencies. In our simulation, a beam resonator with **I** cross-section shape, a familiar structure found in an iron rail or references about mechanics of material, is modeled as illustrated in Fig. 3.22.

Figure 3.22: FEA model of an I-Beam μ -mechanical resonator

For such I-beam resonators, different designs of holes and structural configurations will result in different performances. Through a series of simulations, Table 3.9 shows comparison of performances between a normal beam resonator and an I-beam resonator designed. It is found that the natural frequency has been increased by nearly 25 percent. This increase in natural frequency is due to a significant decrease in effective mass. Although the effective stiffness has also been reduced at the same time, but this reduction, as compared with that of the effective mass, is much smaller. The motional resistance also decreases substantially. However, to realize such designs with holes in cleanroom demands more sophisticated processes and the fabrication cost will certainly be much higher.

Table 3.9: Comparison of Simulation Results between Normal Beam Resonator and I-Beam Resonator Designed

Parameters	Normal Beam Resonator	I-Beam Resonator
Dimensions (μm)	40 x 10 x 4	40 x 10 x 4 Two holes etched with dimensions: 20 x 4 x 3
f_0 (MHz)	20.1	25.0
m_{eff} (kg)	3.02e-012	1.53e-012
k_{eff} (N/m)	48200	37810
C_0 (fF)	35.4	35.4
C_m (fF)	1.62	2.07
L_m (mH)	48.31	19.57
R_m (Ohm)	609.11	384.16
$(1+C_m/C_0)^{0.5}$	1.022	1.028
Max displacement (μm) under $V_p=25\text{V}$, $v_i=10\text{mV}$, $Q=8000$	0.11e-1	0.16e-1

3.6 Discussion and Summary

3.6.1 Issues on Design of μ -Mechanical Resonator with High Performance

3.6.1.1 Consideration on Improving Resonant Frequency

The main purpose of our research is to achieve high operation frequencies while maintaining high Q value. With this objective in mind, following considerations have been made and summarized based on extensive simulations:

- According to equations (3-15), (3-52) or (3-53), in order to increase resonant frequencies, one would like to use low-density material with high Young's modulus and high area moment of inertia, as well as to reduce the feature size of the resonator structure. Small feature size of clamped-clamped beam structures

can be fabricated with the help of MEMS technology or even NEMS technology that scales the characteristic dimensions to a submicron level. But reduction in size will also lead to a decrease in output signal and an increase in the fabrication complexity and cost because it is difficult to minimize such dimensions to several microns in conventional CMOS cleanroom.

- As Michael (1994) believed, low mass and consequently high frequency may be accomplished by using I-beam structure. However, our calculations and simulations also show that the manufacturing complexity involved in fabricating such I-beam structures does not really bring in the additional frequency gain as expected, since its effective stiffness decreases simultaneously with a reduction in effective mass. Nevertheless, this design does bring a reduction in motional resistance. In our simulations, maximum 25 percent frequency gain can be obtained at a natural frequency of 20MHz while slightly reducing its motional resistance by using an I-bar profile, but it remains a challenge for the manufacturing of such a device.
- High Young's modulus and high Q factor materials, such as diamond, single crystal silicon (SCS) and SiC, are preferred as both structure and substrate materials. However, limited by Si-based manufacturing technologies and cost of non-silicon based materials, researches along this direction have remained at laboratory stage.
- Excitation and detection of resonator with higher vibration modes such as longitudinal vibration mode may prove a feasible alternative, however, the layout of the actuation and the sensing electrodes, and the detection of tiny output signal generated at higher vibration modes are its limitations.

In order to be able to sense small displacement (range from hundreds of nano to even sub-nano meter level) and the resultant weak output signals, there are a few general requirements need to be met: higher Q materials such as SCS should be used, smaller air gap spacing g_0 should be ensured, and higher bias voltage V_p is needed. Also signal to noise ratio deteriorates as resonator structures get smaller and it becomes more difficult to detect and separate signal from background noise in this case (John and Yoonkee, 1999; M. L. Roukes, 2000). Reducing the gap size g_0 is the best way to reduce the motional resistance, thereby improving signal sensing in MEMS resonators. In particular, according to the definition of the electromechanical coupling coefficient $h = V_p \frac{\partial C}{\partial y}$ and the formula (3-26), very small electrode-to-resonator gaps (micron to submicron) will also be preferred to improve the electromechanical coupling effect and to achieve sufficiently small port impedance for filters based on micromechanical resonators. Decrease of air gap does not increase the frequency by itself, but it allows possible modifications of other design parameters such as smaller beam length of resonators to enhance operation frequency. To get large enough displacement amplitude which can be effectively sensed, large electrostatic forces need to be generated and applied. Generally, this calls for a higher bias voltage V_p to drive the resonator. However, due to the limitation of the pull-in voltage, both small air gaps and large bias voltage become unfeasible. For those devices integrated with electronic circuitry on a chip, because of the voltage requirement for these ICs, the maximum dc voltage applied across the electrode-to-resonator transducer should be less than 40V. Microfabrication is another factor which affects the formation of the air gap. Sometimes, we cannot get an ideal air gap fabricated due to the limitations of microfabrication capabilities.

3.6.1.2 Issues about Improving Quality Factor

Quality factor Q is an important parameter to be used to describe the transforming effectiveness of a resonator. It is defined as a ratio of stored vibrational energy over lost energy during one cycle of vibration, and can be measured approximately as the ratio between the resonance frequency and the 3dB degressive frequency bandwidth. High Q -factor devices can bring higher sensitivity and lower noise if it is used as a frequency reference (Fred and John, 1995). Because MEMS resonator is a highly electromechanically integrated device, besides the energy loss caused by mechanical factors, electrical losses should also be considered. We believe that the total loss can be expressed as the sum of the mechanical loss, the electrical dissipation and the electrical-mechanical conversion efficiency, and this is discussed below.

- **Mechanical loss factor**

During the operation of MEMS resonators, several possible mechanical mechanisms where energy can be lost need to be considered. Quality factor is directly related to the amount of damping which a vibration system possesses. High damping leads to high loss of mechanical energy of a system to its surroundings through external damping mechanisms such as squeeze-film damping, viscous damping, turbulent flow and acoustic radiation, or through internal damping mechanisms such as thermoelastic dissipation. Usually the total losses caused by various dampings of a system can be added as shown in the following expression:

$$\frac{1}{Q_{total}} = \sum_j \frac{1}{Q_j} = \frac{1}{Q_a} + \frac{1}{Q_i} \quad (3-54)$$

where Q s are the quality factors related to different damping types. The total Q factor of a μ -mechanical resonator may be divided into two main components, i.e., Q_a which

represents the air film damping such as squeeze-film or viscous dissipation, and Q_i which corresponds to the internal material related dissipations.

In an air environment, the lowest Q factor is normally determined by Q_a . For a μ -mechanical resonator with flexural vibration modes, such as the two parallel-plate structure, the most dominant form of damping is squeeze-film damping, which is significant especially for such resonators operated in air. This energy loss mechanism occurs when one structure comes close to another, resulting in a pressure increase (J. B. Starr, 1990). Squeeze-film damping can be modeled as,

$$Q_{squeeze} = \frac{M}{b_{squeeze}} \omega_0 \quad (3-54)$$

where M is the mass of an object, ω_0 is the operating frequency, $b_{squeeze}$ is the damping coefficient which is determined by the fluid viscosity, the ambient pressure and the structure configuration. Another significant source of damping for lateral μ -mechanical resonator, such as comb like structures, is viscous damping, which will dominate when two plates separated by a viscous fluid move parallel to each other. This model assumes a linear velocity profile for the moving fluid underneath the plate while the damping due to ambient fluid motion above the moving plate is considered negligible. However, these models are not applicable in near vacuum conditions where the separation of the two objects becomes smaller than the mean free path of the medium in the gap. Therefore, vacuum packaging is the best way to reduce such air film dampings, though the low pressure packaging adds considerable complexity to the overall device development and cost. In addition, to fabricate holes throughout the proof mass can also help to relieve the build up of pressure and alleviate squeeze-film effects, however, the introduction of holes in such structures increases the complexities of design and microfabrication.

Internal damping in solids can be divided into thermoelastic dissipation, dissipation due to phonon-phonon scattering, lattice defect caused dissipation, etc. (V. B. Braginsky *et al.*, 1985). Thermoelastic dissipation is linked to volumetric changes that produce temperature gradients across the vibration system. Temperature gradients in return produce heat flow that results in conversion of vibrational energy into thermal energy (Terry, 1990). The phonon distribution can be disturbed from equilibrium by the sound waves in a solid and its return to equilibrium brings dissipation. It is also called internal friction. When a resonator is made of high performance materials such as high Q-factor SCS, or by special processes, such as various annealing methods which contribute to stress relaxation mechanisms in a solid and to increasing Q-factor of devices (K. Wang *et al.*, 1997), the contribution of the internal intrinsic Q_i factor to the overall Q-value of the device can be neglected in comparison with the other energy dissipation losses.

- ***Electrical loss factor***

To produce the lowest possible insertion loss and the highest possible isolation, the peripheral electrical structure of a μ -mechanical resonator must be designed carefully. The insertion loss will be affected by mismatch loss, which arises due to the equivalent impedance being different from the reference characteristic impedance, as well as contact resistance loss. The isolation will be affected by the resonator-to-substrate separation which defines the parasitic capacitance. The electrical design of the resonator, therefore, must be carried out in a self-consistent fashion with mechanical and material designs. The performance and quality factor of a μ -mechanical resonator is also affected by the losses associated with conductive silicon substrate, particularly at high frequencies. As discussed in the results of simulations, the degree of those losses depends on the resistivity of the silicon substrate and the thickness of the dielectric

isolation. Increasing the resistivity will reduce the substrate losses and thus increase the quality of the integrated passive components, but a high substrate resistivity will lead to a difficulty in defining an effective RF ground potential in the substrate, although the introduction of a metal ground plane or a silicided polysilicon layer can somewhat compensate such shortcomings (Adolfo 1994; Joachim, 1999).

Highly conductive metal, such as copper and gold, can be selected as signal line to reduce electrical losses. Selecting high resistivity substrate or depositing isolation layer between metal electrode and the substrate can also reduce substrate losses. Other than capacitive sensing, certain detection methods which can be employed to directly measure the vibration displacement of the resonator, such as STM method, may be integrated on chip by using MEMS technologies to eliminate extra electrical loss.

3.6.2 Summary

In this chapter, the working and operating principles of micromechanical resonators are introduced, and some issues regarding the best design practice are discussed. Extensive simulations have been carried out by using different mechanical and equivalent electrical models to analyze the various factors which can affect the performance of resonator devices, and the results are used to guide the subsequent design, fabrication and measurement of micromechanical resonators.

From these simulation results, it can be concluded that the characteristic dimensions of μ -mechanical resonators cannot be reduced unlimitedly due to limitations of microfabrication and electrical signal detection, and the highest 1st natural frequency of the beam resonators designed is less than 150MHz which is also the maximum

resonance frequency so far achieved by Clark's group (John R. Clark, 2000). Their potential good performances and simple fabrication processes make them possible to be used in HF (3 MHz - 30 MHz) or VHF (30 MHz - 300 MHz) bandwidth communication applications in the near future. Resonator structures similar to disk-shape resonator and bar-type resonator with higher order vibration modes have also been designed and simulated. The simulation results have shown they could achieve higher natural frequencies, but their smaller vibration amplitudes need to be further improved so that present electrical signal detection technology of small output current or voltage can be possibly employed to detect them. Therefore, in future work, besides further research on the improvement of the resonant frequency and quality factor, micro detection technologies will also need to be considered to solve the sensing problems of the tiny output signal which is always the case in microresonators. In addition, a new model has also been developed to eliminate the antiresonance effect, and the relevant simulation results have demonstrated that the model is practically achievable. Further research on this proposal needs to be carried out to realize better electrical performance of devices through system-on-chip technology. The actual fabrications of the μ -mechanical resonators designed have also been carried out by using conventional poly-Si micromachining technology, as well as the state-of-the-art SOI technology, and discussions on these fabrications will be introduced in Chapter 4 and Chapter 5.

Chapter 4

Fabrication and Test of Micromechanical Resonators

4.1 Introduction

The continuing demand for miniature devices has sparked a tremendous breakthrough in fabrication of these devices using current IC processing technology. This fabrication technology, namely the micromachining technology, has the ability to fabricate microstructures with both lateral and vertical dimensions that can be controlled within very small tolerances (microns to sub-microns). Silicon micromachining uses the same equipment and processes as those used by the microelectronics and semiconductor industry, which results in the possibility of integrating micromachined devices with CMOS electronics on a single chip. In general, this technology can be grouped into two categories, i.e., bulk micromachining and surface micromachining. Due to its simplicity, low cost and compatibility with IC process, the wet etch technology is likely to remain as a popular micromachining approach.

This chapter will firstly introduce the fabrication processes developed in our work, which are conventional and compatible with current CMOS foundry techniques. Due to similar characteristic parameters used for fabrication, some other type of μ -mechanical resonator/filter designed early such as the disk-shape resonators and the bar-type resonators can be fabricated using the similar processes to the beam resonator in a batch fabrication. The success of a microfabrication process cannot be separated from the support of reliable measurement techniques. During our batch fabrication, a new image measurement method and system has also been researched and developed for inspecting

the geometric parameters of microstructures. Related works will be presented in the following section. In the end, the test techniques and set-ups involved in corresponding electrical/RF measurement are introduced, and some measured results about the static capacitance C_0 , the resonant frequency f , the quality factor Q , etc. of the fabricated beam resonators are presented. These results will be used to evaluate the performances of the designed μ -mechanical resonators, as well as to be the reference for further improvement of design, fabrication process and test technique. The overall process of microfabrication and test line adopted in our work is shown in Figure 4.1.

Figure 4.1: Overall process of fabrication and test of μ -mechanical resonator developed

4.2 Mask Layout Design

Many steps described in our fabrication process deal with the use of some form of photolithography, which requires masks. The design of photolithography masks for MEMS micromachining is generally straightforward. Normally, such designs incorporate relatively large structures (microns to hundreds of microns) compared with the submicron structures that are now incorporated into advanced VLSI (very large scale integration) technologies, and there are also different patterns that correspond to the

different layers possible. When a design is done, not only the dimensions of the layers to be processed but also the deposition or etching order for these layers must be specified by a designer. In addition, the MEMS product developer usually requires that test structures or devices be included on some fabricated wafer. These may be provided by inserting special test patterns at designated locations in the mask field when the step-and-repeat process is at the level of creating the master mask. Therefore, although some suitable CAD softwares in IC application have been used to help design and check the desired layout, a good layout design of MEMS device still needs more understanding of the related fabrication processes and the required test patterns.

In our work, the layout of each mask for pattern transfer of the proposed resonator devices is accomplished using CADENCE software, a popular and synthetical tool for VLSI design. There are two types of masks based on the drawings, i.e., bright field and dark field. In bright field, the design on the mask is the same as the drawing. Whereas, dark field masks have designs which cover the area not covered in the drawings. In our design, a total of six bright field masks are used in fabricating the devices with complete isolation and metallization. Figure 4.2 shows one of the layout drawings, including the beam resonator structure and the overall structure with the specific test pattern for the following electrical/RF measurement. These layouts are named according to their end products produced by pattern transfer through etching process. In Fig. 4.2(b), to match well the dimension of standard probes used in RF network analyzer, the dimension of each probe pad designed is chosen to be $120 \times 120 \mu\text{m}$ and the central distance between two neighboring pads is $150 \mu\text{m}$ for the subsequent dynamic response test.

(a) layout design of the beam resonator, in which different colors and names represent the different layers and functions.

(b) overall layout design of the resonator structure with test pads

Figure 4.2: Example of layout design of beam resonator

4.3 Microfabrication of Designed Structures

4.3.1 Brief Introduction of Microfabrication

For MEMS, as for ICs, silicon is the first choice of the substrate. This is because silicon has both excellent mechanical characteristics and superior electronical properties. In addition, it can be anisotropically etched with high selectivity by several etchants. Popular insulating films are silicon dioxide (SiO_2) and silicon nitride (Si_3N_4), and as well they can be used as the intermediate support layer for free standing MEMS structures. In our polysilicon surface micromachining, PSG (phosphosilicate glass, or P-glass) is used as the sacrificial layer, and the oxide layer will be etched away before the process is completed.

Due to a wide flexibility in geometry and electrode placement, plus the amenability in combining with integrated circuits, polysilicon surface micromachining for MEMS has so far been the preferred technology for fabricating high-Q micromachined resonators (Madou, 1997). The general processes, as shown in Figure 4.3, include deposition, lithography and removal or etching.

Figure 4.3: General wafer processing flow of MEMS micromachining

The main functions of the three processes can be summarized as follows,

- Doping process is used to introduce controlled amounts of impurities into the

bare areas on the silicon (as little as one impurity atom per million silicon atoms).

This allows the formation of p-n diodes or the modification of conductivity in the substrate. Deposition is an additive process by chemical, physical or combined methods to produce a new layer onto the substrate. The new layer would be used as the isolation layer, sacrificial layer, structural layer, bonding pad, etc.

- Photolithography is a way of producing a pattern of bare areas and covered areas on a substrate. It serves as a mask for etching of the silicon dioxide, silicon nitride or layers which need to be processed.
- Etching is a subtractive process and can be described as pattern transfer by chemical, physical, mechanical or combined removal of materials from the substrate, often in a pattern defined by a protective mask layer.

When all these processes are combined, along with metal wires for connections between components and packaging, an integrated MEMS device can possibly be made.

4.3.2 Process Flow of Microfabrication for μ -Mechanical Resonator

The fabrication process used for the development of μ -mechanical resonators designed previously has been optimized by trial and error in our CMOS foundry and it can be categorized as surface silicon micromachining. The fabrication process begins with 6-inch (or 150mm diameter) p-type (100) silicon wafers with 6-100 Ω -cm resistivity. The whole process is similar to that of the Multi-User MEMS Processes (MUMPs) developed by Berkeley Sensors and Actuators Center (BSAC) (David *et al.*, 2000). This process uses polysilicon as structural material, deposited oxide layer such as PSG as sacrificial layer and silicon nitride as electrical isolation layer between the polysilicon and the substrate. The whole fabrication flow employed during processing is illustrated in Figure 4.4.

Figure 4.4: Process flow of microfabrication for μ -mechanical resonator designed

The major steps involved in our fabrication process include: (i) wafer preparation and fiducial etch, (ii) isolation oxide and nitride layers making, (iii) bottom electrode formation, (iv) anchor formation, (v) polysilicon beam making, (vi) gold pads patterning and (vii) release of the vibration structure. This section will introduce these steps and show some fabrication procedures of the beam resonator with schematics.

Firstly a six-inch (100) Si wafer with boron-lightly-doped is labeled and cleaned before it is used to fabricate the devices designed. The wafer is dipped into the buffered hydrofluoric acid (HF) and is rinsed with deionized (DI) water for removing the native oxide and for cleaning the wafer surface respectively. Then, a fiducial mark is patterned and etched into the bare wafer with depth of 6000Å, which is designed for the following photomask alignment to ensure the mask and the wafer are in correct positions relative to each other.

After the photoresist (PR) used for the fiducial etch is wet stripped in Acetone, and the wafer is cleaned with Piranha solution and dried by a dry spinner, the fabrication sequence continues with the fabrication of two isolation layers. The layers are formed by successive depositions of LPCVD (low pressure chemical vapor deposition) TEOS (tetraethoxysilane) oxide with 300Å thickness at 700 °C ~ 750 °C, and of LPCVD low-stress silicon nitride with 1500Å thickness at 850 °C in the standard furnace. The dioxide layer serves as a buffer between the substrate and the subsequent silicon nitride layer, and also as an ion implant barrier; the silicon nitride film with tensile stress can prevent the compressively stressed oxide layer from bowing, and also serves as an electrical isolation layer between the bottom electrode and the substrate. Fig. 4.5(a) shows the wafer cross section after the nitride layer deposition. Then the nitride layer in P⁺ contact

areas (as shown in Fig. 4.2(b)) is etched by CF_4 etchant to prepare for the following ion implantation. With energy of 150keV and concentration of 5×10^{15} , boron ions are implanted through the nitride window to the oxide layer and into the P^+ areas of the p-type substrate. The doped areas will become the ground planes and the electrical interconnects of the test pad. The use of ion implantation is because this technology can be carried out in room temperature quickly and has higher uniformity. Since the implanted atoms are seldom in the desired locations within the silicon lattice, it is necessary to follow the P^+ implantation step with a post annealing process for activation of the implanted atoms and reparation of the damaged substrate lattices. Thus, after implantation process, the wafer is transferred into the annealing furnace with quartz boat at around 1000 °C and held for half to one hour.

Subsequently, a 3800Å polysilicon film (denoted as poly 0) is deposited by LPCVD at about 580 °C with the SiH_4 deposition source and successively followed by the phosphorous implantation with PH_3 source and with energy about 100keV to form the electrode with better conductive characteristics. Then the annealing process is carried out again to electrically activate the ion diffusion and to significantly reduce the internal stress in the polysilicon layer. After 30mins of annealing at 1000 °C in nitrogen ambient, poly0 is patterned by photolithography, a process that includes the coating of the wafer with photoresist, exposure of the photoresist with the appropriate mask and developing the exposed photoresist to create the desired etch mask for subsequent pattern transfer into the underlying layer. Such steps are schematically shown in Fig. 4.5(b). The sheet resistance test is successively carried out by using the four-position probes measurement which is defined as ohm per square meter in superficial resistance of the doped areas. At the end of this phase, unprotective poly 0 layer is etched by CF_4 reaction gas in an RIE (reactive ion etching) chamber. These substeps can be seen from Fig. 4.5(c) and (d).

In succession, a 300Å TEOS oxide is deposited on poly 0 by LPCVD and another 700Å phosphosilicate glass (PSG) layer is then deposited in the standard furnace. The PSG layer is more resistant to the polysilicon etch chemistry than the photoresist, thus leads to better transfer of the pattern onto the polysilicon. In our process, the PSG layer will be etched to produce a hard mask for the subsequent polysilicon etch and will be removed at the end of the release process to free the resonant structure from the polysilicon layer. The wafer with the PSG layer (shown as Fig. 4.5(e)) is patterned with the mask layer named anchor and etched by RIE. This step provides anchor holes (shown in Fig. 4.5(f)) that will be filled by the next polysilicon layer.

After fabrication of anchor holes, another 2μ m polysilicon layer (poly 1) is deposited by LPCVD as shown in Fig. 4.5(g). Then the same processes of phosphorous implantation and annealing as those for poly0 are performed again. The poly1 layer is lithographically patterned using a mask designed to form the structural layer and the remaining polysilicon is removed by RIE. All mechanical structures have hitherto been fabricated. After photoresist strip in PRS solution, the wafers need to be dipped into the BOE (buffered oxide etching) solution for about 90 seconds to remove the oxide and open the bond-pad areas.

The subsequent step is the sputtering of a seed metal layer of 800Å Cr/2400Å Au as illustrated in Fig. 4.5(h). The Cr layer is to improve the adhesion of gold; the gold layer provides electrical pads for probing, bonding and electrical routing. A thicker Au layer is subsequently plated to a thickness of 2μ m. The wafer is patterned lithographically with the mask named gold and the metal is wet etched with Aqua Regia solution. After the photoresist descumming process in O₂ plasma, the thin residual layer of photoresist is

removed. The process is now complete and the wafer can be coated with a protective layer of photoresist for later wafer dicing.

The final step in the fabrication is the release of the sacrificial oxide layer or the PSG layer, which will leave the poly1 structure free standing to move. The release process includes the following substeps: First, the whole wafer is diced into single chips. These dices are carefully selected with the help of microscope, placed in wafer pads with holes and followed by the cleaning process. After that, the boat is submerged into the fresh Acetone solution (or other solution for photoresist stripping) for several minutes to remove the residual photoresist. The superficial color of the dices will change from brown to dark blue which is the same color as that of the oxidation. The boat is transferred into a tank of DI water to rinse, and flushed with isopropanol (IPA), then sprayed by air gun. This substep helps the dices to free themselves from the remains and to become dry faster. Then it is placed onto the hot plate for drying. The third substep is the device release process. After the removal of photoresist, the sacrificial oxide layer also needs to be removed (shown as Fig. 4.5(i)), using a process called the device release process. The release is performed by immersing the boat into a wet solvent bath of 49% HF acid (or BOE solution) in room temperature for 3-4 minutes to remove the sacrificial layer. The advantage of HF is that it etches away the sacrificial oxide layer without significantly affecting the properties of polysilicon material. The etching process is followed by rinsing the HF in DI water for about 30 minutes. Then, methanol is used for final rinsing solution to enhance drying for about 5 minutes. Each transfer between containers has to be done as quickly as possible to prevent the sticking, a common problem associated with the wet release process. The used solution should have lower surface tension coefficient to help reduce the possible sticking between the resonator and the electrode pad. An oven is pre-heated to a temperature of 90 °C. As soon as the

process of methanol rinsing completes, the dices are quickly transferred into the oven for approximately 2 hours. After this, the chips are sorted and shipped for test. In this release process, as submicron gaps are required, the ability to clear out etch residuals from gaps during release etching becomes very important, and the surfactant-enriched hydrofluoric acid solutions are often used to enhance the quality of released devices.

(a) A 300Å TEOS oxide (SiO_2) layer and a 1500Å low stress silicon nitride (Si_3N_4) layer using the gas mixture of dichlorosilane and ammonia are successively deposited on the p-type silicon wafer. The wafer has been marked, cleaned and fiducially etched.

(b) A blanket layer of 3800Å polysilicon (Poly 0) is deposited with SiH_4 by LPCVD. Next, the Poly-Si layer is doped with phosphorous implantation and a 1000°C annealing is carried out for half an hour, which is to electrically activate the ion diffusion and to reduce the internal stress in the poly0. The wafer is then coated with ultraviolet (UV)-sensitive positive-photoresist with 2μm thickness.

(c) The photoresist is lithographically patterned by exposing to UV light through the first level mask (Poly 0) and by developing the exposed area with specific developer.

(d) The unprotective polysilicon is removed by RIE. After the etch step, the photoresist is chemically stripped by Acetone or PRS solution. This process of patterning the wafers with photoresist, etching and stripping the remaining photoresist is used repeatedly in the microfabrication.

(e) A 300Å TEOS and a successive 700Å PSG layer are deposited on the wafer by low pressure chemical deposition (LPCVD). They are used as the sacrificial layer.

(f) The oxide2 is re-coated with photoresist and then is lithographically patterned for anchor formation. The unwanted oxide is removed by RIE and the photoresist is striped.

(g) Another 2μ m thick polysilicon layer is deposited by LPCVD followed by the phosphorous implantation, half an hour annealing and RIE etch.

(h) The wafer is coated with photoresist and the metal layer (gold with the thin adhesion layer Cr) is lithographically pattern. Then the resist and unwanted metal are removed in a resolvent bath.

(i) The structure is released by immersing the chips into the HF or BOE resolvent. The Poly 1, i.e. the beam structure, can be observed by optical microscope.

Figure 4.5: Schematics of fabrication steps along A-A' cross-section (marked in Fig. 4.2).

The dimensions of every layer are not to scale.

The similar fabrication processes have also been used to fabricate other μ -mechanical resonator structures designed previously such as the disk-shape resonator, bar-type resonator and high frequency filter. Figure 4.6 and Figure 4.7 show some photos of the fabricated μ -mechanical resonators taken by optical microscope and scanning electron microscope (SEM).

(a) photo of resonator structure with metal pad taken by optical microscope

(b) SEM photo of side view of the beam resonator and electrode

(c) zoomed view of the beam structure shown in (b)

Figure 4.6: Example photos of clamped-clamped beam resonator

(a) SEM photo of fabricated disk-shape resonator

(b) zoomed side view of disk-shape resonator

Figure 4.7: Example photos of disk-shape μ -mechanical resonator

In the following sections, two important testing technologies used in our batch fabrication, i.e., 3D structural dimensions measurement and electrical performance test, together with related test results will be introduced and discussed.

4.4 Image Measurement Method and System for 3D Dimensions Inspection

During microfabrications of μ -mechanical resonators and other MEMS devices, many micro detection technologies and apparatus, such as SEM, film stress analyzer, impedance analyzer etc., have been used to measure and control structural properties. The measurement of geometrical parameters of MEMS microstructures becomes indispensable, because with the reinforcement of the size effect in micro-domain, the accuracy of geometrical size has been very important to the performance of MEMS devices. Most microscopic measurement methods, such as optical probe, SEM and atomic force microscope (AFM), cannot be employed easily during the fabrication because of their narrow measurement range and rigorous requirements of measurement environment. Since current fabrications of such microstructures are mainly based on IC processing techniques, the accuracy of micromachining relies on the control of processing conditions and fabrication experience. To inspect and control the 3D dimensions of microstructures fast and accurately, a newly developed image measurement system based on CCD (Charge Coupled Device) photoelectric technology has been developed (Wang *et al.*, 2003).

4.4.1 Measurement Theories

Based on different optical imaging models and imaging components, measurements in both depth and plane orientations can be carried out using the proposed system developed with different imaging theories and relevant optical path models.

- **Measurement of depth based on grey image**

The depth measurement based on grey image utilizes the relationship between the illuminance of measured surfaces and the grey levels of the corresponding areas of the image. Referring to Liu's (1998) and Ma's (1998) works, we established a model as shown in Figure 4.8 and derived the measurement criteria as follows: A discal light source model is assumed to simplify the derivation of results and the real experimental conditions. Its radius is assumed to be R and radiosity L_e . The measured surface element dA is under the light, and the distance between them is h and the centerline is OO_a .

Figure 4.8: Simplified radiation model on the surface element to be measured

To determine the irradiance I_t on dA , a polar coordinate system is established in the light source. The radiation light element dP is assumed, which radiates light energy to dA and its area can be calculated as $dP = r \cdot dr \cdot d\alpha$. If the angle between P and OO_a is θ , the projective area of dP in the light emission direction dPO_a can be regarded as $dP \cos \theta = r \cdot dr \cdot d\alpha \cos \theta$. The steric angle $d\omega$ constituted by dP and dA is $d\omega = dA \cos \theta / (PO_a)^2$. So the energy stream from dP to dA can be calculated as,

$$\begin{aligned}
d\mathbf{f}_e &= L_e \cdot dP \cdot \cos\mathbf{q} \cdot d\mathbf{w} \\
&= L_e \cdot r \cdot dr \cdot d\mathbf{a} \cdot \cos\mathbf{q} \cdot \frac{dA \cos\mathbf{q}}{(PO_a)^2}
\end{aligned} \quad (4-1)$$

To substitute $\cos\mathbf{q} = h/\sqrt{h^2 + r^2}$, $(PO_a)^2 = h^2 + r^2$ into (4-1), one has,

$$d\mathbf{f}_e = L_e \frac{h^2 dA}{(h^2 + r^2)^2} r dr d\mathbf{a} \quad (4-2)$$

Through integration, the total energy emitted from whole light source to dA can be computed. That is,

$$\begin{aligned}
\mathbf{f}_e &= \int_0^R \int_0^{2p} L_e \frac{h^2 dA}{(h^2 + r^2)^2} r dr d\mathbf{a} \\
&= L_e \frac{pR^2}{h^2 + R^2} dA
\end{aligned} \quad (4-3)$$

So the irradiance L_i of dA becomes,

$$L_i = \frac{\mathbf{f}_e}{dA} = L_e \frac{pR^2}{h^2 + R^2} \quad (4-4)$$

For SCS (single crystal silicon) basal body by surface micromachining, the superficial light diffusion intensity L_d is directly proportional to irradiance L_i , and has no correlation with the diffusion direction. It is mainly influenced by the material properties. The diffusion intensity L_d , the material diffusion coefficient r_d and the irradiance L_i of the measured surface have the following relationship,

$$L_d = r_d L_i \quad (4-5)$$

When the visual angle of camera is small (the cosine value of that angle can be approximated to be 1), the irradiance L on the surface of photoelectric sensor can be approximately written as,

$$L = \frac{p}{4} L_d \left(\frac{d}{f} \right)^2 \quad (4-6)$$

where d is the diameter of aperture and f is the focal length of the imaging lens. In the working range of CCD sensors, L is directly proportional to the grey level g . Upon

integrations of (4-4), (4-5) and (4-6), the relationship of g and h can be deduced to become,

$$g = \frac{KL_e}{h^2 + C} \quad (4-7)$$

where K and C are constants of the measurement system.

During the measurement, a bunch of light with certain wavelength casts on the surface to be measured, and the height difference of the surface will cause a change of spatial density distribution of the emitted light. In our system, the height of the light source, the camera and the basal body are fixed. So the grey level g_b of the basal surface is pre-determined, while the grey level g_n of the measured surface varies with the machining difference of the beam. By measuring the grey difference between g_b and g_n , the real depth between the beam and the basal surface can be calculated. Bearing this objective in mind, the formula (4-7) should be modified to become,

$$h^2 = \frac{KL_e}{g} - C \quad (4-8)$$

Upon differentiating and taking approximation, one has,

$$2h\Delta h = -\frac{KL_e}{g^2} \Delta g \quad (4-9)$$

To substitute the height H and the corresponding grey level G of basal surface into h and g respectively in above equation, Δh can be established as,

$$\Delta h = -\frac{KL_e}{2HG^2} \Delta g \quad (4-10)$$

In the experiment, Δh and Δg are defined as absolute values. By calibration with geometrical measurement methods, such as mechanical probe or confocal microscope, and suitable data processing, an experimental linear function relationship between Δh and Δg can be established.

- **Planar size measurement based on geometrical image**

The planar size measurement based on geometrical image utilizes the perspective projection theory and the specific processing algorithms. As shown in Figure 4.9, a Cartesian coordinate system is established on the lens plane of the camera.

Figure 4.9: Perspective projection and imaging model

Its origin O is located in the center of the lens, and its Zaxis is coincided with the optical axis of the camera. An image plane will be formed which lies in the distance f (f is the focal length of the camera). Another coordinate system xoy is then established on this image plane, with its origin o at coordinates (0, 0, f) and its x-axis and yaxis parallel to the X-axis and the Y-axis respectively. A spatial object point P(X, Y, Z) is projected onto the image plane through viewpoint O and becomes an image point P'(x, y). According to geometrical relationship, coordinates (x, y) can be determined by the following formulas,

$$x = f \cdot X / Z \text{ and } y = f \cdot Y / Z \quad (4-11)$$

Based on the projective invariability of parallelism between two spatial parallel lines, if the expressions of the two lines on the image plane are,

$$Ax + By + C = 0 \text{ and } A'x + B'y + C' = 0 \quad (4-12)$$

Then their intersection point coordinates on the image plane will be,

$$\left(\frac{BC' - CB'}{AB' - BA'}, \frac{CA' - A'C'}{AB' - BA'} \right) \quad (4-13)$$

Based on the above coordinates and distance formula, the distance (if parallel) of the two lines can be ascertained.

From imaging theory, the optical path for planar size measurement is shown in Fig. 4.10. Through zoom lens, the measured object forms an optical image on the CCD light-sensitive element array. In the output port of the camera, video signal can be acquired and transformed into digital image by sampling and quantizing process. The measured areas will be extracted from the image. After image processing, the maximal and minimal number of rows or columns of the extracted edge can be established. The pixel span among the edge can consequently be determined. This span multiplied by the scale coefficient K of the system will lead to the actual dimension of the object to be measured.

Figure 4.10: Optical path for planar size measurement

When object distance is fixed, the scale coefficient K should be derived through experiments as below,

$$K = \frac{W_p}{N_p} \quad (4-14)$$

where W_p is the actual size of the standard sample, and N_p is the pixel span of the

measured images of the relevant sample. Here, K represents the real physical size corresponding to a pixel in the working distance. In order to get the optimal solution, K should be the average values obtained from repeated calibrations.

4.4.2 Structure of Image Measurement System

The structure of the proposed measurement system is shown in Figure 4.11. This system consists of five main parts: optical imaging, video signal processing, digital image processing, result output and adjustable mechanism.

Figure 4.11: Structure of image measurement system

The optical imaging part is the most important of the system, which determines the form and quality of images, and influences the mode of the subsequent information processing. The objects to be measured, the measurement requirements and the measurement conditions should be considered carefully in order to design a good optical subsystem. The video processing subsystem performs the sampling and the quantizing of the imported analog signal. It decides the spatial resolution, the volume of image data and the computational complexity. Its digital output is analyzed and processed in the image processing part. Through specific algorithms, the needed information is extracted from the original images and displayed on output devices. The mechanical supports and

accessories integrate all the subsystems into a single measurement system and provide a reliable positioning accuracy. The arrows in Fig. 4.11 indicate the transfer of information among subsystems. The planar array CCD sensor (753 x 582 pixels with sensitivity ratio 0.08Lx), fluorescence and parallel light sources, micro object lens (focus length f 20mm, numerical aperture 0.5) and zoom lens (focus length f 6mm), specific video card and image processing algorithms have been designed and tested.

4.4.3 Information Processing Flow of System

For different measurement requirements, such as two-dimensional or three-dimensional, the imaging theories and relevant image processing technologies to be used are also different. Therefore, the information processing procedure based on the same hardware devices is adopted separately as shown in Figure 4.12 (a) and (b). The main difference between the two charts is the idiographic algorithm of image processing in the dashed box in Fig. 4.12(a). Based on the photometric information in the grey images, the processing flow for depth measurement places the emphasis on the conservation and extraction of the original grey level from measured areas. Whereas the planar size measurement focuses itself on the exact localization of measured contour. For different contours, such as line, circle, rectangle and free-curve, the available algorithms are also different.

By calibrating with SEM and establishing the relationship between the luminosity of measured surface and the grey level in the relevant images of the beam structure, the depth size can be obtained with an absolute error smaller than 2 microns and a relative error to be within 1% (Wang *et al.*, 2003). And with the same system but different imaging lens and light sources, the planar size can also be measured by utilizing the perspective projection imaging theory and relevant algorithms. The attained relative

error of the planar size is less than 2% and the repeatable precision is higher than 1 μm (Wang *et al.*, 2003). The imaging processing is less than one millisecond, which depends on the hardware level and the complexity of processed pattern. The whole procedure of inspection includes arrangement of tested devices, adjustment of optical and imaging components as well as manual extraction of inspected area with present system.

(a) information processing flow for depth measurement

(b) information processing flow for planar size measurement

Figure 4.12: Information processing flow for 3D dimensional measurement

During our fabrication of resonator structures, using the image measurement system and its information processing, it is observed that the measured results were close to the designed values and the variation of planar dimensions is less than 1%. This demonstrates that our fabrication process is feasible and there is no substantial deviation from the designed dimensions.

4.5 Test Structure and Set-up for Electrical Performance Measurement

Two main targets for electrical performance test have been carried out, and these are the C-V characteristics test of the on-die resonator and frequency response test of the packaged resonator chip. After the release process, the dies are selected under optical microscope and their C-V values are successively measured to get the impedance characteristics of static capacitance of the structure and to evaluate the effects of different release methods. The chips with good impedance characteristics and no structural fracture will be wire bonded and packaged. Then frequency response test is carried out to measure the dynamic response of the resonator, such as the resonant frequency, the quality factor Q and the output gain. The basic testing configuration can be illustrated in Figure 4.13.

Figure 4.13: Schematic of the electrical test configuration

4.5.1 C-V Test and Analysis

Capacitance (C) – Voltage (V) measurement, or in short, C-V test, is a testing method used to verify the proper functionality of the device by simply measuring the capacitance response of the device under some applied voltage. The schematic diagram of the C-V test set-up in our work is shown in Fig. 4.14.

Figure 4.14: Schematic diagram of C-V measurement set-up

A 1kHz ac input signal is exerted on the test structure by using the probes of HP4284A Multi-Frequency LCR meter. In this measurement, Cp/Rp function of the LCR meter is selected. The dc voltage is applied and added by setting the bias option. The capacitances between probe1 and probe3 (defined as group1), between probe1 and probe2 (group2), between probe2 and probe3 (group3), are measured respectively. Measurement of C-V characteristics of group1 is the main objective since from which we can derive the static capacitance between resonator and its bottom electrode, together with the change of this capacitance by adjusting the bias voltage. Group2 and group3 are accessorial tests employed to evaluate the conductivity of input and output electrodes to ground. In Table 4.1, the measured C-V characteristics of group1 corresponding to beam resonator of B1~B5 are listed. These results can be used to estimate the different

impedance characteristics of the test structures and accordingly to evaluate the different effects of release methods. The unit of capacitance is pF while that of voltage is V. The maximum input dc voltage of LCR meter is 40V.

Table 4.1: C-V Characteristics of Beam Resonator Fabricated

Release Conditions: HF etch 5mins, oven heat and dry 1hour					
	B1	B2	B3	B4	B5
C0 @ 0V (pF)	1.37	2.25	1.85	0.92	2.17
Pull-in Voltage V_{pull} (V)	3 -1	1 -2	20 -20	$\geq \pm 40$	$\geq \pm 40$
Release Conditions: HF etch 5mins, SCC and dry					
	B1	B2	B3	B4	B5
C0 @ 0V (pF)	2.25	1.81	1.02	1.16	1.16
Pull-in Voltage V_{pull} (V)	1 -1	2 -2	25 -25	$\geq \pm 40$	$\geq \pm 40$

From above results, we can find that different release methods have different effects on the gap formation and hence different capacitances, and that the measured static capacitances C_0 are larger than those of simulation results listed in Table 3.6. It shows that the parasitic capacitances associated with bond pads, metal signal lines and unremoved impurities (particles in solvent, photoresist, etc.) have affected the actual capacitance value of the devices fabricated. Therefore, to eliminate these parasitic factors, optimization of layout design and improvement of fabrication processes such as release methods and critical cleaning process are necessary.

4.5.2 Test Set-up and Measurement Results of Frequency Response

The fabricated μ -mechanical resonators with good C-V characteristics will be packaged and subsequently RF characterization will be performed. In general, the dynamic response measurement of a resonator can be modeled either as a one or n-port electric network depending on how the resonant structure is driven and how the output signal is sensed. In our frequency response measurement, the test configuration is modeled as a two-port network, in which a dc voltage is applied to the structure, an ac input voltage is exerted at the driving electrode pad, and the resultant ac output signal is sensed at the sensing electrode pad. As shown in Figure 4.15, the packaged resonators are tested in a probe chamber with tens to hundreds of mTorr pressure. The dc voltage is provided by Agilent Power Supplier. The input signal is provided and the output signal is detected off-chip by a RF network analyzer. Vector Network Analyzer HP8753D (working frequency range: 30kHz to 3GHz), having the coaxial cable connector with 50 Ω characteristic impedance and the standard probes with 150 μ m-interval ground-signal-ground pins, was used to determine the frequency response of the beam resonator developed. Before test is conducted, the network analyzer needs to be calibrated. The measured data, typically consisting of the real and imaginary parts of the forward gain S21 for frequency points over some frequency span, were extracted from the HP8753D and stored as an ASCII file for further processing. The amplitudes of bias voltage V_p and the input signal V_i should be carefully chosen to avoid overdrive, to ensure high enough signal-to-noise ratio as well as to prevent ionization breakdown. The MMA (MEMS Motion Analyzer) vacuum probe station is used for contacting the packaged devices.

Figure 4.15: Set-up for frequency response analysis of the resonator

As stated in section 3.4.5, the scattering parameter S_{21} , which represents the forward gain coefficient in a two-port network and is expressed approximately as the ratio of the output voltage to the input voltage, has been measured and the results for the cases of beam resonators B2, B3 and B4, whose simulated 1st natural frequencies are 5MHz, 10MHz and 58MHz respectively, are shown in Figure 4.16(a)~(c). Multipoint averaging has been used to reduce the noise effect. From the data shown in Figure 4.16(b), $f = 8.06\text{MHz}$ is identified as the operating frequency which is near the maximum output gain. Q value can be calculated approximately by $f_0/\Delta f_{-3\text{dB}}$ and it is about 1000 from this particular measured forward gain S_{21} of resonator B3. In Fig. 4.16(c), there appears no obvious resonance peak because a high motional resistance about 2100Ω (referring to Table 3.6) together with a high power dissipation arises at the high resonance frequency in the case of B4. Nevertheless, the frequency responses for other μ -mechanical resonators, such as B5, disk-shape resonator and bar-type resonator, though successfully fabricated, have not yet been measured because of their weak output signals under the limited input power when off-chip measurement were carried out.

(a) Beam 2, $V_p = 1$ V, $P_{in} = -25$ dBm

(b) Beam 3, $V_p = 5$ V, $P_{in} = -20$ dBm

Figure 4.16: Frequency responses of the beam resonators

In former harmonic simulations in section 3.4.3, a high vacuum environment ($Q=8000$) is assumed and the structural damping existed in the material is also neglected, while in reality, the squeeze-film damping existed in these commonly packaged devices caused not only the non-linearity phenomenon in above frequency response curve but also the frequency shift. The damping effect will change the measured resonant frequency in actual testing environment based on $\omega_r = \omega_0 \sqrt{1 - \zeta^2}$ (ω_0 is natural frequency and ζ is damping ratio of the vibration system). From the test results, the measured natural frequencies are not as close to those of the theoretical predictions as what we would expect. The errors between the analytical and measured 1st natural frequencies are about 10% for the resonator of B2, 20% for B3 and 26% for B4, respectively. It has been found that the Q-factor of the polysilicon material is low and varies with processes. In the following section, we would seek to discuss some of these reasons based on the comparisons between present results and those of corresponding references.

4.6 Discussion and Summary

4.6.1 Discussion of Factors Influencing the Performance of Fabricated Resonator

In this section, we will discuss some factors which influence the final performance of the resonators from the points of view of design, fabrication and measurement.

- *Design factors*

It is obvious that the theoretical models are just the idealizations of the real physical structures. In these models, some parameters, such as the properties of materials and structural dimensions, may be varied with different fabrication processes. For example, the ion implantation and annealing process for polysilicon beam may change the material properties and cause tensile or compressive internal stress in vibration structure, which will lead to frequency shift. Some other parameters, such as anchor dissipations, distributions and magnitudes of internal stresses and moments, squeeze air film damping and material damping etc., are neglected or simplified in the analytical models, but they play substantially important roles in the real world. The selection of these parameters should be carefully considered. Another important factor causing the frequency shift is the bias voltage. The frequency variation with bias voltage comes from the introduction of the electrostatic stiffness. In this case, system stiffness consists of structural stiffness and electrostatic stiffness. Structural stiffness is positive because the force increases when a spring is stretched. However, electrostatic stiffness of a parallel plate capacitor is negative. The attraction force generated between the plates depends not only on the applied voltage, but also on the resonator position. As shown in (3-24) and (3-25), it will decrease non-linearly with an increasing gap of the parallel-plate capacitive transducer. Thus the transducer behaves as an additional spring with a negative stiffness that is joined to the resonator. As a result, this effective electrical spring will cause the stiffness of system lowering and make the resonant frequency shifting. For the parallel plate

capacitively transducerd clamped-clamped beam resonators, Clark (1999) has deduced the resonance frequency including the bias effect,

$$f_0^* = f_0 g \left(1 - \frac{k_e}{k_m}\right)^{1/2} \quad \text{where } k_e = V_{pn}^2 \frac{C_0}{g_0^2} \quad (4-15)$$

in which, k_m is the effective mechanical spring constant, k_e is the effective electrical spring constant which is generated by the nonlinear dependence of capacitance of electrode-to-resonator transducer on displacement, V_{pn} is the voltage difference between the dc bias and the voltage on the electrode, g is a scale factor that models the effects of surface topography and is dominated by anchor step-up effects. It can be found out that the center frequency decreases as the dc bias increases because the voltage-controllable electrical stiffness reduces the stiffness of the system, and the influence of this factor on the natural frequency has been verified experimentally. In our circumstance, the maximum error caused by the bias effect can be nearly 2%~3%.

- ***Fabrication factors***

Our consideration in fabrication factors is the influence of the release step, which is the last process step to form the air gap between the resonant structure and the bottom electrode. As shown in Fig. 4.17, an ideal release will leave nothing in the air gap. Thus a pure air or vacuum capacitor can be formed. However, the real situations are often like those shown in plot (c) below, in which the remainders of the sacrificial layer and the drops of the cleaning fluid coexist within the released gap. The measured impedance characteristics will hence be different due to the presence of parasitic capacitance. More seriously, the remainders may sometimes form a short circuit. Attractive capillary forces will also be generated since the encapsulated fluid tends to pull deformable microstructures into contact with their substrates. That is the common sticking problem associated with wet release process. Different release, cleaning and drying methods have

been tested to evaluate their influences on the resonator performance.

Figure 4.17: Illustration of the use of sacrificial layer to form a raised and released structure

In a typical surface micromachining, a series of film depositions and lithographic patterning processes are usually involved. High-quality thin films are often either grown or deposited at elevated temperatures. Because their thermal expansion coefficients are different from that of the silicon substrate, films of these materials tend to have residual stresses at room temperature when they are deposited on silicon substrates. This is a topic of particular concern in MEMS. Residual stresses can be detrimental or advantageous depending on the applications of the device, and therefore must be carefully considered during the design of the fabrication processes. The characteristics of the oxide, particularly its thickness uniformity and surface morphology, are also important because they will affect the characteristics of the final finished device. Sacrificial oxides are often phosphorus doped. As a result, the phosphorus atoms can

diffuse into adjacent polysilicon layers during heat treatments. Doping uniformity of the oxides is therefore very important to ensure desired characteristics of the eventual devices. Based on these considerations, optimization of fabrication processes need to be carried out further. From the point of view of fabrication, another new process using the state-of-the-art SOI wafer and relevant technologies has also been researched and developed to improve the performance of current devices, and this part of work will be introduced in the following Chapter 5.

- **Measurement factors**

Some environmental factors, such as the temperature, the pressure and the humidity within the test chamber will lead to the variations of resonance frequency and the degradation of Q-factor. For example, under different chamber pressures, the output gain and the Q values will become different, as shown in Figure 4.18. In addition, the different network model and configuration for test circuit will lead to different measurement results.

(a) frequency response of unpackaged resonator B3 at 760T (atmospheric), $V_p=8V$, 0dBm ($V_i=0.22V$)

(b) frequency response of packaged resonator B3 at 300mT, $V_p=5V$, $-13dBm$ ($V_i=0.05V$).

Improved signals are obtained after packaging and bonding the devices.

Figure 4.18: Frequency response functions under different pressures

As discussed in section 3.6.1, for any integrated MEMS devices, besides the inherent parasitic capacitance between the structure and the electrodes, and between the electrodes themselves, one should also be aware of the effect of parasitic resistances and capacitances due to substrate, which will contribute to the overall noise level and slow down the speed of the response of the system. The values of these parasitic components greatly depend on the layout and design, and their influences on the performance of a resonator also depend on the substrate properties. Figure 4.19 shows the measured frequency response results of beam resonators B3 and B4 obtained using high resistivity Si substrates. Compared with corresponding results shown in Fig. 4.16, it is obvious that the performance has been improved by using high resistivity substrate.

(a) B3 response with high resistivity N^+ substrate. $V_p = 13V$, $P_{in} = -5dBm$ (24 averaging), $Q \sim 1830$

(b) B4 response with high resistivity N^+ substrate. $V_p = 30V$, $P_{in} = 0dBm$ (16 averaging), $Q \sim 169$.

Figure 4.19: Frequency response of B3 and B4 with high resistivity substrates

4.6.2 Summary

In this part of the work, new processes using conventional polysilicon surface micromachining technology have been researched and developed successfully to fabricate various μ -mechanical resonators designed early. In addition, during this process, a new image measurement method and system for 3D microstructure inspection has also been developed and employed in our design work, which shows characteristics of adequate accuracy, high reliability and convenient measurement requirements. The static impedance characteristics and the dynamic frequency responses of the beam resonators with relatively low operating frequencies have been measured with a two-port network model, while other types of μ -mechanical resonators designed with high operating frequencies and high order vibration modes have not yet been measured because of their large motional resistances and tiny output signals even though they have been successfully fabricated. Based on the measurement results, several advantages of micromechanical resonator have been drawn. These are characterized as simple structural configurations with small feature sizes, potential applications in HF or VHF applications and compatibility with CMOS technology. Discussions on the effects of design, fabrication and measurement on the performance of devices have also been carried out, and it has been found that in order to achieve better resonator performance, challenges in new design methodology for improving operating frequency beyond GHz, in development and optimization of microfabrication processes to reduce the parasitic effects, and in development of new measurement method to effectively detect small output signal, should have to be tackled in future research work. To meet some of these challenges, a new process using the state-of-the-art SOI wafer and relevant technologies has also been researched and developed to improve the performance of current resonator devices, and this part of work will be introduced in the next Chapter 5.

Chapter 5

Development of Micromechanical Resonators using SOI Technology

5.1 Introduction

Recent advance in SOI (silicon-on-insulator) technology has generated increasing interest in their applications to IC industry, such as high speed CMOS ICs, smart power ICs and three-dimensional ICs. At the same time, research and development of devices with SOI wafer together with its corresponding microfabrication technologies are becoming promising in creating MEMS devices for mechanical, physical, chemical and optical applications, because SOI wafers can offer prominent advantages over bulk Si wafers, e.g., fewer process steps are needed for isolation, power consumption of device is lower, thicker and flatter films can be made than surface micromachining, and most importantly, parasitic capacitances and leakage current for both devices and electrical interconnections are reduced because of the existence of an insulating layer between the active silicon structure and the silicon substrate.

In our work, the introduction of SOI technology has enabled us to overcome some shortcomings that exist in the conventional polysilicon (poly-Si) micromachining, such as the internal stress built up in high temperature film deposition and the sticking effect due to wet release as discussed in Chapter 4. Furthermore, although polysilicon provides flexibility in mechanical properties, geometry and number of possible structural layers, it generally remains as a poor substitute for single crystal silicon (SCS), especially in

relation to its electrical properties. Table 5.1 gives some comparison of the properties of single crystal silicon and polysilicon.

Table 5.1: Comparison of Material Properties of SCS and Poly-Si

Material Property	SCS	Poly-Si
Young's modulus (10^{11} N/m ²)	1.90 (111)	1.61
Intrinsic Q factor at room temperature	6×10^5	Varies
Fracture strength (GPa)	6	0.8 - 2.84
Thermal conductivity (W/cm·K)	1.57	0.34
Residual stress caused by thermal processing	None	Varies
Resistivity	Depends on doping	Always higher

To improve the performance of μ -mechanical resonators developed earlier which employ polysilicon as structural material and are fabricated using conventional polysilicon surface microfabrication technology, another type of beam resonator which employs SOI wafers and corresponding technologies have been developed successfully. The relevant fabrication process and test results will be presented, compared and discussed in this chapter.

5.2 Working Principle of the Proposed μ -Mechanical Resonator

The schematic model of the newly developed μ -mechanical resonator is illustrated in Figure 5.1. In this model, clamped-clamped beam resonator is electrostatically coupled between the bottom electrode and the Si bridge. The working and design principles of this type of resonator is the same as those introduced in Chapter 3. Generally speaking,

the beam resonator is vibrating flexurally when its first mode vibration is excited by the input excitation signal and sensed from the sensing electrodes. In this schematic, the high frequency input signal comes from the bottom electrode, the top electrode provides dc bias voltage as well as electrical port for sensed output signal.

Figure 5.1: Schematic model of clamped-clamped beam resonator developed using SOI technology

The 1st natural frequency of this clamped-clamped beam resonator can be derived from the formula (3-15), and can be written as

$$f_0 = 1.03 \sqrt{\frac{E}{\rho}} \frac{h}{l^2} \quad (5-1)$$

where E is Young's modulus of SCS, ρ is the material density, h is the height and l is the length of the Si bridge. The effective stiffness of such flexural clamped-clamped beam resonator can be calculated as,

$$k_{eff} = 32E \frac{Wh^3}{l^3} \quad (5-2)$$

in which W is the width of the Si bridge. Then the effective mass of the beam resonator becomes,

$$m_{eff} = \frac{k_{eff}}{(2pf_0)^2} \quad (5-3)$$

Corresponding the same BVD model, its equivalent electrical parameters can also be calculated based on equations (3-40) and (3-41).

5.3 Fabrication Process using SOI Technology

5.3.1 Introduction to SOI Wafer

Many different SOI materials have been developed over the years, but two are being extensively used for IC production, i.e., SIMOX (separated by implanted oxygen) and SFB (Si fusion bonded) wafers.

In the SIMOX process, a standard silicon wafer is implanted with oxygen ions and then annealed at high temperature. The oxygen and silicon are combined to form a silicon oxide layer beneath the wafer surface. To minimize wafer damage, the oxygen is sometimes implanted in two or more passes, each followed by an anneal. The thickness and depth of this oxide layer are controlled by varying the energy and dose of the implantation and the anneal temperature. In some cases, a CVD process is used to deposit additional silicon on the top layer.

As illustrated in Figure 5.2, the SFB wafer process starts with an oxide layer, with the desired thickness typically from 0.25 to 2μ m, being grown on a standard SCS substrate.

Figure 5.2: Si fusion bonded wafer production

This wafer is then bonded to another wafer, with the oxide sandwiched in between. No mechanical pressure or other forces are applied during the bonding. The sandwich is then annealed at 1100°C for about 2 hours in a nitrogen ambient, leading to a strong binding between the two wafers. One of the wafers is then ground to a thickness of a few microns using mechanical tool and CMP (chemical-mechanical-polishing) processing. The crystalline perfection of the former silicon wafers in SFB is completely preserved in the SOI layer as the wafers do not suffer from implantation induced defects. By using plasma etching, wafers with a top Si layer thickness of as little as 1000Å with total thickness variation of less than 200Å can be made. SOI layers with 2μm thickness are more standard and are adopted in our fabrication.

Different with conventional poly-Si surface micromachining, SOI machining involves dry anisotropic etching to etch a pattern onto the Si layer on top of the insulator. These

structures can then be made free by etching the buried sacrificial SiO_2 insulator layer, which has a thickness of 400nm with very high reproducibility of 5nm and uniformity of $<\pm 5$ nm, especially in the case of SIMOX wafer. SOI wafers have been employed to produce an etch stop in such mechanical devices as pressure and acceleration sensors, high temperature sensors and ISFETs (ion selective field effect transistor). The SFB wafer offers more versatile MEMS approach due to its associated potential for thicker single crystal layers and the option of incorporating buried cavities and facilitating packaging. During the fabrication of micromechanical devices, the underlying silicon oxide can become a sacrificial layer that is etched away at the end of the process to free the mechanical structures such as vibrating beam, cantilever and diaphragm.

5.3.2 Layout Design of SOI-based Beam Resonators

Figure 5.3: Example of layout design of SOI beam resonators

As shown in Figure 5.3, a total of four masks are designed for pattern transfer in our SOI μ -mechanical resonator fabrication. In which, one is for glass substrate fabrication, and

three of them are for SOI wafer fabrication. Referring to the earlier Figure 5.1, the shallow trench frame is used to determine the beam length by etching out an air gap; the deep trench frame will isolate the resonator structure from other Si substrate and open the windows for probing the signal pads; the top electrode pad controls the areas of dc bias pad and output signal pad on the SOI wafer; the drawing of signal line and ground pad is patterned onto the glass substrate with a thin metal layer.

5.3.3 Development of Fabrication Process

There are several ways to process SOI wafers, but the bond and grind back is a mature method that gives good material processability for MEMS devices. Nowadays, a large percentage of commercial and academic MEMS development is also focused on the DRIE (deep reactive ion etching) of SOI materials. Based on the experience and available facilities in our cleanroom, the whole process of development of the new μ -mechanical resonator is divided into three stages, and they are (i) SOI wafer fabrication to construct the beam resonator structure, (ii) glass wafer fabrication to shape the bottom electrode, and (iii) bonded wafer fabrication to form the air gap and the support of the beam resonator. Each part of work will be presented schematically in the following.

The process starts with the SOI wafer fabrication (shown as Fig. 5.4(a)), and at this stage, the main process steps include:

1. Wafer marking, cleaning and standard fiducial mark fabrication which is used as a common alignment base.
2. Si pattern and shallow trench etch. As shown in Fig. 5.4(b), the top of SOI wafer is coated with $2\mu\text{m}$ thick positive photoresist, photolithoprinted with designed mask (shallow trench frame), exposed with $180\text{mj}/\text{cm}^2$ UV energy, and then

developed. Necessary bake steps are needed at 90~110°C during this process. The patterned wafer is sent into etching chamber to excavate shallow grooves onto SCS layer. The chamber for Si etching has a pressure of 100mTorr, and RF power of 400W. The flow rate of etchers HBr:Cl₂ is 40:40 sccm. After 120secs of etching, a shallow trench with 5000Å thickness is fabricated. This trench will form the air gap and anchors of the beam resonator. The wafer is then transferred into another chamber for photoresist strip with O₂ plasma. Subsequently, the processed wafers need to be cleaned with Piranha solution for 20 mins, DI water rinse and spin drying. To ensure a well alignment with the bottom electrode later, the depths of every etched trench should be measured and recorded at the end of this step.

3. Si pattern and deep trench etch to form the beam resonator structure. In the pattern process of this step, the same process used in step 2 is repeated and the mask of deep trench frame is used. The patterned wafer is thereafter sent into deep Si plasma etching chamber (STS ICP etcher/system) for DRIE reaction, which has an alternate process of etch and passivation in every cycle. The frequency of matching RF network is 13.56MHz, and the base pressure of chamber is 1.2mTorr. In etch phase, the reaction gases are C₄F₈, SF₆ and O₂. Their flow rate is 30:100:10 sccm. In passivation phase, only C₄F₈ reacts and its flow rate is 160 sccm. The Si:resist selectivity is 85:1, the sidewall profile is approximate 90°. The total reaction time for 5µ m thick Si etching will take about 8mins and the etch process will stop until it reaches the oxide layer. Post cleaning is also needed for subsequent wafer bonding. The schematic drawing of this process is given in Fig. 5.4(c).

(a) SOI wafer cleaning and preprocessing

(b) shallow trench etching to form air gap

(c) deep trench etching to form beam structure

Figure 5.4: Main processes for fabrication of SOI wafer

The process for glass wafer fabrication can be concurrently carried out with the fabrication of SOI wafer. The main steps are described as follows:

1. Pyrex (Corning 7740) glass preparation, marking and cleaning with H₂SO₄:H₂O₂ solution.
2. Frontside 600 Å Cr/2400 Å Au deposition. As shown in Fig. 5.5(a), 2400 Å Au layer is deposited onto the glass substrate in a dc sputtering chamber. To improve the adhesion of gold, a 600 Å Cr film is sputtered between the Au and glass.
3. Bottom electrode pattern and etch, as shown in Fig. 5.5(b). The wafer with blanket Cr/Au layer is patterned with the designed mask (signal line and ground pad), developed and then dipped into the Aqua Regia solution for about 25secs

until the unprotected Au is stripped. The unwanted Cr is also wet etched in a specific etchant.

4. The residual photoresist is stripped in PRS3000TM solution for about 30mins and dump rinsed. To keep the glass wafer clean, a fresh PRS solution is needed and it is better to further clean the glass surface with fresh Nano strip solution.
5. Anodic bonding with prepared SOI wafer frontside to frontside to form the air gap in a resonator. Using manual aligner, one of the fabricated SOI wafers is aligned accurately with a fabricated glass wafer. The pair is fixed and clamped on a specific jig carefully, and is then conveyed for anodic bonding. Under 350°C, 20e-3mBar chamber pressure and 800V dc voltage, the bonding time takes one and half hour. The bonded wafer is shown schematically as Fig. 5.5(c).

(a) glass cleaning, and sputter Cr/Au with 3000 Å thickness

(b) bottom signal line and pad formation

(c) wafer bonding (not scaled)

Figure 5.5: Fabrication of glass substrate

After anodic bonding, the main subsequent processes for the bonded SOI-glass pair include:

1. SOI wafer backside thinning down to about 30 μ m by mechanical grinding and polishing, as shown in Fig. 5.6(a).
2. Top electrical pad formation. The top electrode pad pattern is transferred onto the Si surface using common UV photolithography and the mask of top electrode pad. Positive photoresist is used as the mask for the following etching. To make an electrical ground for DRIE processing, a blanket Al with 500Å thickness is evaporated subsequently onto the backside of the glass wafer in a vacuum chamber of E-Beam evaporator. This step is shown in Fig. 5.6(b).
3. DRIE Si etch till stop on oxide layer and resist strip. The patterned wafer is then sent into STS ICP chamber for Si etching. The base pressure of the chamber is set to be 0.1mTorr. In etch phase, the flow rate of reaction gases SF₆:O₂ is 130:13 sccm. This phase will last 6secs in one cycle. In passivation phase, the flow rate of C₄F₈ is 110 sccm and will last 5secs in every cycle. The total reaction time for 30 μ m thick Si etching is about 30mins until the underneath oxide layer is reached. Then the wafer is dipped into the PRS3000 solution to remove the photoresist. The final result of this step is illustrated in Fig. 5.6(c).
4. Oxide wet etch with BOE. Using the processed SCS layer as mask, the wafer is dipped into BOE (6:1) solution for about 15 mins to remove the underneath oxide layer. As demonstrated in Fig. 5.6(d), this etch stops onto the structure Si and forms an open pad. BOE has a little reaction to Si, while it etches the glass wafer selectively. So after this process, the glass substrate will also become thinner. To avoid this problem, a RIE etch with CHF₃ reaction gas may be used to substitute the wet oxide etch.

5. 5000Å Au deposition on Si side. After cleaning process, a 5000Å Cr/Au film is sputtered onto the Si surface. Then a negative photoresist with 5μm thickness is coated and developed. The mask (top electrode pad) is used again for photolithography. However, this time the photoresist over window area is not removed, the photoresist in other area will be decomposed. Dip the wafer into Aqua Regia and Cr etchant again to remove the unprotected Cr/Au metal layers. The final results are displayed in Fig. 5.6(e) and (f).
6. Blank Si etch with DRIE and resist strip. As shown in Fig. 5.6(g), the wafer is sent into STS ICP chamber to remove the large area of Si substrate, and then is dipped into the PRS 3000 to remove the residual photoresist.
7. 2μm thermal oxide etch with BOE or RIE. The last step is to etch the large area of thermal oxide layer from the Si resonant structure. BOE has a quick etch rate of 1000~2000 Å/min. While it attacks the glass substrate, it also easily leads to a sticking of Si bridge to the substrate because of the liquid tension. So dry etching method is also tried. The final fabricated beam resonator is demonstrated in Figure 5.6(h).

(a) top Si layer grinding

(b) PR coating and patterning, 500Å Al deposition on backside of glass

Si DRIE etching and stop onto oxide layer

(c) Si dry etching and stop onto oxide layer

oxide wet etching and stop onto Si layer

(d) SiO₂ wet etching with BOE and stop onto Si layer

Negative photoresist coating with 5 μm thickness

(e) Au deposition and negative PR coating

(f) patterning and Au wet etching

(g) Si dry etch

(h) oxide removal

Figure 5.6: Post-bonding processing

A number of clamped-clamped beam resonator with various dimensions and various electrical pads were fabricated. In Figure 5.7, some example photos of the fabricated μ -mechanical resonators are displayed. The measured results will be presented in next section.

(a) frontside view of μ -resonator

(b) zoomed view of beam structure

(c) backside view of μ -resonator

Figure 5.7: Example photos of fabricated beam resonator

Compared with the previous processes developed for the poly-Si resonator fabrication, in the case of SOI resonator fabrication, an accurate alignment between the SOI wafer and glass substrate during wafer bonding will determine if the SCS bridge and the bottom electrode can be matched well, and consequently whether the resonator can work

normally. Similar problem also generates extra challenge in our process because a transferring action from aligner to bonding chamber is necessarily required after alignment. In general, one technique used for bonding alignment is the fabrication of holes in both the device wafer and the substrate, followed by bonding in a specially designed fixture. However, the accuracy achievable with this technique is only around 50 μm . Higher alignment accuracy ($\sim 2.5\mu\text{m}$) has been achieved by using a bonding machine equipped with an in situ optical alignment set-up. An infrared aligner modified to hold two imprinted wafers face to face, while projecting an infrared image of the surfaces to a viewing screen, is typically used. An array of elaborately designed alignment marks can provide good alignment results. Alignment jig can also be constructed and used for accurate ($\sim 5\mu\text{m}$) wafer-to-wafer alignment. Although the position accuracy of an adopted projection alignment is better than 5 μm in our anodic bonding of Si-Glass, misalignment cannot be eliminated completely, especially in the case of manual aligning, and it has led to the failures of many devices just because of poor alignment accuracy.

Another remarkable process is to saw the finished silicon wafer into individual dice. Most of the time, after the wafer is probed, it is mounted onto a sticky-tape and put onto the dicing saw, whose sawblade consists of a thick-shaped hub with a thin rim impregnated with diamond grit and rotates at a speed of several thousands of r.p.m. To avoid effect of the cutting impact on the bonding of the wafer and the possible disengagement of the bonded pair, optimal dicing parameters as well as good bonding results must be established before the dicing takes place. Because amorphous glass Pyrex 7740 matches very well with silicon in coefficient of thermal expansion, the internal stress caused by thermal mismatch during bonding will be very small. However, some air bubbles will still possibly occur in the fringe of bounded wafers. The reason for

this may be that the bonded surfaces are not clean, or that the process parameters fluctuate during bonding. The improvement on fabrication processes need to be investigated further. In addition, following example of improved designs as shown in Figure 5.8, which provides more bare areas around the resonant structure for bonding, reveals good bond strength than the designs shown in Fig. 5.3.

Figure 5.8: Improvement of resonator design by increasing the bonding areas

5.4 Test Results

The test pattern and set-up for measuring the electrical performance of the SOI resonator are the same as those introduced in Chapter 4. For frequency response measurement, the network analyzer HP8753D was again used. The resonator was excited by input electrode using ac signal v_i and the output signal was detected through the output pad. An adjustable dc bias voltage between the bottom electrode and the resonator was applied. The measurement was just carried out on-wafer at normal atmospheric pressure, and the measured frequency response of forward gain S_{21} is shown in Figure 5.9(a). Using the functions of signal processing provide by 8753D, we also verified our idea (referred to the model shown in Fig. 3.7) of compensating the antiresonance which

occurs in typical capacitive sensing measurement of μ -mechanical resonator. The processed result is shown in Fig. 5.9(b), which proves that this tactic is feasible from the point of view of signal processing and the physical realization of such operation though system-on-chip should be researched further.

(a) original measured results of S_{21} , 16 points averaging

(b) processed result for subtracting static capacitance to eliminate the antiresonance effect

Figure 5.9: Measured and processed results of frequency response

(a) Response of resonator using SOI technology. Test conditions: $V_{\text{bias}}=12\text{V}$, $P_{\text{in}}=-5\text{dBm}$, at atmospheric, no averaging, $Q \sim 150$, on wafer test.

(b) Response of B3 with high resistivity N^+ substrate. Test conditions: $V_{\text{bias}} = 10\text{V}$, $P_{\text{in}} = -5\text{dBm}$, no averaging, $Q \sim 120$, on wafer test.

Figure 5.10: Comparison of response of resonator using SOI technology and B3 using polySi micromachining

In Figure 5.10, the dynamic responses of the SOI resonator and the conventional polySi resonator are compared. We can find that when the Si substrate of the previous resonator becomes glass substrate and the polySi beam is replaced by a beam of SCS material, the Q-factor of such a SOI based resonator is improved and the noise level is reduced, even though the air gap spacing of the polySi resonator (1000Å) is much smaller than that of the SOI resonator (2000Å). In Table 5.2, on-wafer measurement results for the 5MHz resonator are tabulated.

Table 5.2: Comparison of Simulation and Test Results

	Simulation Values	Measured Values
Dimensions (μm) $l \times W \times h$	90 x 10 x 5	90 x 8.8 x 5
1 st Frequency (MHz)	5.73	5.44
Breakdown Voltage (V)	< 60	>40
Static Capacitance (pF)	0.042 (with 2000Å air gap)	0.028~0.32
Resistance of Si beam (Ohm)	~280	~370

Compared Table 5.2 with Table 4.1, it can be found that the breakdown voltage of such SOI based resonator has been improved to become more than 40 volts. The actual dimensions of devices are not matched well with their designed counterparts. The reason may be due to the BOE or CHF_3 which has eroded Si layer while etching the oxide layer. Although both oxide etching methods have high selectivity to Si, long time exposure into these erosive substances will inevitably lead to some Si being removed. The residual resist, impurity particles or oxidized layer lead to the measured capacitance and resistance much larger than the simulated ones. In addition, the metal pad and probes will contribute considerably to the parasitic effects. So far, only on-wafer measurement results are available. Optimization of fabrication processes, on-die measurement and test

for packaged devices will be carried out in our future work.

5.5 Summary

To overcome some shortcomings that exist in the foregoing poly-Si micromachining, such as the internal stress and the sticking effect, as well to take the advantage of better material properties of SCS, a new process for fabricating μ -mechanical resonator using SOI wafer and its relevant microfabrication technology have been developed successfully to improve the performance of the previous designed polySi based resonators. For easy reference, Table 5.3 summarizes the main differences in characteristics of the polySi and SOI based resonators.

Table 5.3: Comparison between Conventional and SOI μ -mechanical Resonators

	Conventional Poly-Si Process	SOI Process
Structure material	Polysilicon	Single crystal silicon
Substrate material	Si (100), need isolation layer	Pyrex glass
Fabrication type	Surface fabrication, resultantly the thickness of PolySi layer is not much big.	Bulk fabrication: the thickness of resonant beam can be from microns to tens microns.
Process complexity	Mature processes	Depending on bonding and alignment results
Air gap and anchor formation	Wet etching to remove the PSG sacrificial layer, which leads to the sticking because of liquid tension	Dry etching the shallow trench and anodic bonding to constrain the both ends of resonant bridge
Mask numbers	4	4
Break down voltage (V)	Varied	> 40
Performance	Need vacuum environment; Much noise and insertion loss	Higher Q value in air; Low noise and insertion loss
Cost	cheap Si wafer (<US\$0.5/piece)	expensive SOI wafer (>US\$50/piece)

Compared with the results of conventional poly-Si based resonator, the SOI resonator has the same operating principle as that of the polySi based ones, while the SOI based resonator possesses some major preferred processability due to its absence of high temperature processing and wet etching release in conventional surface micromachining. SOI resonator also shows better static impedance characteristics (higher breakdown voltage, smaller static capacitance) and dynamic frequency response performance (higher Q-factor, lower noise level). However, high cost of SOI wafer and accurate alignment requirement during fabrication are the main obstacles for the commercialization of SOI-based resonant devices.

No matter which fabrication technology is employed, because of the limitations of the current MEMS technology in further reduction of feature size and the current technical difficulties in weak signal detection, practically applicable resonators with higher resonant frequencies up to GHzs can hardly be achieved when a lower order mechanical vibration mode is assumed. To meet high frequency application requirement, a new design methodology, the TFBARs technology, has been researched in this project as another potential method to achieve workable resonators with resonance frequencies up to GHz. Related work on design and development has been carried out and will be presented next in Chapter 6 and Chapter 7.

Chapter 6

Design and Simulation of Thin Film Bulk

Acoustic Wave Resonators

6.1 Introduction

As summarized in Table 2.1, various acoustic devices with different vibration modes have been researched to seek high resonant frequencies with high quality factors of resonators since 1960's. Thin film bulk acoustic wave resonator (TFBAR, or FBAR) is one of the major breakthroughs of bulk acoustic wave (BAW) technology developed in recent years (Krishnaswamy *et al.*, 1990; Ewald *et al.*, 1998; Qing *et al.*, 2001). Unlike surface acoustic wave (SAW) resonators where the acoustic waves only oscillate on the surface of the piezoelectric substrate, TFBAR devices have acoustic wave resonating through the body of the piezoelectric materials such as Aluminum Nitride (AlN) and Zinc Oxide (ZnO). Because of this, TFBAR resonators have much smaller size, better power handling and higher operational frequencies up to 7.5 GHz, which is ideal for wireless communication applications. Another attractive advantage of such devices is its compatibility with current thin film semiconductor process. Although TFBAR technology has been researched for a long time, the challenges in relevant technologies, such as extremely precise and uniform film thickness for frequency control, exact acoustic coupling and minimum stress for good reliability, have not been resolved satisfactorily, and thus a high volume production of the TFBAR devices (resonators, filters, oscillator etc.) has not yet been realized.

Considering the limitation of achievable frequency range of foregoing μ -mechanical

resonators, and the good characteristics and potential commercialization of TFBARs, applicable researches in this field have also been carried out in our work, concentrating on improving the quality-factor of existing resonators for above GHz RF applications from the points of view of new structural designs and high-performance piezoelectric material development. This chapter will introduce the working principles of TFBARs and discuss the issues that could influence the TFBARs' design and performance based on various simulation results such as FEM frequency analysis and equivalent impedance characteristic analysis. A versatile simulation program has been developed using Matlab and the four-layer Mason model, and the results can be used to analyze the impedance characteristics of a resonator with thickness excitation modes and with different structural configurations. Based on the design specifications of high frequency (>1 GHz), small volume and good manufacturability, two newly developed resonator structures, namely the electrode-isolation and serial-resonator configurations, will also be presented and discussed in this chapter.

6.2 Theory of Thin Film Bulk Acoustic Wave Resonators

Two important theories are involved in our complete resonator design, that is, the bulk acoustic wave theory which provides the working and design principles of bulk acoustic wave resonators and for which two good references can be found in Auld's (1973) and Rosenbaum's (1988) works, and the microwave transmission line theory which decides how an electrical signal with microwave frequency and low power is efficiently transmitted to a resonator from a signal source and is efficiently received by peripheral conditioning circuits, and on which basic discussions can be found from many RF/Microwave engineering references. For easy reference, this and next section will give a comprehensive introduction to these theoretical foundations.

6.2.1 Working Principle of TFBARs

For a TFBAR resonator to work, there must be two essential ingredients: the first is the existence of an acoustic cavity, and the second is a mechanism through which electrical energy can be converted into acoustic energy. The type of device which can perform such energy conversion is that made of piezoelectric materials, such as AlN, ZnO or PZT. The first requirement can be satisfied by designing a large acoustic impedance mismatch between the two interfaces, thus “trapping” the acoustic energy into vibrating body. Essentially, TFBAR is an electromechanical transducer which couples the mechanical properties (stress and strain) and the electrical properties (electric field and electric displacement) of a piezoelectric crystal. The simplest configuration of TFBARs is the sandwiched structure with metal-piezoelectric-metal layers as shown in Figure 6.1(a), in which the metal layers are used as the upper and lower electrodes, and the AlN film is used as piezoelectric transducer. When an alternating electrical potential with specific frequency is applied across the electrodes, the entire piezoelectric layer will expand and contract because of the piezoelectricity effect, creating a vibration of crystal lattice parallel to the applied electric field direction (longitudinal vibration) or perpendicular to electric field direction (shear vibration), as illustrated in Figure 6.1(b).

(a) model of resonant structure with thickness excitation (TE) modes

(b) longitudinal and shear vibration mode of AlN crystal lattice in the presence of an electric field E

Figure 6.1: Schematic illustration of the working state of TFBARs

The piezoelectric media essentially performs an energy conversion through the interactions between mechanical stress and electrical charge. Therefore, the general constitutive equations for piezoelectric media with linear elasticity are expressed in terms of mechanical and electrical variables as (R. Lerch, 1990),

$$\begin{aligned} T_m &= c_{mm}^E S_m - e_{mn} E_n \\ D_n &= e_{nm} S_m + \epsilon_{nn}^S E_n \end{aligned} \quad (6-1)$$

where, T_m and S_m are components of mechanical stress and strain vectors, D_n and E_n are the components of electric flux density and electric field intensity vectors, c_{mm}^E, e_{mn} and ϵ_{nn}^S are components of elastic stiffness, piezoelectric and dielectric constants of the piezoelectric material, respectively. Also, subscript m is an integer of 1 to 6 and subscript n is 1 to 3. And the equations related to acoustics are expressed through Newton's second law, together with the definition of strain as,

$$\begin{aligned} \nabla_{nm} \cdot T_m &= \rho \frac{\partial^2 u_n}{\partial t^2} \\ \nabla_{mn} \cdot u_n &= S_m \end{aligned} \quad (6-2)$$

where ∇_{nm} is the partial gradient matrix, u_n is the displacement vector and ρ is the

material density. Similarly, the equations related to electrostatics are expressed as the divergence of electric flux density and the gradient of electric potential as,

$$\begin{aligned}\nabla \cdot \mathbf{D}_n &= 0 \\ -\nabla \mathbf{f} &= \mathbf{E}_n\end{aligned}\quad (6-3)$$

where ∇ is the partial gradient operator under rectangular coordinate system and $\mathbf{f}$ is the electric potential. As an important design target, the natural frequency of an acoustic resonator can be written as follows (Rosenbaum, 1988),

$$\mathbf{w}_n = \frac{v_a}{t} ((n\mathbf{p})^2 - 8k_t^2)^{1/2} \quad (n=1, 3, 5, \dots) \quad (6-4)$$

where k_t is the electromechanical coupling constant of piezoelectric material, v_a is the phase velocity of acoustic wave in piezoelectric stack and t is the characteristic dimension in wave propagation direction. In thickness excitation (TE) modes, t is the thickness of piezoelectric film. High resonant frequencies can be achieved by using one of the harmonics of the fundamental resonance, however, insertion loss associated with higher harmonic modes is always much higher. In our current device design, we only consider the fundamental resonant frequency in TE modes. Letting $n=1$ in equation (6-4) and neglecting k_t^2 whose value is only 2%~8% for AlN and ZnO crystals, the fundamental natural frequency of the resonator in thickness vibration can be approximately derived as,

$$\mathbf{w}_r = \frac{\mathbf{p}v_a}{t} \quad (6-5)$$

The acoustic velocity v_a of a piezoelectric resonator is determined not only by the material properties of piezoelectric crystal, but also by the propagation properties of acoustic wave in bulk piezoelectric layer. In Rosenbaum's (1988) works, by solving the eigenvalues and the eigenvectors of the stiffened Christoffel equation, the phase velocities v_a and the corresponding polarization directions have been resolved based on equations (6-1)-(6-3), and v_a can be simplified to become,

$$v_a = \sqrt{\frac{c^E + \frac{e^2}{s}}{r}} \quad (6-6)$$

It is obvious from (6-6) that the presence of piezoelectricity effect influences the propagation characteristics of the acoustic transducer since they are functions of electric and piezoelectric properties, and this makes piezoelectric transducer different from the common acoustic or mechanical sensors.

From above descriptions of TFBARs, resonant vibration occurs in the bulk body of the piezoelectric transducer, rather than being only confined to the surface of the piezoelectric substrate which is the case for SAW devices. One distinctive advantage of such resonator is its intrinsically better power handling characteristics as compared with the interdigitated structures used in SAWs, especially at high frequencies where the pitch of the interdigitated structures must be reduced to become extremely small. As a result, the piezoelectric membrane of a TFBAR device is able to provide a very high Q mechanical/acoustic resonance. Small volume is another advantage of TFBARs. According to the relationship of $v = f\lambda$ (i.e., wave speed = frequency x wavelength), it is understandable that for a given resonant frequency f , sound wave which travels at a speed of several hundreds or thousands of meters per second will have much shorter wavelength than that of the electrical or electromagnetic wave which transmits approximately at the speed of light. Consequently, the dimensions for an acoustic resonator are usually several orders of magnitude smaller than that for a coaxial-based resonator (a common resonator in RFIC designs). And like SAW devices, TFBAR devices can be easily integrated on to a semiconductor chip when materials and fabrication technologies employed are compatible with the standard IC processes.

6.2.2 Structural and Equivalent Electrical Models of TFBARs

As shown in Figure 6.2(a), a four-layer model is adopted in our equivalent impedance simulation and analysis, which considers the multi-layer effect on the performance of device and is more representative of the real device characteristics than the model shown in Fig. 6.1(a).

(a) four-layer structural configuration of resonator

(b) Mason equivalent circuit model including front and rear layers and acoustic loads (Rosenbaum, 1988)

Figure 6.2: Structural and equivalent electrical models of bulk acoustic wave resonator

In this model, the structural configuration comprises a piezoelectric crystal layer, sandwiched between two metal plates, and supported by a nonpiezoelectric substrate. When an ac signal is applied to the metal electrodes, an alternating electric field is established, forcing the crystal to vibrate in unison with the input signal. At the same

time, the metal electrode will also vibrate together with the transducer, producing the acoustic emission to its neighboring layers. Figure 6.2(b) shows an equivalent electrical circuit model (known as Mason model) of this four-layer structure, in which Z_i stands for the acoustic impedance, t_i for thickness and k_i for wave number of each corresponding layer. This model includes the acoustic attenuation and impedance of all four layers by characteristic parameters Z_i , t_i and k_i , and thus provides a more accurate solution for the design simulations of TFBAR devices. Furthermore, when more layers need to be deposited and analyzed, the four-layer Mason model can also be easily extended by introducing relevant parameters (Z , t and k) of these extra layers. When the thickness of the substrate t_4 is very close to zero and the thickness of the metal layer is less than $1000\text{\AA}$ (which is the case for our real fabrication), the structural configuration of Figure 6.2(a) degenerates to that shown in Figure 6.1(a), and the Mason model effectively becomes the BVD (Butterworth-Van Dyke) equivalent circuit model as shown in Figure 6.3, which has also been used as an earlier model for μ -mechanical resonator analysis. Additionally, a piezoelectric resonator operating at or near its resonance frequency can also be simply yet effectively characterized using BVD equivalent circuit model.

Figure 6.3: BVD equivalent circuit model for BAW resonator (Rosenbaum, 1988)

In this BVD model, the acoustic attenuation of the materials is represented by the equivalent motional resistance (or radiation resistance) R_m . The motional inductance L_m and the motional capacitance C_m define the resonance frequency of the resonant circuit. For thickness excitation modes, the static/clamped capacitance C_0 characterizes the

physical properties of the piezoelectric layer and can be calculated as,

$$C_0 = \frac{\mathbf{e}_r \mathbf{e}_0 A}{t} \quad (6-7)$$

in which e_r is the relative dielectric constant of the piezoelectric material, A is the effective electrode area and t is the thickness of the piezoelectric layer. The motional resistance in the BVD model can be expressed by the following formula (Rosenbaum, 1988),

$$R_m = \frac{\mathbf{p}^3 h}{8k_t^2 \mathbf{r} \mathbf{e}_r \mathbf{e}_0 A \mathbf{w}_r v_a} \quad (6-8)$$

where, η is the viscosity coefficient of the piezoelectric material. It is obvious that the motional resistance is inversely proportional to the resonance frequency $\mathbf{w}_r$, the effective electrode area A and the acoustic velocity v_a . The motional capacitance C_m can be written as,

$$C_m = \frac{8}{\mathbf{p}^2} k_t^2 C_0 = \frac{8k_t^2 \mathbf{e}_r \mathbf{e}_0 A \mathbf{w}_r}{\mathbf{p}^3 v_a} \quad (6-9)$$

and the motional inductance L_m can be found as,

$$L_m = \frac{\mathbf{p}^3 v_a}{8k_t^2 \mathbf{e}_r \mathbf{e}_0 A \mathbf{w}_r^3} \quad (6-10)$$

Also, similar to (3-47) and (3-48) in the case of μ -mechanical resonators, the series resonant frequency f_r and the parallel resonant (or antiresonant) frequency f_a are given as,

$$f_r = \frac{1}{2\mathbf{p}} \sqrt{\frac{1}{L_m C_m}}$$

and

$$f_a = \frac{1}{2\mathbf{p}} \sqrt{\frac{C_0 + C_m}{L_m C_m C_0}} = f_r \sqrt{\frac{C_0 + C_m}{C_0}} = f_r \sqrt{1 + \frac{1}{C_r}} \quad (6-11)$$

in which the capacitance ratio C_r (or C ratio) is defined as the ratio of the clamped capacitance C_0 to the motional capacitance C_m . At series resonance, the total impedance will be minimum and only motional resistance and capacitive reactance caused by C_0

exist. However, at parallel resonance, the total impedance will be maximum and the output signal will be minimum. The quality factor Q of such device can be calculated as,

$$Q = \frac{1}{2\pi f_r Z_m C_0} \left(\frac{f_a^2}{f_a^2 - f_r^2} \right) \quad (6-12)$$

where Z_m is the motional impedance evaluated at frequency f_r , together with the values of R_m , L_m and C_m . Based on these formulas and parameters, we will analyze various effects on the performance of TFBAR devices by using impedance characteristics simulation results as will be discussed in Section 6.4.

6.2.3 Process Flow of Program for Impedance Characteristics Analysis

Using the four-layer structure and its equivalent circuit model shown in Figure 6.2, a MATLAB simulation program has been developed for analyzing the frequency and impedance characteristics of the TFBARs based on the characteristic dimensions, the acoustic properties of the piezoelectric layer, the metal electrode layer and the substrate layer. Figure 6.4 illustrates the information processing flow in this program, which includes the attenuation and impedance effects of all four layers and can be used to calculate the overall impedance characteristics of the resonator. After some further modification, it can also be developed to compute the impedance characteristics of multi-layer resonators and filters. The simulation results will be used to guide our designs and optimization of the TFBAR devices. Also, more accurate and advanced equivalent electrical models have been investigated when mechanical, dielectric and piezoelectric losses associated with vibration need to be considered and the equivalent circuit elements are expressed with imaginary components (Kim *et al.*, 1993). However, for our design analysis and simulation, the Mason model has been found to be accurate enough to analyze the performance of the TFBARs when they vibrate in TE modes and at frequencies close to fundamental natural frequencies.

Figure 6.4: Information processing flow of the program for impedance analysis of TFBARs

6.3 Microwave Transmission Line Design

Besides BAW resonator, a complete TFBAR system operating above GHz should consider the microwave transmission line and relevant conditioning circuit as well in order to accurately represent its dynamic model performance. A transmission line is a pair of parallel metal conductors exhibiting specific characteristics due to its distributed capacitance and inductance along its length. In monolithic microwave integrated circuit (MMIC) design, the transmission line is an essential interconnection media amongst discrete devices or integrated systems, and it must be considered and designed carefully for optimal power handing. In our work, coplanar waveguide (CPW) and microstrip are employed as such connector linking TFBAR devices to peripheral conditioning circuit and ground pad.

6.3.1 Microwave Transmission Line Theory

In continuous dc circuits or low frequency ac circuits, many transmission line effects do not appear to be significant enough to warrant an attention. However, at higher frequencies (e.g. above GHz), the wavelength of the electrical signal propagating through a transmission line becomes comparable to the propagation distance. When a signal (voltage or current) is suddenly applied to one end of a transmission line, a voltage “wave” or a current “wave” is produced which propagates along the line at a speed close to light. Two things become noticeable when this situation occurs: (i) a parameter called characteristic impedance Z_0 becomes very important, and (ii) since the voltage or current to be measured becomes variable along the signal line in this case, the constant power becomes a preferable measurand in the world of high frequency applications.

The characteristic impedance of a transmission line is the resistance it would exhibit as if it were infinite in length. It defines the average behavior for the entire line or circuit, and is purely a function of the capacitance and inductance distributed along its length. Uniform impedance along the line is important to achieve optimal power transfer. Commonly, in MMIC design, the most effective way to minimize the impact of transmission line effects on circuit behavior is to match the line's characteristic impedance Z_0 with the load impedance. If the load impedance is equal to the line impedance, then any signal source connected to the other end of the line will "see" exactly the same impedance, and will have exactly the same amount of current drawn from it, regardless of the line length, because under this condition of perfect impedance matching, line length only affects the amount of time delay of the signal from the source to the load. On the other hand, as demonstrated in Figure 6.5, if a transmission line is not perfectly matched, some of the input power P_i will be transmitted to the load as P_t while some will be reflected back to the source as P_r . However, perfect matching of line and load impedances is not always practical or possible. So the trick is to design the Z_L to be as close to the Z_0 as possible, and Z_0 close to the source impedance Z_s . For a best compromise between power handing and lowest attenuation for coaxial lines in peripheral circuit, the input resistance for most RF and microwave instruments and cables adopts 50Ω or 75Ω characteristic impedances as standard (Pozar, 1990).

Figure 6.5: Schematic illustration of power distribution in high frequency application

6.3.2 Design of Transmission Line

In our TFBARs design, two types of transmission line are used, i.e., CPW and microstrip line, which are commonly employed in current MMICs. Figure 6.6 shows the schematics of the two transmission lines and their characteristic dimensions, in which W stands for the width of the signal line, G for the distance between the signal line and the ground line, t for the thickness of the metal layer and H for the height of the substrate. Their desired characteristic impedances are determined by these crucial dimensions and the relative dielectric constant of the substrate material.

Figure 6.6: Microwave transmission lines used in TFBARs and their characteristic dimensions

The characteristic impedance of the microstrip line can be calculated as (David, 1990),

$$Z_0 = \begin{cases} \frac{60}{\sqrt{e_{eff}}} \ln \left(\frac{8H}{W} + \frac{W}{4H} \right) & \text{for } W/H \leq 1 \\ \frac{120\pi}{\sqrt{e_{eff}} \left[\frac{W}{H} + 1.393 + 0.667 \ln \left(\frac{W}{H} + 1.444 \right) \right]} & \text{for } W/H > 1 \end{cases} \quad (6-13a)$$

$$e_{eff} = \frac{e_r + 1}{2} + \frac{e_r - 1}{2} \frac{1}{\sqrt{1 + 12H/W}} \quad (6-13b)$$

in which e_{eff} is the effective dielectric constant of the substrate. The calculation of characteristic impedance of CPW is more complicated. Brian (1991) however described

a simple yet accurate expression which is used to analyze the CPW line with bottom ground plane,

$$Z_0 = \frac{60p}{\sqrt{e_{eff}}} \frac{1}{\frac{K(k)}{K(k')} + \frac{K(k_1)}{K(k'_1)}} \quad (6-14a)$$

in which,

$$k = \frac{W}{W + 2G}, \quad k' = \sqrt{1 - k^2} \quad (6-14b)$$

$$k_1 = \frac{\tanh(\frac{p}{4} \frac{W}{H})}{\tanh(\frac{p}{4} \frac{W + 2G}{H})}, \quad k'_1 = \sqrt{1 - k_1^2} \quad (6-14c)$$

$$e_{eff} = \frac{1 + e_r \frac{K(k')}{K(k)} \frac{K(k_1)}{K(k'_1)}}{1 + \frac{K(k')}{K(k)} \frac{K(k_1)}{K(k'_1)}} \quad (6-14d)$$

where $K(k)$ is the complete elliptic integral of the first kind.

Figure 6.7: Complete circuit model including TFBAR and transmission lines

In our research, the use of CPW provides a more important design and fabrication method for making contact with a TFBAR device than the microstrip. Furthermore,

CPW provides a well-defined ground plane and thus avoids the introduction of stray inductances, which arise when a wire bonding is used. With such transmission line, on-wafer or on-die measurements can also be easily performed using ground-signal-ground probes provided by network analyzers. To accurately assess the influence of the CPW or microstrip, based on the model shown in Figure 6.7, the overall transfer functions of a TFBAR device including the transmission line can be approximately derived by cascading the transmission lines and a TFBAR (Qing *et al.*, 2001),

$$\begin{aligned}
 S_{11} &= \frac{Z + \frac{Z_0^2 - Z_s^2}{Z_0} (gL)}{2Z_s + Z + \frac{ZZ_s + Z_0^2 + Z_s^2}{Z_0} (gL)} \\
 S_{21} &= \frac{2Z_s}{2Z_s + Z + \frac{ZZ_s + Z_0^2 + Z_s^2}{Z_0} (gL)} \quad (6-15)
 \end{aligned}$$

where γ is the wave propagation constant, L is the total length of the transmission line, Z_0 , Z_s and Z are the characteristic impedances of the transmission line, the source and the TFBAR, respectively. When $Z_0 = Z_s$, i.e., the characteristic impedance of the transmission line is the same as the source impedance, (6-15) can be simplified to become,

$$\begin{aligned}
 S_{11} &= \frac{Z}{(2Z_s + Z)(1 + gL)} \\
 S_{21} &= \frac{2Z_s}{(2Z_s + Z)(1 + gL)} \quad (6-16)
 \end{aligned}$$

The effect of the transmission line can be neglected because γL is always small in GHz. However, if the characteristic impedance of transmission line is not equal to the source impedance, the CPW or microstrip will influence not only the magnitude of S_{11} , but also the series resonant frequency, thus contributing to the overall TFBAR response. Ideally, the transmission line connected to a TFBAR should be so designed that it possesses an impedance of about 50Ω.

The dimensions of the CPW as well as the microstrip designed in our work were carefully selected in order to achieve a characteristic impedance close to 50Ω, thereby minimizing its influence on the extraction of TFBAR properties. All these transmission lines are formed by patterning the metal layer (gold or aluminum) on a high-resistivity silicon substrate with thickness of 670 μm and relative permittivity of 11.8. Typical dimensions of some designed CPW and microstrip lines are enumerated in Table 6.1.

Table 6.1: Parameters of CPW and Microstrip Line Designed

Type	W (μm)	G (μm)	t (μm)	ϵ_{eff}
CPW I	195	120	0.1	6.49
CPW II	120	70	0.1	6.42
CPW III	188	120	0.7	6.44
Microstrip	530	--	0.1	7.75

6.4 Simulation and Analysis of Performance of TFBARs

To design a bulk acoustic wave resonator or filter with high operating frequencies and high performances, many parameters need to be considered carefully and synthetically. Besides the material properties of piezoelectric film (such as density, stiffness constants, dielectric constants, piezoelectric constants, electromechanical coupling coefficients, acoustic attenuation etc.), the properties of input signals, metal electrodes, middle layers (for stacked filter structure) and substrate also play important roles in the design of a TFBAR device. Analytical analysis and calculation of the effects of these parameters have proven to be very difficult and cumbersome, even just along the vibration principal

axes. Consequently, computer aided analysis and design tools should be developed and used. Desired natural frequencies and operating vibration modes can be obtained through repeated numerical simulations. Some finite element methods (FEM) in piezoelectric applications have been reported in recent years (Tapani *et al.*, 2000). In following simulations, a FEM harmonic analysis using ANSYS and an impedance characteristics analysis using our developed software program have been carried out to achieve the best designs of TFBAR devices.

6.4.1 Properties of Materials used in Simulation

According to formulas (6-1)-(6-3), for calculations of wave propagation characteristics (v_a, f_0, g etc.) and 3D FEM simulations, related vectors of material constants are needed. AlN and ZnO are the two popular piezoelectric materials developed with IC processes and both have crystal structures belonging to hexagonal system as illustrated in Figure 6.1(b). For this type of system, the stiffness matrix (unit: N/m²) has the following form,

$$c = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{bmatrix} \quad (6-17a)$$

As $c_{66} = (c_{11} - c_{12})/2$, there are only five independent parameters in this matrix. The form of the piezoelectric stress matrix (unit: C/m²) is expressed as,

$$e = \begin{bmatrix} 0 & 0 & 0 & e_{14} & e_{15} & 0 \\ 0 & 0 & 0 & e_{24} & e_{25} & 0 \\ e_{31} & e_{32} & e_{33} & 0 & 0 & 0 \end{bmatrix} \quad (6-17b)$$

As crystal structures of AlN and ZnO belong to the class of $6mm$, in this matrix $e_{15} = e_{24}$, $e_{31} = e_{32}$ and $e_{14} = e_{25} = 0$, and only three independent parameters exist. Two independent

parameters are found in the relative permittivity matrix, which is written as,

$$\mathbf{e} = \begin{bmatrix} \mathbf{e}_{11} & 0 & 0 \\ 0 & \mathbf{e}_{11} & 0 \\ 0 & 0 & \mathbf{e}_{33} \end{bmatrix} \quad (6-17c)$$

In our simulations, AlN is assumed to be the piezoelectric material used for TFBAR devices, and the reason for this will be explained in Chapter 7. Other material constants used were all extracted from relevant authentic literatures (Carlotti *et al.*, 1995; Dubois and Muralt, 1999; NSM Archive, 2003) and some of them are summarized in Table 6.2.

Table 6.2: Main Properties of Materials used in Simulations

	Density (kg/m ³)	Acoustic impedance (10 ⁶ kg/m ² s)	Q (at 1GHz)	Permittivity ϵ_r
AlN (002)	3260	35.7~36.9	2000 ~ 7000	8.5
Al	2700	17.14	1000	--
SiO ₂	2200	8.9	500	3.8
Si ₃ N ₄	3100	35.97	500	7
Si <1, 0, 0> long	2300	19.8	3000	11.9

6.4.2 Frequency Response Simulation and Impedance Characteristics

Analysis of TFBARs

6.4.2.1 Symmetrical Model for FEM Simulation

As shown in Figure 6.8, to reduce computational time and memory requirement, a quarter symmetrical model is adopted in frequency response simulation by introducing properly the boundary conditions. In our research, we used high resistivity (2000-10000 Ω -cm) Si wafer as substrate and adopted the backside etching to remove the substrate

from the working area of TFBARs. The piezoelectric layer is edge-supported. In ideal case, all of the energy is confined to the piezoelectric transducer. Therefore, the substrate effect is neglected in our simulations to analyze approximately the performance of the devices designed, and in this model three layers are included: the top Al layer, the middle AlN layer and the bottom Al layer. The bottom layer has a boundary $5\mu\text{m}$ larger than the boundary of the top layer, and this extended area is all clamped as the boundary constraints. Different characteristic dimensions and shapes were simulated to assess their effects on the performance of TFBARs.

Figure 6.8: Quarter symmetric model, parameters and boundary constraints for frequency simulation of TFBARs with rectangular electrode

6.4.2.2 Flexural Vibration Modes in Al-AlN-Al Membrane

In lower order vibration modes, the elastic flexural plate wave (FPW) modes become dominant in the rectangular shaped diaphragm vibration. Although the natural frequencies of such modes are much lower than those in thickness excitation modes, we use these FPW modes in practice to measure the mechanical and piezoelectric properties of the piezoelectric materials, as well as for large displacement electroacoustic sensing and actuation applications.

(a) 1st order mode shape with $f_1 = 2.3\text{MHz}$ (b) 2nd order mode shape with $f_2 = 7.0\text{ MHz}$

Figure 6.9: Low order mode shapes of the TFBAR diaphragm structure designed

Figure 6.9 shows the 1st order and the 2nd order mode shapes and their corresponding frequencies in FPW vibration modes. The thickness of the simulated AlN layer is $1.8\mu\text{m}$, the top electrode is $0.7\mu\text{m}$ and the bottom electrode is $0.2\mu\text{m}$. The effective area of both electrodes is $100 \times 100\mu\text{m}$.

6.4.2.3 Frequency Response in Thickness Excitation (TE) Modes

Because a thin diaphragm has an infinite number of vibration modes, when thickness excitation modes are of interest, using frequency response analysis will be more convenient for us to find the required frequency characteristics and the corresponding mode shapes. Figure 6.10 shows a dynamic response plot and the corresponding displacement profiles at resonance and antiresonance. Here, the same structural configuration as that of Figure 6.9 is assumed, a 1V voltage is applied onto the Al electrodes and the stored charge is set as the output result. A visible current peak and valley occurs at frequencies of 3.06GHz and 3.08GHz, which represent the resonance and antiresonance at fundamental TE modes. At resonance, the piezoelectric membrane

expands and contracts evenly in thickness direction, while in the vicinity of the antiresonance, the displacement profile of the membrane presents irregularity. There are also some peaks and valleys caused by unwanted modes (spurs) in lower frequency range, but these spurious responses are far away from the working frequency and are weak in magnitude that they will not influence substantially the operation of the resonator designed.

(a) Frequency response of TFBAR membrane with thickness excitation mode

(b) displacement profiles at $f_r = 3.06\text{GHz}$.

(c) displacement profiles at $f_a = 3.08\text{GHz}$

Figure 6.10: Frequency response and corresponding displacement profiles at resonance and antiresonance

6.4.2.4 Simulation of Thickness Effects of AlN Film

For a TFBAR device working at TE modes, the thickness of piezoelectric layer is the most important factor that affects its resonance frequencies, the impedance characteristics of the device, the availability of fabrication methods and so on. Figure 6.11 shows the effect of the thickness of piezoelectric layer on the frequency response of TFBARs. Following the previous structural configuration, the thickness of the AlN layer is changed to become $5\mu\text{m}$, the frequency at series resonance is then lowered to about 1.1GHz . Compared with Figure 6.10(a), some unwanted responses occur in a closer range of the working frequency. It is shown that decreasing the resonator dimension will allow the unwanted modes to be removed far enough away from the main resonance that they do not interfere with the device operation.

Figure 6.11: Frequency response simulation for 5μ m thickness AlN layer

A 3D FEM harmonic analysis provides a convenient and visualized way for observing structural performance of a TFBAR device designed, while considering the whole electric circuit analysis similar to the one performed in μ -mechanical resonator simulation, it is essential to extract the equivalent electrical parameters using accurate Mason model for optimization of the device design, and a synthetic program has been developed in this project for such purpose. Once the equivalent parameters are known by solving Mason model, we can further determine the electric performance of resonators or filters designed using BVD model and standard circuit analysis. Table 6.3 shows the simulation results of AlN thickness effects on the fundamental frequency, the Q-factor and the equivalent electrical parameters corresponding to the BVD model. Here, we assume the electrode area is $100 \times 100 \mu\text{m}$, the thickness of the top electrode and the bottom electrode is $1000 \text{\AA}$, and the thickness of AlN film changes from $1 \mu\text{m}$ to $5 \mu\text{m}$. As the thickness increases, the fundamental natural frequency in TE modes and the clamped capacitance C_0 decrease nonlinearly, whereas the Q-factor increases. The motional resistance R_m also increases with thickness, but the value is away below the 500

characteristic impedance preferred. The C ratio also increases with thickness and this means that the serial resonance will be brought closer to the parallel resonance when the operation frequency is lowered. It is also found that frequencies below 1GHz require relative thick piezoelectric layers ($>5\mu\text{m}$), which will be difficult to fabricate with sputtered AlN films due to long deposition time and internal stress problem.

Table 6.3: Thickness Effects of AlN Film

t (μm)	1.0	2.0	3.0	4.0	5.0
f_r (GHz)	4.39	2.56	1.76	1.34	1.08
f_a (GHz)	4.83	2.61	1.78	1.36	1.09
Q	27.27	152.22	372.70	654.73	979.71
R_m (Ohm)	4.27	17.60	23.32	24.32	24.69
L_m (H)	4.22e-9	1.67e-7	7.87e-7	1.90e-6	3.58e-6
C_m (F)	3.11e-13	2.32e-14	1.04e-14	7.49e-15	5.12e-15
C_0 (F)	7.52e-13	3.76e-13	2.51e-13	1.88e-13	1.50e-13
C Ratio	2.4	16.2	24.1	25.1	29.3

The acoustic device is characterized by its equivalent electrical impedance which is a complex function of the frequency and the material constants of the elements that make up the device. At resonance, only resistance R_m and capacitive reactance caused by C_0 exist. Compared with μ -mechanical resonator, the motional resistance of TFBARs is much smaller, while as discussed early, this value is required to be close to 500 for efficient energy transmission. According to (6-8), R_m is inversely proportional to the frequency, and a very high frequency will limit this resistance to only few ohms, which will lead to the design of external matching elements more difficult. Therefore, to meet the requirements of impedance matching and fabrication, the thickness of AlN film must be optimal. From Table 6.3 and according to (6-12), the Q-factor will be improved

because the resonance frequency as well as the clamped capacitance decreases when the thickness of AlN film increases, even though the acoustic attenuation increases under this circumstance.

6.4.2.5 Metal Electrode Effects on the Performance of TFBARs

Metal layer plays another important role in designing a high performance TFBAR device. Compared with electrical loss, the reduction of Q-factor caused by the metal layers due to increased acoustic attenuation along wave propagation path is more dominant, especially in high frequency (above 1GHz) applications. Using the impedance characteristics simulation again, we concentrate ourselves on the effects of the thickness and the area of the metal electrodes on the performances of TFBARs. A sputtered Al film is used as the electrode material because of its intrinsically high Q-factor and compatibility with AlN in fabrication. When the thickness of AlN layer is kept as 5 μ m, the area of electrodes is kept as 100 x 100 μ m and assuming the thickness of electrodes changes from 1000Å to 1 μ m, the simulation results are listed in Table 6.4.

Table 6.4: Thickness Effects of Electrodes

t (μ m)	0.1	0.3	0.7	1.0
f_r (GHz)	1.08	1.04	0.98	0.94
f_a (GHz)	1.09	1.06	1.01	0.97
Q	979.71	588.28	371.88	313.81
R_m (Ohm)	24.69	32.84	42.98	48.66
L_m (H)	3.58e-6	2.96e-6	2.60e-6	2.58e-6
C_m (F)	6.12e-15	7.94e-15	1.02e-14	1.12e-14
C_0 (F)	1.50e-13	1.50e-13	1.50e-13	1.50e-13
C Ratio	24.5	18.9	14.7	13.4

It is obvious that the resonant frequency, the Q-factor and the C ratio have decreased, while the motional resistance has increased to near 500 as the thickness of the electrode increases from 0.1 μm to 1 μm . When the thickness of AlN layer is kept as 5 μm , the thickness of metal layer is kept as 0.1 μm and assuming the area of electrodes changes from 150 x 150 μm to 50 x 50 μm , simulation results for the effect of various areas are listed in Table 6.5. It can be found that when the area decreases, the resonant frequency, the Q-factor and the clamped capacitance also decrease. The motional resistance can be improved to become near 500 when an electrode size of 50 x 50 μm is used.

Table 6.5: Area Effects of Electrodes

Dimensions (μm)	150 x 150	100 x 100	80 x 80	50 x 50
f_r (GHz)	1.08	1.08	1.07	1.03
f_a (GHz)	1.09	1.09	1.09	1.10
Q	1127.5	979.7	841.4	343.6
R_m (Ohm)	12.19	24.69	32.04	49.51
L_m (H)	2.03e-6	3.58e-6	4.01e-6	4.73e-6
C_m (F)	1.07e-14	6.12e-15	5.52e-15	5.04e-15
C_0 (F)	3.39e-13	1.50e-13	9.63e-14	3.76e-14
C Ratio	31.7	24.5	17.4	7.5

According to the results shown in Table 6.4 and Table 6.5, when the thickness of the metal layer increases or its effective electrode area decreases, the following differences are noticeable: (i) the resonance frequency has been reduced, (ii) the Q-factor has been lowered, and (iii) the equivalent impedance characteristic has been changed. Based on these simulation results, the reasons can be analyzed as follows.

The metal electrode reduces the resonance frequency by its presence as part of the

acoustic path of the transducer, or it acoustically “loads” the transducer. This effect is more prominent with metal material with low acoustic velocity and high acoustic attenuation such as gold. Compared with the effective area, the resonance is determined to a large degree by the electrode thickness. It can be found that when the thickness of electrode layer increases from 0.1 μm to 1 μm , as much as 13% frequency shift will be produced. As the thickness of AlN layer decreases further or the resonance frequency increases, the effect of the metal loading on the frequency shift will also be much higher. To ensure the operation frequency designed, any increase in the metalization will require a decrease in the transducer thickness. Therefore, the metal electrode thickness should be as thin as possible to reduce its loading effect.

The main decrease in device Q-factor is a result of the high metal attenuation. In high frequency applications, the increase of thickness of metal layer will produce more acoustic attenuation in the metal layer and lead to lower Q-factor. The decrease of effective area of metal layer will reduce the working area and the acoustic impedance of the transducer. Consequently, less acoustic energy will be reflected and confined within the vibrating piezoelectric layer and thus leading to lower Q-factor of device. Based on the simulation results shown in Table 6.4 and Table 6.5, it is obvious that both increasing the thickness and decreasing the area of metal electrodes have led to a reduction in Q-factor.

The equivalent impedance depends on the acoustic properties of all layers and on the frequency, while according to simulation results, the values of reactive component C_m and L_m do not vary dramatically. For a given operating frequency, only the electrode area determines and influences the values of C_0 . Optimal resonator operation requires designing the motional resistance well below 50 Ω so that the device does not reflect the electric energy. According to (6-8), the motional resistance is inversely proportional to

the area of the electrode. When the area of the metal layer decreases, the effective working area and the clamped capacitance of the device also decrease, causing the radiation resistance to increase. In TFBAR design, the area is an effective factor to control the impedance matching to the source resistance (usually 50Ω). However, from Table 6.5, to achieve this value, extremely small effective areas are needed. Such small areas can lead to difficulty in bonding as well as degradation of device performance such as excessive acoustic diffraction.

In our actual fabrication, the bottom electrode thickness is of 0.2 μm, while the top electrode thickness is about 0.2 μm~0.7 μm, after taking into consideration of the requirement of the low resistance of the signal line. From the point of view of fabrication, the bottom metal plane serves a more important function, because in sputtered piezoelectric film technology, this metal plane provides an ordered growth “bed” for the AlN film and holds the film firmly to the substrate.

Besides the rectangular shape, resonator with circular electrode shape has also been simulated to verify the electrode shape effect on the performance of TFBARs. Figure 6.12(a) shows a quarter symmetric model used in such a simulation, where the Al-AlN-Al sandwiched structural and parametric configurations are similar to the model shown in Figure 6.8.

(a) quarter symmetric model for circular electrode shape verification

(b) simulation result of frequency response

Figure 6.12: Model and simulation of TFBARs with circular electrode shape

Here, the assumed thickness of the AlN layer is $1.8\mu\text{m}$, the top electrode is $0.7\mu\text{m}$, the bottom electrode is $0.2\mu\text{m}$, and the area of electrodes is $10000\mu\text{m}^2$ (equivalent to $100\times 100\mu\text{m}$), the frequency response of the model is simulated and shown in Figure 6.12(b). Compared with Figure 6.10, this model presents similar frequency characteristics in terms of resonance (3.07GHz) and antiresonance (3.09GHz), while its output current with the same applied voltage is lower than that of the model with rectangle electrode shape, and more spur responses appear in a closer range to the operating frequency. It seems the electrode shape has no prominent effects on the performance of the device as far as structural analysis is concerned, while further investigation on its electrical effect need be carried out.

6.4.3 Discussion of Simulation Results

For our particular research purpose, the performance of TFBAR devices is characterized by high operating frequency and high quality factor. After neglecting some factors such as ohmic loss of metal layer, dielectric loss of piezoelectric layer and temperature stability, we acquired the characteristics of the frequency response, the Q-factor and the equivalent impedance of TFBAR devices designed by using FEM and Mason models and corresponding simulations. This simplification is necessary because it is difficult to optimize all the design factors simultaneously, and theoretical and fabrication limitations always need trade-offs in the design of commercial devices. As shown in Figure 6.4, the structural parameters and the acoustic properties of all layers in the acoustic path have been considered and included in the simulation program developed.

According to (6-5), working at TE modes, acoustic velocity of piezoelectric crystal is a critical factor in frequency design which mainly relies on the properties of piezoelectric material such as stiffness, piezoelectric constant, permittivity constant and density. The use of high performance piezoelectric material always leads to high performance devices. Once a piezoelectric material is selected, the thickness of the piezoelectric film is the only design factor in TE modes. As discussed early, thickness is critical because it is the only characteristic dimension which determines the operating frequency of TFBARs and further determines other performances of devices designed such as Q-factor and impedance characteristics. However, because the metal loading effect can cause a frequency shift as shown in Table 6.4 and Table 6.5, the actual operating frequency of the device will possibly deviate from the designed value and careful attention must be paid to both transducer thickness and metal loading effect. To achieve higher frequency, the thickness of piezoelectric layer must be made smaller. From the point of view of

fabrication, TFBAR device for high frequency applications can be easily made because a low resonant frequency (below 1GHz) will need large amount of time to deposit the required half-wave thickness, which will lead to problems such as excessive internal stress, charge accumulation in reaction chamber and low production efficiency as discussed in Chapter 7. For example, the sputtering rate of AlN film in our work is about 420Å/min, thus a 5μm thickness layer requires nearly 2 hours of deposition time and more total production time. It's found that thick film will lose partly or completely its characteristic properties (Wang, 1993), and tend to be highly stressed and invariably peel off the substrate. However, from the point of view of impedance characteristics, because the motional resistance varies inversely with frequency, a very high frequency resulting from a thin piezoelectric film can limit the motional resistance to only few ohms, which is far away from the desired 50Ω. Therefore, to meet the requirements of design and fabrication, the thickness of AlN film cannot be designed too thin or too thick and an optimal thickness needs to be established.

In TE vibration modes, metal loading is caused by the electrode plane in acoustic propagation path. At low frequency or with thin metal film, the primary effect of the metal layer is to lower the series and parallel resonant frequencies rather than to alter resonator performance significantly. However, at high frequency or with thick metal film, the metal layer begins to constitute an increasingly greater percentage of the overall thin film resonator structure. In the case without electrode, the Q-factor of TFBAR device is determined only by the quality factor of the piezoelectric material, whereas in the case with electrodes, it is a weighted average of the two quality factors of the metallization and the piezoelectric crystal. Because the metal plane is essentially a low-Q and nonpiezoelectric layer, it begins to degrade device performance by lowering the Q-factor of the device. In this case, metal electrodes need to be considered as lossy acoustic

transmission lines, and the BVD model and the corresponding formulas are not available. From the intuitive viewpoint, thin metal layer and large area are preferred, while other performances will be degraded such as lower motional resistance and bigger volume. Therefore, the electrode parameters must be designed carefully and synthetically by simulation and by experiment. The effects of different thickness, area and shape of metal electrodes on the performance of devices designed have been simulated and analyzed. It is also found that the metal loading associated with the thickness and the area of metal electrodes has greater influence on the performance of TFBAR devices than the shape of electrode does.

The substrate attenuation is always a critical factor in wideband device design (such as filters and wideband delay lines), in which the piezoelectric layer is rigidly attached to a substrate and a close acoustic impedance match between transducer and substrate is required for an efficient energy transfer. However, for high-Q TRBAR devices, the attenuation in the substrate needs to be substantially reduced, and consequently the acoustic wave can be reflected back and forth many times before attenuating in piezoelectric transducer. As shown in Figure 2.1, in a conventional TFBAR structure, the acoustic wave in the piezolayer is often isolated from the substrate by backside etching to form a suspended membrane, or by sacrificial layer etching to form an air gap, or by carefully building up the middle layers to form an acoustic Bragg reflector. In our present research, the silicon substrate has been removed from the acoustic path by wet or dry etching, or by using electrode-isolation structure (which will be introduced in next section), and thus this effect is not included in our simulation. In addition, in our actual fabrication, Si substrate with high electrical resistivity (2000-10000 $\Omega\cdot\text{m}$) has been used to reduce the electrical power dissipation due to microwave signal propagation.

In general, TFBAR device based on AlN material has high acoustic velocity and high operating frequency. Many Q-detractors, which depend on the acoustic and electric properties of all layers in the acoustic path, will exist as the possible forms of attenuation and electric loss in the substrate, attenuation and dielectric loss in the piezoelectric transducer and attenuation and ohmic loss in the metal planes, etc. Especially, at microwave frequencies, the metal layer begins to constitute an increasingly greater percentage of the overall resonator structure and to degrade device performance by lowering its Q value. Based on foregoing simulation results and the realizability of microfabrication using MEMS technologies, some possible measures are being taken into account to reduce the dispersion of these factors and thus improve the Q-factor of devices. They are:

- Reduction of power diffusion and electric loss to substrate by using isolator layers, high resistivity substrates and further, electrode-isolation structure. Based on these assumptions, corresponding technologies such as modeling, design and fabrication of newly developed configurations have been further researched in our work, and will be introduced in Section 6.5.
- Optimization of designed parameters for good electric and acoustic impedance matching to realize efficient transmission of electric energy and conservation of acoustic energy in vibration body. Matching the device is complicated because its resistive component depends on frequency and its reactive component varies with the acoustic parameters of the various layers. Therefore, external matching elements (usually inductor, capacitor or RF transmission line) or matching network (LC tuning network) technologies will be essentially researched and designed.

- Development of high quality metal materials with low attenuation, and using substrates with low electric resistance and low acoustic attenuation.
- Development and optimization of high performance piezoelectric materials with preferred crystal orientation, fine grains, low acoustic attenuation, low internal stress, etc. for high frequency and high Q resonator applications. The work on development of high performance AlN material with optimal deposition parameters has been carried out and will be introduced in Chapter 7.

6.5 Introduction of Newly Developed Designs

Based on above discussion and simulation results, two novel designs of TFBAR resonators are developed, simulated and analyzed in our research, to further improve the performance of the conventional TFBAR devices and to solve the problems associated with fabrication. One is the electrode-isolation configuration, which is used to eliminate the electrode effects on the performance of resonators. Another is the serial-resonator configuration, which is developed to meet the requirements in device fabrication.

6.5.1 Electrode-isolation Configuration Design

As discussed earlier, in high frequency applications, the metallic loading effect as well as the acoustic attenuation in substrate are two critical Q-detractor factors. One obvious improvement of resonator Q at high frequency requires the metal and the substrate be removed from the acoustic path. To achieve this, a so-called BVA (which means “in a box with improved ageing”) structure was firstly introduced by Raymond Besson in 1976, which demonstrated good performance in low frequencies (2~5 MHz) application with 1~2 mil air gap. At frequencies of a few megahertz, Q-factors of quartz BVA structure have been reported to have approached its material limit (R. Besson and U.

Peier, 1980; Jerry and R. Besson, 1993). Building on this idea, together with advances in current MEMS technology, a new electrode-isolation structure has been proposed in our research to obtain a zero-mass-loading effect and a resultant high performance resonator. Figure 6.13 shows the schematic of this design, in which the electrodes are separated from the AlN layer by an air gap distance of d . At the same time, the substrate is also isolated from the acoustic path without using backside etching process. Hence, the acoustic wave produced in AlN layer will not propagate into the substrate and no acoustic attenuation occurs in the substrate as well.

Figure 6.13: Structural configuration of electrode-isolation design

It is obvious that in this model the metal electrodes have been stripped off from the vibrating piezoelectric layer, and the application of excitation and the sensing of response can be performed through the electric field of the metal-piezo capacitors. Thus, this proposed electrode-isolation structure will provide a maximum acoustic energy reflection E_{ref} which can be calculated using the following formula,

$$E_{ref} = \left(\frac{Z_{piezo} - Z_{air}}{Z_{piezo} + Z_{air}} \right)^2 \cdot 100\% \quad (6-18)$$

in which Z_{piezo} and Z_{air} are acoustic impedances of the piezoelectric layer and the neighboring air layer respectively. In our configuration, because Z_{piezo} is much larger than Z_{air} , the energy reflected from the interface between the AlN film and the air gap, other than the metal film or the substrate in the case of conventional TFBAR structures,

will be close to 100%. That means more acoustic energy can be confined or trapped within the vibrating piezoelectric layer.

The equivalent circuit model including the effect of air gap in such an electrode-isolation design can be established as a resonator in series with an air gap capacitor C_s in the corresponding BVD model as shown in Figure 6.14.

Figure 6.14: Equivalent circuit model for electrode-isolation structure

Based on this model, the total impedance can be derived as,

$$Z' = -\frac{1}{\omega C_s} \cdot \frac{C_0 + C_m + C_s - \omega^2 L_m C_m (C_0 + C_s)}{C_0 + C_m - \omega^2 L_m C_m C_0} \quad (6-19)$$

Compared (6-19) with equation (3-45), the denominator form in the impedance expression and the resultant parallel resonant frequency remain unchanged, while its numerator and the corresponding serial resonant frequency has been modified to become,

$$\begin{aligned} \omega_r' &= \frac{1}{\sqrt{L_m C_m}} \sqrt{1 + \frac{C_m}{C_0 + C_s}} \\ &= \omega_r \sqrt{1 + \frac{C_m}{C_0 + C_s}} \end{aligned} \quad (6-20)$$

From (6-20), the resonant frequency of such design will be improved by the introduction of the series capacitor C_s . Thus the resonant frequency and antiresonant frequency will be brought closer together. This problem becomes more serious at high frequency. To be practically useful above 1 GHz frequency range, the gap between the AlN layer and the

electrodes must be extremely small to improve the C_s value and enhance the electric field, and thus special microfabrication techniques are necessary.

Assume the thickness of AlN is $5\mu\text{m}$ and the Q-factor of material is 6800, Table 6.6 shows the simulation results of conventional TFBARs with $0.1\mu\text{m}$ thick Al electrodes and results of the electrode-isolation structure with $0.1\mu\text{m}$ air gap. It is concluded that the frequency shift can be eliminated and the Q value for the overall resonator can be improved by introducing such electrode-isolation structure due to the absences of the metal loading and the acoustic attenuation in the electrodes. The improvement has been found to be especially obvious for those piezoelectric materials with low loss, and for cases where the loss of the metal electrodes becomes dominant. From the results in Table 6.6, the frequency shift due to the metal loading effect has not occurred in such novel design, the Q-factor has been greatly improved, while the impedance in this case has been reduced significantly, which will lead to a more severe mismatch between the impedance of the resonator and the impedance of the external tuning circuit at resonance. Therefore, more consideration and optimization should be taken into account for such designs.

Table 6.6: Comparisons of Q-factor with and without Al Metals

Area of Electrodes	0.1 μm Al electrodes			0.1 μm Air gap		
	f	Q	Z	f	Q	Z
300 x 300	1.03GHz	1700	5.21	1.02GHz	5800	0.86
150 x 150	1.02GHz	1670	17.4	1.02GHz	5670	3.47
80 x 80	1.01GHz	1403	45.9	1.02GHz	5470	12.2

Another comparison result of different configurations of TFBARs and electrode-isolation structures is illustrated in Figure 6.15. It can be found, at operating frequency of 1GHz, the Q value of such electrode-isolation structure is much higher than that of the conventional TFBARs with metal electrodes, and with the air gap being further reduced, the Q-factor can be improved further. Referring to the ideal resonance frequency determined only by the AlN layer, the effect of frequency shift of electrode-isolation resonator has been reduced, and with the air gap decreasing, the operating frequency will be much closer to the ideal frequency.

Figure 6.15: Simulation results of different configurations of conventional and electrode-isolation designs

According to the simulation results, we think this novel design is feasible in improving the Q value as well as in stabilizing the operating frequency of the TFBAR devices. Some specific measures and microfabrication technologies will be adopted to reduce the influence of the series capacitance and to improve the fabrication capability.

6.5.2 Serial-resonator Configuration Design

During the fabrication of TFBAR devices, although many etchant and etching methods, such as 100°C HF/H₂O or hot H₃PO₄/CH₃COOH/HNO₃ solution (referred as PAN etch) have been found to be able to etch the AlN material, they unfortunately also attack aluminum. However, in a conventional TFBAR design as shown earlier in Figure 2.1(a), to probe the output signal from the bottom electrode pad, an open via is necessarily required to be fabricated by etching through the AlN layer. To avoid the attack on the Al electrode patterns while etching the AlN layer, and to be compatible with existing CMOS cleanroom processes, a serial-resonator configuration has been put forward, designed and developed in our research. This design employs the ladder architecture shown in Figure 6.16, in which the bottom electrode is used as the signal (displacement current) channel, the excitation signal is applied to one of the top electrodes, while the sensed signal is output from another top electrode.

Figure 6.16: Cross-section schematics of a serial-resonator configuration

The equivalent circuit model of this design can be constructed by piling up two BVD models serially. Nevertheless, with the help of EM3DS, which is the first 3D EM (electromagnetic) analysis software including modeling of FBARs with pure thickness excitation modes, we have simulated directly and compared the performances of the serial-resonator configuration and the conventional TFBAR device. The models for a conventional TFBAR and for our novel design are shown in Figure 6.17. In both cases,

the thickness of AlN film is $1.8\mu\text{m}$, the thicknesses of the bottom and the top electrodes are $0.2\mu\text{m}$ and $0.7\mu\text{m}$ respectively, the effective electrode area is $100 \times 100\mu\text{m}$ and the transmission lines CPW I with designed parameters listed in Table 6.1 are included. The gap spacing between the top electrodes is $150\mu\text{m}$. A 2-port analysis is basically performed by enclosing the DUT (device under test) in a perfect rectangular waveguide.

(a) simulation model for a conventional TFBAR structure

(b) simulation model for a serial-resonator structure

Figure 6.17: 3D EM simulation models for a TFBAR device and a corresponding serial-resonator device with CPW I designed in Table 6.1

The simulation results are expressed with the S-parameters S_{11} and S_{21} in dB unit and are displayed in Figure 6.18.

(a) simulated S-parameter results of TFBAR device designed

(b) simulation results of corresponding serial-resonator structure

Figure 6.18: Simulation results of TFBAR and corresponding serial-resonator structure

Compared with the simulation results of the serial-resonator structure with those of the conventional TFBAR, the serial and parallel frequencies are not influenced, the Q-factor

has been improved from about 118 to 230, the insertion loss of the serial-resonator structure has been degraded from -0.09dB to -0.29dB, and its return loss has also been degraded from -22.4dB to -16.9dB. In this proposed configuration, the two resonators serialized are identical and they have the same characteristic dimensions. Therefore, the operating frequency will not be changed greatly, and this configuration increases the equivalent electrical impedance to become about two times than that of the single resonator, which will make the matching network design be easier at resonance to some extent. The increase of effective vibrating area can also increase the acoustic impedance of the transducer and traps more acoustic wave within the vibrating body. It is considered that the serial-resonator structure will not greatly change the performance of the conventional TFBAR device, while it makes the fabrication much easier to carry out due to the absence of the etching of AlN layer. However, one obvious disadvantage of such proposed design is that a larger electrode area is required in fabrication for patterning and etching, and the dimensions of the final product will be much larger than that of the conventional TFBAR product. This design has been fabricated using our developed high performance AlN material and the relevant microfabrication processes in CMOS cleanroom, which will be presented in Chapter 7.

6.6 Summary

In this chapter, the working and design principles of TFBAR devices are introduced. Extensive simulations have been carried out and summarized based on FEM and characteristic impedance analysis using equivalent Mason model and our developed program. It is found that characterized by the thin film thickness, high acoustic velocity and low Q-factor of piezoelectric material, TFBAR devices can have high operating frequencies above GHzs, but low quality factors in the range of hundreds to thousands.

For such high frequency applications, the metal layer begins to constitute an increasingly greater percentage of the overall thin film resonator structure, and thus the metal layer becomes one of the main Q-detractors in the overall device design, and influences the frequency responses and the equivalent impedance characteristics to a great extent when either the thickness or the area of metal electrode changes. Based on these findings, two newly developed designs, i.e. serial-resonator configuration and electrode-isolation structure, have been proposed from the points of view of improving the fabrication ability and the Q-factor of current devices. The simulation results have demonstrated that these designs have better performance than that of the conventional devices. Based on simulation results and deposition parameters available for AlN growth, the design parameters of various TFBAR devices and microwave transmission lines have been determined. Development of high performance AlN piezoelectric material and TFBAR devices designed has also been carried out and this will be introduced in Chapter 7.

Chapter 7

Development, Fabrication and Test of AlN

Piezoelectric Material and TFBAR Devices

7.1 Introduction

For a TFBAR device, its best achievable quality factor is strongly dependent on the intrinsic Q values of the used piezoelectric materials when acoustic losses resulted from the attenuations and reflections of the metal layers and dielectric layers are eliminated. During fabrication, a poorly grown piezoelectric crystal will usually be highly stressed and will most probably contain a high density of grain boundaries, air pockets, impurities, etc. These defects will usually have dimensions comparable to an acoustic wavelength and will hence scatter or absorb the vibration acoustic wave. In general, improving crystal growth conditions could result in a significant reduction of power losses due to these defects. Therefore, high Q-factor is closely correlated with the growth conditions and the resultant properties of the piezoelectric materials (M. –A. Dubois *et al.*, 1998; M. –A. Dubois *et al.*, 1999; H. P. Löbl *et al.*, 1999).

To realize high performance TFBARs, researches on development of high quality AlN film with preferred crystal orientation and material properties, together with the requirements for optimal fabrication conditions (such as high deposition rate, high thickness and low residual stress), have been carried out firstly. This chapter will introduce our work on the development and characterization of AlN piezoelectric thin film, including the fabrication and preliminary test results of TFBARs. This chapter also

seeks to discuss and to provide possible solutions to the current problems associated with the development of high performance of TFBAR devices.

7.2 Preparation and Characterization of Piezoelectric Material

7.2.1 Introduction to Piezoelectric Material and Deposition Mechanism

Nowadays, the available piezoelectric materials for high performance TFBARs applications have been mainly concentrated on the polar materials with hexagonal wurtzite crystal class, such as AlN and ZnO (as shown in Fig. 6.1(b)), because thin films of these compounds could possess a strongly oriented polycrystalline fibered structure. ZnO is a potential candidate for such applications but it has some drawbacks due to which high electrical resistance, high breakdown voltage and low dielectric losses are difficult to achieve. As a promising semiconductor material currently being developed, AlN has been used as passivation and dielectric layers for various microelectronics, optics, surface acoustic wave devices and RFIC applications. Compared with ZnO, AlN would certainly be a good alternative for TFBARs, due to its excellent piezoelectric property, high acoustic velocity, wide-band-gap ($E_g=6.2\text{eV}$), high electrical resistivity ($>10^{14}\Omega\text{-cm}$), high breakdown voltage and low dielectric loss. When compared with conventional PZT piezoelectric material, although the electromechanical coupling coefficient of AlN film is nine times smaller than that of PZT film, its static dielectric constant is forty times smaller than the corresponding constant of PZT, together with its process compatibility with IC processes, which makes AlN better choice of piezoelectric material used for MEMS devices and for high frequency applications. In addition, its low thermal expansion coefficient ($4.6\text{ppm}/^\circ\text{C}$) and high thermal conductivity ($80\sim200\text{W/mK}$) provide opportunities for us to achieve a small thermal drift, a characteristic that is important for controlling the stability of internal stresses and the

desired frequency of TFBARs during fabrication. Table 7.1 shows some comparisons of the three piezoelectric materials commonly employed.

Table 7.1: Comparison of Main Material Parameters of AlN, ZnO and PZT

	Acoustic velocity v (m/s)	Electromechanical coupling coefficient k_t^2	Dielectric constant ϵ_r
AlN	11400	0.029~0.065	8.5
ZnO	6340	~0.078	8.8
PZT	4500	0.20~0.30	350

Although fabrications of ZnO and PZT film have been successfully accomplished in a number of laboratories worldwide, growth of AlN piezoelectric film has been proven to be a much more difficult task. A variety of the state-of-the-art techniques have been researched and developed for the realization of AlN thin films, including reactive evaporation, sputtering, cluster ion beam, molecular beam epitaxy (MBE), spray pyrolysis, etc. AlN films were managed to have grown using metal-organic chemical vapor deposition (MOCVD) at very high temperature (1150°C ~ 1250°C) (M. T. Duffy *et al.*, 1973). Although epitaxial AlN films fabricated in this way exhibited some promising properties suitable for TFBAR applications, such a high growth temperature and the substrates required (e.g. sapphire and Si(111)) were not compatible with the current IC technology. With the maturity of reaction mechanism and the development of microfabrication technology, sputtering method has gradually become a key approach and has to some extent been proven to be a success in the deposition of highly fiber-oriented AlN layers. Most efforts have been focused on magnetron sputtering of AlN preparation. An alternative technique is the reactive sputtering which has produced a preferred *c*-axis growth of AlN film at low temperature (H. Okano *et al.*, 1992).

Considering the advantages of reactive sputtering, the available facilities and the cost of microfabrication in CMOS cleanroom, we are focusing ourselves on developing AlN thin film using pulsed DC reactive sputtering technique. Deposition parameters are established through trial and error. As illustrated in Fig. 7.1, the AlN reactive sputtering

Figure 7.1: An illustration of the reactive sputtering in our process, where the Al atom is striped by the high-energy ion and reacts with the N atom to form AlN.

developed in our research is a hybrid procedure involving both physical and chemical reactions. Its reaction mechanism can be explained as follows. Firstly, mixed Ar and N_2 gas discharges with applied DC power supply and generates a plasma substance. The particles, including Argon ions (Ar^+) and Nitrogen ions (N^+), are energized in DC electric field, and then bombard the Al target, resulting in Al atoms being sputtered out. The sputtered Al atoms then bond with N atoms to form AlN molecules. This reaction can take place in plasma regions as well as on substrate surfaces. The energetic species, either as positive ions neutralized and reflected from the target or as sputtered negative ions that are accelerated away from the target, can impinge onto the substrate surface. These adatoms (Al, N or AlN) diffuse on the substrate surface and eventually settle down to a stable site to form the required AlN film. During this procedure, the AlN

material properties will be dependent on two factors: (i) transportation and reaction of adatoms in the area between the electrodes, and (ii) diffusion of adatoms on substrate surface. Although the actual detailed mechanism is still not very clear, these microscopic particle movements can be controlled by macroscopic process parameters. The first factor depends on the applied electric field, which is determined by the DC power and the mean free path (MFP) of molecules (determined by gas pressure). The second factor depends on substrate temperature. The adatoms diffusion on substrate surface is also significantly influenced by the incidence of energized particles, because kinetic energy may have been converted to thermal energy. AlN has two common phases, i.e., cubic (*c*-AlN) and hexagonal (*h*-AlN). It is widely accepted that hexagonal (*h*-AlN) is a closely-packed Wurtzite structure, and in the (002) orientation, its *c*-axis is perpendicular to the substrate surface and its crystal basal plane parallel to the substrate possesses the lowest surface energy and the maximum atomic density with either all aluminum or nitrogen atoms. Therefore, the nucleation takes place on *h*-AlN(002) easily, the growth is along *c*-axis and the (002) plane is the fastest growing plane (N. Fujimura *et al.*, 1993). In an ideal situation (adatoms have enough time and energy to reach the most stable position), the impinging atoms rearrange themselves at crystal site in (002) plane and accumulate along *c*-axis, and in this case, nonepitaxial polycrystalline *h*-AlN films normally exhibit a preferred growth in the (002) direction. From another point of view of device, it is also well verified that the better the AlN film grows along (002) orientation, the stronger the TFBAR responses and the lower the wave propagation losses are.

7.2.2 Development of AlN Film

Using the process described above, AlN piezoelectric films have been deposited onto different substrates by using Al as sputtering target with different Ar to N₂ ratios. These

thin films are deposited *in situ* at various substrate temperatures between 300°C and 500°C in order to improve structural properties of the AlN layers. The choice of substrate and its orientation are also very important to achieve highly oriented AlN thin film. The post thermal processing, i.e., the rapid temperature annealing (RTA), has also been used to further improve the crystalline properties of the AlN material.

Figure 7.2 shows the diagram of the Varian M2i modular sputtering system, which is used for our AlN deposition. Wafers are loaded into this system via dual cassette module, while AlN film is deposited in one of the process modules. The transfer module moves wafers between dual cassette module and process module. The deposition parameters, including the temperature, the gas flow rate, the applied DC power and the deposition time, are controlled by the computer.

Figure 7.2: Varian M2i modular sputtering system

Physically, an Al-Si-Cu (Al 98.5%, Si 1% and Cu 0.5%) target with 99.999% purity is first placed on cathode, while the substrate holder is connected to the anode and is grounded. The space between the cathode and the anode is typically 5~8cm. High purity Ar (99.999%) and N₂ (99.999%) gases are introduced into the deposition module. When a DC voltage is applied, the plasma is generated through gas discharge, leading to a

bombardment against the target by energized particles. The sputtered Al atoms are taken away from the target, react with N based particles, and eventually deposit onto substrate surface, resulting in a growth of AlN film.

In order to improve the purity of the film grown, high module vacuum is required. In our system, the base pressure in deposition module for AlN deposition is 2.0×10^{-8} Torr, and the base pressure of Al deposition module is 8.9×10^{-9} Torr.

The conventional DC power supply in this system has been replaced with a pulsed DC power supply because of the dielectric isolation of the AlN film. In a plasma-related deposition process of insulator material, charge accumulation frequently occurs on the target surface and aggravates as deposition continues, causing a potential configuration and a discharge condition to drift in time. To alleviate such charging effect on AlN insulator surface, pulsed DC power supply is adopted. The maximum power output in our process is 10kW and frequency can be adjusted in a range between 0 and 350kHz.

The key problem for the deposition of these films is to control precisely the crystal orientation and the properties on the various electroded surfaces. Two strategies have been executed in this work: AlN on Si (AlN/Si) and AlN on Al grown on Si (AlN/Al/Si). The first case is to investigate the basic mechanism and the process parameters of AlN film growth onto the bare Si substrate. In the latter case, the purpose is to investigate deposition of AlN on Al, which will be used as the bottom electrode in TFBAR devices. To form AlN/Al/Si structure, an Al film with a thickness from 1000Å to 7000Å is firstly deposited in one module, and then the processed wafer is immediately transferred to another module for AlN deposition. The deposition conditions for Al and AlN films are listed in Table 7.2 and Table 7.3, respectively.

Table 7.2: Deposition Parameters of Al Films

Target	Al-Si-Cu (99.999%)
Substrate	6" Si(100) wafer
Base pressure of deposition module (Torr)	8.9×10^{-9}
Substrate temperature ($^{\circ}\text{C}$)	150
DC power (kW)	2.4 ~ 9.1
Ar gas flow rate (sccm)	35
Deposition pressure (mTorr)	3.0

Table 7.3: Deposition Parameters of AlN Films

Target	Al-Si-Cu (99.999%)
Substrate	6" Si(100) wafer, Al/Si(100)
Base pressure of deposition module (Torr)	2.0×10^{-8}
Substrate temperature ($^{\circ}\text{C}$)	150 ~ 500
DC power (kW)	1 ~ 6
Ar gas flow rate (sccm)	20 ~ 80
N ₂ gas flow rate (sccm)	10 ~ 40
Deposition pressure (mTorr)	1.8 ~ 7.3
Deposition time (sec)	600 ~ 3000, depend on film thickness

7.2.3 Characterization of Properties of Deposited AlN Film

Having successfully deposited the AlN films using pulsed DC sputtering system, the properties of AlN films need to be analyzed. X-ray diffraction (XRD) is used as a direct means of evaluation of the crystal structure of the AlN film. A comparison between X-ray diffraction diagrams will indicate the optimal conditions for highly oriented AlN

deposition. The elemental compositions of AlN material are evaluated by sputtering and analyzing the sample surface of AlN thin film using Auger electron spectroscopy (AES) or second ion mass spectroscopy (SIMS). And the residual stress inside the film is measured by thin film stress and measurement system. Other characterization results regarding the properties of AlN film, such as refractive index and deposition rate are also introduced and discussed in this section.

7.2.3.1 Analysis of Crystal Structure of AlN Film

Primarily, the crystal structure of AlN films is characterized and analyzed as one of the most important material properties. Siemens D5005 x-ray diffractometer in a lock coupled (θ - 2θ) mode with an incident x-ray wavelength of $1.540\text{\AA}$ was used. The desirable crystal structure of AlN film for TFBARs application as discussed is the *h*-AlN with its *c*-axis perpendicular to its substrate. In such ideal case, the only representative peak expected is the *h*-AlN(0002) at a θ value of 36.04° . The crystal structure of AlN films have been studied systematically by recording the XRD patterns of the AlN films deposited at different conditions, from which the dependence of the XRD patterns on deposition parameters has been established.

- **DC power effect**

Figure 7.3 demonstrates the XRD patterns of AlN/Si and AlN/Al/Si wafers deposited at various DC powers. To eliminate the effect of thickness on the diffraction intensity, all the films were kept at the same thickness of $1.5\mu\text{m}$. The *h*-AlN(002), *h*-AlN(101), *h*-AlN(102) and *h*-AlN(103) peaks can be observed, indicating polycrystalline structure in these films. However, for the films deposited at 3kW and 4kW, *h*-AlN(002) peak is much stronger than others, indicating that a highly (002) oriented *h*-AlN film can be

obtained at intermediate DC powers. The temperature and pressure associated with each deposition are labeled as shown in the figures.

(a) AlN/Si substrates

(b) AlN/Al/Si substrates

Figure 7.3: XRD patterns under different DC power and substrates

However, the orientation preference pattern changes when the film thickness is increased to $2.5\mu\text{m}$ under the same deposition conditions. As shown in Fig. 7.4, the h -AlN(002) peak intensity in the film deposited at 3kW becomes weaker, whereas a strong h -AlN(002) peak appears in the film deposited at 2kW compared to the diffractograms shown in Fig. 7.3(a). This may possibly be due to the change of electric field configuration because of the charging effect on AlN surface, leading to a change in atom transportation and deposition rate. However, such condition may not necessarily be true and further investigation in this area is necessary.

Figure 7.4: XRD patterns of AlN films deposited on Si at various DC powers.

The film thickness is $2.5\mu\text{m}$

- **Substrate temperature effect**

The temperature dependence of the crystal structure of the AlN/Si films is shown in Figure 7.5, which reveals the preferred orientation of (002) for the films deposited at temperatures below 400°C . A temperature at 530°C has led to a deterioration of the

orientation preference. These experiments were carried out at high deposition pressure (7.3mTorr) and high DC power (4kW). Further investigation has found that at a low deposition pressure of 1.8mTorr and a low DC power of 1kW, high (002) orientation could be obtained at a temperature as low as 150°C. The temperature effect on crystal structure may be explained as that the Al and N adatoms have sufficient mobility to form *c*-axis oriented structure even at a temperature of 200°C or lower, whereas a substrate temperature at 530°C leads to degradation of film quality. Similar phenomenon was also reported by W. Y. Chiu *et al.* (2002), who attributed this degradation to the establishment of a lower energetic state at high atom mobility.

Figure 7.5: XRD patterns of AlN films deposited at various temperatures with a DC power of 4kW and film thickness of 1.5μm

- **Gas pressure effect**

Figure 7.6 illustrates the XRD patterns of AlN films grown on Si(100) substrate at various gas pressures ranging from 1.8mTorr to 7.3mTorr. The DC power was kept 1kW, the substrate temperature was set at 150°C, and the Ar:N₂ flow rate ratio was fixed at 2:1.

The thickness of films was 5000Å. It is obvious that h -AlN(002) peak intensity is strongly dependent on the pressure, and decreases dramatically as the pressure increases. At low pressures, the AlN film is highly oriented with the preferred orientation of (002). There are two spurious peaks occurring 2θ values of 61.8° and 65.9° and they are not originated from AlN film. Although the orientations of these two peaks are not determined, they are believed to be related to the substrate orientation.

Figure 7.6: XRD patterns of AlN films grown at various gas pressures, while Ar:N₂ flow rate ratio was kept as 2:1.

- *Ar and N₂ flow rate ratio effect*

Keeping the gas pressure at 7.3mTorr, the substrate temperature at 400°C, the DC power at 3kW, the XRD scans of AlN films deposited on Si(100) at various Ar:N₂ flow rate ratios ranging from 1:2 to 5:1 have been recorded and are shown in Fig. 7.7. The thickness of films in this case was 1μm. It is clear that at Ar:N₂ ratios of 2:1 or 1:1, a highly (002) oriented AlN film could be obtained.

Figure 7.7: XRD patterns of AlN films grown at various Ar and N₂ flow rate ratios

7.2.3.2 Analysis of Morphology of AlN Film

The morphologies of growth of AlN films can be observed by scanning electron microscopy (SEM) for cross section, thickness measurement and for top view observation. Typical SEM cross sectional images of AlN/Si and AlN/Al/Si are demonstrated in Figure 7.8, in which the columnar structure of AlN film can be observed either on Si or Al. In Figure 7.8(b), clear interface between AlN and Al indicates a smooth Al surface.

(a) AlN/Si structure

(b) AlN/Al/Si structure

Figure 7.8: Typical SEM cross sectional images of different structures

Fig. 7.9 provides a direct evidence on the gas pressure effect on AlN crystal structure deposited on Si. It can be seen from these SEM photos that as the deposition pressure increases from 1.80mTorr to 7.3mTorr, the AlN grain size decreases from 100nm to 10nm, and in the meantime the structure of the AlN becomes looser.

(a) under 1.80mTorr

(b) under 4.05mTorr,

(c) under 7.3mTorr.

Figure 7.9: SEM top view images of AlN/Si deposited at 150°C, 1kW and under different gas pressures, the magnification is 50000.

7.2.3.3 Measurement of Refractive Index of AlN Film

The refractive index of AlN film is deduced by measuring the $\cos \mathbf{D}$ ($\mathbf{D}$, the phase of refraction coefficient) and $\tan \mathbf{Y}$ ($\mathbf{Y}$, the ratio of two values of reflection coefficient in both polarization) with the ellipsometry. The measured data are curve fitted using Chauchy dispersion equation to find out a credible refractive index (n) as well as the thickness and the extinction coefficient (k) of the AlN film, provided the error resulting from the curve fitting is small enough. The incident wavelength used in this measurement is 6320Å. The range of refractive indices is dependent on crystal structure of the film. In general, a value ranges from 1.8 to 1.9 is for amorphous film, that from 1.9 to 2.1 is for polycrystalline film and 2.1 to 2.2 for single crystalline film (Levinshtein *et al.*, 2001).

In our experiment, the refractive indices of AlN/Si wafers have been measured, and Figure 7.10 presents the variation of measured refractive index values with applied DC

powers, in which the substrate temperature, the gas flow rates and the film thickness are indicated in the figure, together with the curve fitting error values associated with each measurement point. At a DC power range from 2kW to 4kW, the refractive indices measured were in a range of 2.04 to 2.10, implying a polycrystalline structure of the films. The higher index n values at 3kW and 4kW than that at 2kW could be attributed to the increase of packing density within the compact structure of the film. The variation of the n values is consistent with the XRD results shown in Fig. 7.3(a) that DC powers of 3kW and 4kW produce a higher orientation preference when the thickness of the film is less than $2.5\mu\text{m}$. For the film deposited at 6kW, a high n value of 2.26 is not consistent with the XRD results shown in Fig. 7.3. However, the fitting error in this case is 0.11, implying that this estimated n value is less reliable. It is also found that the fitting error increases with film thickness. A reliable fitting result could be obtained with the film thickness less than $2000\text{\AA}$.

Figure 7.10: Refractive indices variation with applied DC power

7.2.3.4 Analysis of Residual Stress in AlN Film

The total residual stress in films can be written as the sum of the intrinsic stress and the thermal stress:

$$\mathbf{S} = \mathbf{S}_{\text{int}} + \mathbf{S}_{\text{th}} \quad (7-1)$$

The intrinsic stress results from the structure of the growing films, such as chemical reaction, doping, lattice mismatch during rapid deposition. The thermal stress is due to the difference of coefficients of thermal expansion (CTE) between the film and its substrate:

$$\mathbf{S}_{\text{th}} = E_f (\mathbf{a}_f - \mathbf{a}_s) \Delta T \quad (7-2)$$

where E_f is the Young's modulus of the film, $\mathbf{a}_f$ and $\mathbf{a}_s$ are CTEs of the film and the substrate, and ΔT is the temperature difference between deposition and measurement (S. Wolf and R. N. Rauber, 2000). Much theoretical calculation and experimental work on intrinsic stress has been carried out. It is commonly accepted that tensile stress is due to a porous and open microstructure, while compressive stress is attributed to a dense structure with impurity addition (H. Windishmann, 1991; I. H. Kim and S. H. Kim, 1995). And energetic particle bombardment on the film surface may favor compressive stress and denser microstructure. Transition from tensile to compressive stress has been observed as input power increases (K. Kusaka *et al.*, 2000). It is also believed that a high deposition rate can affect the intrinsic stress via the shortening the movement time of adatoms, leading to the formation of porous microstructure. Similarly, residual stress will also inevitably develop in the AlN film due to the mismatch of the lattice parameters and the coefficients of thermal expansion between the film and the substrate. High residual stress in a film may cause micro-cracks and even result in film peeling off from the substrate. Therefore, stress control is also essential for AlN film formation.

In this work, the pressure influence on the residual stress of AlN/Si films has been investigated and residual stresses have been measured by using the thin film stress and measurement system. As shown in Fig. 7.11, the residual stress values have been found to be tensile in a range from $1.1 \times 10^9 \text{ dyn/cm}^2$ to $4.0 \times 10^9 \text{ dyn/cm}^2$ for a AlN film deposited onto Si substrate. The residual stress increases with gas pressure first and it then drops when gas pressure is further increased. A slight stress relief has been observed 24 hours after deposit and this may be attributed to the crystalline slip (S. Wolf and R. N. Rauber, 2000) or to the surface oxidation (H. Windishmann, 1991).

Figure 7.11: Relationship between residual stress and deposition pressure. The solid circle is the immediate data after deposition at 400°C. The open circle is data measured after 24 hours. The solid square is for the immediate data after deposition at 150°C, and DC power was 1kW.

Thermal stress s_{th} can be calculated using equation (7-2), assuming the CTE of Si to be $4 \times 10^{-6}/\text{K}$, of Al to be $20.3 \times 10^{-6}/\text{K}$, of AlN to be $5.27 \times 10^{-6}/\text{K}$, and the Young's modulus of AlN film to be 300GPa (Gregory, 2000; NSM Archive, 2003). For AlN/Si deposited at 400°C, the thermal stress s_{th} has been found to be $1.44 \times 10^9 \text{ dyns/cm}^2$; for AlN/Al/Si

deposited at 400°C, the s_{th} is 1.71×10^{10} dyns/cm², and for AlN/Al/Si deposited at 150°C, the s_{th} is 5.85×10^9 dyns/cm².

7.2.3.5 Results of Micro-cracks in AlN Film Deposited on Al/Si Substrates

High residual stress may cause micro-crack in AlN film. For AlN film deposited on Si wafer, no such problem has been encountered, and the AlN surface is smooth. However, for AlN/Al/Si, as shown in Figure 7.12 (a), severe cracks can be observed and the AlN

(a) deposition conditions: DC power for Al deposition was 3.64kW, DC power for AlN deposition was 2kW, $T_s=400^\circ\text{C}$, Ar:N₂= 80:40(sccm).

(b) deposition conditions: DC power for Al deposition was 2.42kW, DC power for AlN deposition was 1kW, $T_s=150^\circ\text{C}$, Ar:N₂= 20:10(sccm).

Figure 7.12: Micrographs of surface of AlN/Al/Si wafers under different deposition conditions, the magnification is 200.

surface is quite rough. The thicknesses of the Al and the AlN layers are 3000Å and 2.5μm. The deposition rates set for Al and AlN during deposition were 7000Å/min and 1000Å/min respectively. The appearance of micro-cracks is probably attributed to three reasons: (1) a rough Al surface and hence poor AlN quality due to too high Al deposition rate; (2) a loose AlN structure led by high AlN deposition rate; (3) a remarkable thermal stress in the AlN film induced by a large difference between the CTE constants of Al

and AlN at high AlN deposition temperature. Based on these considerations, three strategies have been employed: reduction of AlN deposition rate, reduction of Al deposition rate, and lowering down of AlN deposition temperature. An example of improvement of surface morphology of AlN/Al/Si can be observed from Figure 7.12(b) when optimized deposition parameters, which are shown in Table 7.4, are used. Eventually, with these parameters, a crack-free AlN film on Al/Si substrate has been achieved.

Table 7.4: Parameters for Crack-free AlN/Al/Si Deposition

Temperature (Al)	150°C
Ar flow rate (Al)	35sccm
Deposition pressure (Al)	3.0mTorr
DC power (Al)	2.42kW
Deposition rate (Al)	1600Å/min
Temperature (AlN)	150°C
DC power (AlN)	1kW
Ar flow rate (AlN)	20sccm
N ₂ flow rate (AlN)	10sccm
Deposition pressure (AlN)	1.80mTorr
Deposition rate (AlN)	420Å/min

In Figure 7.12, the AlN/Al/Si wafer has a Al thickness of 3000Å and AlN thickness of 2.5µm. Furthermore, crack-free AlN film with thickness as large as 4.3µm has already been successfully deposited on Al/Si substrate. Similarly, XRD analyses have indicated the highly preferred orientation along its *c*-axis in thus deposited films, as shown in Figure 7.13, in which the thicknesses of AlN films under test are 2.5µm and 4.3µm, respectively. Due to high AlN thickness, the underlying Al diffraction signal becomes too weak to be observed and the strong peak at 65.9° is presumably from Si substrate.

Figure 7.13: XRD patterns of AlN/Al/Si samples

Comparison between thermal stress values clearly indicates the existence of micro-cracks in the AlN film deposited on Al/Si substrate at a high temperature of 400°C. While for those AlN films deposited on Si at 400°C or on Al/Si at 150°C, thermal stresses become so small that micro-cracks can be avoided.

7.2.3.6 Composition Analysis of AlN Film

AlN films were deposited on Si at various Ar and N₂ flow rate ratios, while keeping other deposition parameters as constants. Figure 7.14(a) shows their surface chemical elemental fractions measured using AES. The Al and N compositions are in a range of 40% ~ 50%, which translates to a Al/N atomic ratio to be from 0.78 to 1.25 (referred to Fig. 7.14(b)). For the film deposited at 400°C, 7.3mTorr and 3kW, around 10% O was detected. As the temperature, the deposition pressure and the DC power are reduced to 150°C, 1.8mTorr and 1kW, the O composition in the film is reduced to less than 5%. The correlation between the O composition and the deposition parameters has yet to be established, and we surmise the reduction of O composition is probably attributed to the reduction in temperature and deposition pressure. It is also notable that compositions do

not vary with the Ar:N₂ flow rate ratio at low temperature, low pressure and low DC power. However, due to the insulation of AlN material, the charging effect on AlN surface caused by electron beam incidence might affect the measurement results. Therefore, second ion mass spectroscopy (SIMS) is probably a better way for AlN composition analysis in this case.

(a) compositions of AlN films deposited at various Ar and N₂ flow rate ratios

(b) Al/N composition ratios varied with Ar:N₂ flow rate ratios. The solid symbols correspond to the film deposited at 400°C, 7.3mTorr and 3kW. The open symbols correspond to the film deposited at 150°C, 1.8mTorr and 1kW.

Figure 7.14: Compositions of AlN films under different deposition conditions

7.2.3.7 Deposition Rate Analysis

The deposition rate is determined by target sputtering and atom transportation in the deposition chamber. To date, most of the reported deposition rates of AlN film are less than 100Å/min. However, for batch industrial production, a higher deposition rate is obviously required. In this experiment, the deposition depth is measured by the mechanical probe which scans the deposition plane and records the stage difference between the substrate and the patterned film. The deposition rate is the depth of the film grown divided by the deposition time. For a given gas pressure and Ar:N₂ flow rate ratio, Figure 7.15(a) shows a linear increase of deposition rate with the applied DC power in our system, and a maximum deposition rate of 1500Å/min can be achieved at 6kW. In such cases, AlN films are deposited on Si(100) wafer at 400°C with Ar and N₂ flow rate of 80sccm and 40sccm. Similar results of linear increase of deposition rate were also obtained in H. Y. Joo *et al.* (2000). Figure 7.15(b) demonstrates an increase of deposition rate with Ar/N₂ flow rate ratio. Further investigation has indicated that the deposition rate is not affected by the substrate temperature, nor by the substrate types (Si or Al/Si).

(a) under different applied DC power

(b) under different Ar:N₂ flow rate ratio

Figure 7.15: Variation of deposition rate with different deposition conditions

7.2.4 Summary on the Development of AlN Film

In this part of the work, crystal structures of AlN films deposited under various conditions have been systematically studied. The dependence of XRD patterns on the deposition parameters, including the DC power, the substrate temperature, the gas pressure, and the Ar:N₂ flow rate ratio has been established. It is observed that highly oriented AlN films with preferred orientation along *c*-axis can be deposited at low DC powers (1kW~4kW), low temperatures (150°C~400°C) and low gas pressures (1.80mTorr~4.00mTorr). Additionally, Ar:N₂ flow rate ratio also has influence on the orientation preference of the film, that is, intermediate Ar and N₂ ratio (1:1~2:1) leads to a highly *c*-axis oriented growth.

The crystal structure of AlN films is determined by the kinetic energy of adatoms and the diffusion time on substrate surface. When the DC power is low (2kW) and the pressure is high, the adatoms do not have sufficient kinetic energy for rearrangement, leading to a poor film quality. On the other hand, an extremely high DC power (6kW) will lead to a very high deposition rate. The time for adatoms diffusion in this case is too short for them to reach their stable positions. As a result, strong *h*-AlN (002) peak can only be observed in XRD patterns for intermediate power supplier, as shown in Fig. 7.3.

Gas pressure is another important external parameter which influences the adatoms transportation process. The mean free path of gas particles is inversely proportional to gas pressure. High gas pressure causes frequent collisions and hence energy losses in the scattering processes. Fig. 7.6 and Fig. 7.9 shown earlier provided a clear information about pressure effect on crystal quality. Improvement of orientation preference and grain size has been observed as gas pressure decreases.

The influence of the fraction of Ar gas in gas mixture involves gas discharge. As it is generally more difficult to have a discharge in a molecular gas than in a noble gas, Ar gas is easier to become discharged than N₂ gas. Increase of the fraction of Ar causes high plasma density, high particle energy, and in turn high deposition rate, as shown in Fig. 7.15(b). Therefore, at a low fraction of Ar, the energy level of the species is not sufficient to realize a *c*-axis growth. However, a high fraction of Ar leads to a high deposition rate, and atom diffusion time becomes too short for *c*-axis growth. Such conclusion has been supported by the results shown in Fig. 7.7.

Taking into consideration of the various factors that affect the AlN deposition process, in order to achieve a highly (002) orientation and crack-free AlN film required for TFBAR

application, optimal conditions have to be established, such as those shown in Table 7.4. These are low pressure (1.8mTorr), low temperature (150°C) and intermediate Ar:N₂ flow rate (20:10 sccm). Using such process parameters, AlN film suitable for TFBARs applications has been obtained and its material properties are shown in Table 7.5.

Table 7.5: Summary of AlN Properties Achieved

	Highly (002) Orientation	Stoichiometry	Refractive Index	Deposition Rate	Thickness	Crack Free
Achieved properties	Yes	0.78~1.25	2.04~2.10	200~1500Å/min	< 4.3µm	Yes

7.3 Fabrication and Preliminary Results of the Proposed TFBAR Design

Based on the analysis and simulation results in Chapter 6, together with the development of AlN piezoelectric material discussed so far in this chapter, successive progresses had been made on the research and development of the microfabrication processes of the proposed TFBAR designs, including resonators, filters and relevant transmission lines. Compared with fabrication processes of µ-mechanical resonators discussed earlier, processes required for TFBARs fabrication turn out to be much simpler in layout designs, fewer steps, and the achievable device performance depends mainly on the quality of the AlN film grown. This section will discuss the fabrication and preliminary results of the proposed TFBAR design.

7.3.1 Layout Design

(a) example of symmetrical design of serial-resonator configuration. The area of electric pad is $100 \times 100 \mu\text{m}$, the center distance between two neighboring pads is $150 \mu\text{m}$, and the window for backside wet etching is $1055 \times 1055 \mu\text{m}$. Considering possible alignment error, the boundary of bottom electrode is $5 \mu\text{m}$ bigger than the top electrode.

(b) example of filter design constructed by single TFBARs. A T-type configuration is demonstrated.

Figure 7.16: Examples of layout designs for TFBARs and filter fabrication

There are in total three masks involved in the device fabrication of present design, and they serve as the bottom electrode pattern, the top electrode pattern and the backside etch

pattern. Verification structures on the effects of different areas and shapes of electrodes, of different types and characteristic impedances of transmission lines, and of different configurations of filters have been designed. Figure 7.16 shows two examples of T type filter and resonator with serial-resonator configuration and rectangular electrode shapes. In this design, there are two different backside patterns, which are used to form the suspended membrane. One is used for wet etching (solid-lined box) and another for dry etching (dash-lined box). In our mask set, the transmission line from pad to TFBAR devices is CPW and the optimized dimensions to achieve 50 Ω characteristic impedance are given earlier in Table 6.1.

7.3.2 General Process Flow

Figure 7.17: General process flow for TFBARs fabrication

The general process flow in our TFBARs fabrication is schematically shown as Fig. 7.17. Throughout the flow of the processes, the deposition of piezoelectric layer is the most

critical process to ensure the success of a device's fabrication. The underlying principles and the experimental results of our pulsed DC reactive sputtering developed for AlN film growth have been discussed earlier in this chapter. Other processes, such as wafer processing and test, metal deposition and etching, are quite mature with the present CMOS cleanroom technologies. The detailed steps adopted in our work will be introduced in the following section.

7.3.3 Fabrication Process

Figure 7.18 schematically illustrates the structural configurations and the relevant parameters of the fabricated devices, in which a Silicon Nitride (Si_3N_4) layer serves both as a support membrane and an etch barrier layer, and a Silicon Oxide (SiO_2) layer is used as the isolation layer. The process starts with 6" N-type Si wafers. To reduce the parasitic contributions from mobile charges in the normal low-resistivity (1-100 $\Omega\cdot\text{cm}$) Si substrate, high-resistivity (1000-20000 $\Omega\cdot\text{cm}$) Si substrate is used for the fabrication of the device.

Figure 7.18: Cross-section configuration and parameters of fabricated device

The main process steps are described as follows and the corresponding schematics are shown in Figure 7.19:

1. To start with, wafer marking and cleaning with 15:1 HF solution for 10 seconds,

then DI water rinsing for 6 times and spin drying.

2. Standard alignment mark pattern, photolithography and development for fiducial mark fabrication, which is used as a common alignment base in subsequent processes. Then the wafer is cleaned again with 15:1 HF solution for 10secs, DI water flushing for 6 times and spin drying again.
3. A 1500Å thick Si_3N_4 film is grown successively in a standard furnace under 780°C, 200 sccm flow rate of NH_3 reaction gas and for nearly one-hour thermal reaction, as illustrated in Fig. 7.19(a).
4. Next, an oxide layer with compressive internal stress is deposited to compensate the tensile stress in the nitride layer. In a furnace chamber with 150mTorr base pressure, 720°C, 100sccm flow rate of TEOS for about half an hour reaction, a 2000Å thick oxide layer is deposited on the nitride layer. This layer, together with the previous nitride layer, serves as the electric isolation layer for high frequency applications. The device after this reaction is shown in Figure 7.19(b). Finally, the wafer is dipped into a 100 °C Piranha solution ($\text{H}_2\text{SO}_4:\text{H}_2\text{O}_2 = 3:1$) to rinse for about 5 minutes.
5. To balance the remnant stress in the previous depositions of nitride and oxide layers, a backside deposition of a nitride layer is followed. In a 25mTorr chamber of 420 °C, with the flow rate of reaction gases $\text{N}_2:\text{SiH}_4:\text{NH}_3 = 1800:195:75$ sccm and for 8secs reaction, a PECVD deposition is carried out to produce a 1000Å nitride layer onto the backside of the Si substrate.
6. The wafer is then transferred to our modular sputtering system, i.e. Varian M2i PVD chamber, to be deposited a 2000Å blanket Al metal for subsequent bottom electrode pattern, as shown in Fig. 7.19(c). The optimized deposition parameters used are listed in Table 7.4. To improve the adhesion of Al, a thin film of Ti with 500Å thickness is deposited first between the oxide layer and the Al layer.

7. In succession, the wafer with deposited Al layer is coated with 2 μ m thick positive photoresist, photolithoprinted with designed mask and exposed with 180mj/cm² UV energy, and subsequently developed with specific developer. The patterned wafer is sent to the etching chamber, which, for Al etching, has a chamber pressure of 200mTorr and a RF power of 750W. The flow rate of etchants BC₃:C₂ is 40:25 sccm. Under these process parameters, an etching rate about 4000Å/min has been achieved. After 30secs of etching, the wafer is then transferred into another chamber for photoresist strip with O₂ plasma. The pressure in this chamber is 2Torr, the RF power is 1400W and the flow rate of O₂ gas is 3000 sccm. After Al etching, a 20 mins cleaning process is needed in ACT690 solution to remove the superficial particles meanwhile to prevent Al film from attacking by conventional cleaning solutions. The final resultant device after this step is shown in Fig. 7.19(d).
8. The wafer is again sent into M2i for AlN deposition. Using the relevant parameters listed in Table 7.4, a 2 μ m thick AlN film is deposited at 150 °C for a reaction of about 50mins. The result is plotted in Fig. 7.19(e).
9. The processes of 6 and 7 are then repeated here for a 7000Å PVD Al deposition and the top electrode pattern. The schematics of such processes are shown in Figure 7.19(f) and (g).
10. After the cleaning process, the backside nitride layer of the wafer is patterned and etched using RIE (reactive ion etching) method to open a window for subsequent Si substrate etching. The reaction chamber has a pressure of 60mTorr, a power of 235W and a flow rate of combined gas CHF₃:O₂ 31:2.6 sccm. Under these process parameters, the etch rate for nitride layer is about 420Å/min, and the etching will stop as soon as the Si substrate is reached.
11. The last step in a wafer-level fabrication is the etching of the unprotected Si

substrate. Using the nitride layer as hard mask, KOH wet etching or DRIE dry etching can be carried out to form the suspended piezoelectric membrane. A 35% in weight KOH solution at 75 °C is a common etchant for Si etching in microfabrication, while DRIE is getting more and more popular for deep Si etching because of its prominent advantages of smaller etching area, higher etch rate, better vertical and sidewall profile, more accurate dimension control and cleaner to device and environment. Whichever etching method is used, the Si etch will stop once it reaches the oxide and nitride layer. Afterwards, the wafer is sent to the RIE etcher chamber again to remove the frontside nitride and oxide layers and consequently to form the suspended membrane. The final device after this process is schematically shown in Fig. 7.19(h).

(a) 1500 Å thick nitride layer (Si_3N_4) deposition to form an etching stop and electric isolation layer

(b) TEOS LPCVD deposition to form SiO_2 isolation layer

(c) PVD deposition of 2000 Å thick Al at 150 °C

(d) Al etching and photo resist strip to form bottom electrode

(e) AlN reactive sputtering at 150 °C

(f) Al PVD deposition at 150 °C

(g) Al etching and PRS to form top electrode pattern

(h) Si backside etching to form the suspended membrane

Figure 7.19: Schematic illustrations of main process steps for TFBARs fabrication

Following these process steps, AlN films have been grown and TFBAR devices have been fabricated. In Figures 7.20 and 7.21, some TFBAR devices are illustrated.

(a) frontside view of resonator

(b) backside view of resonator

(c) SEM photo of fabricated resonator with highly (002) oriented AlN film

Figure 7.20: Optical and SEM images of fabricated TFBAR resonator with serial-resonator configuration and rectangular electrode pattern

Figure 7.21: Other examples of fabricated TFBAR devices

Although the deposition parameters for the growth of AlN films have been achieved, the stress problem in device fabrication has not yet been resolved to date. It has been found that the stress in a TFBAR device strongly depends on every deposition condition and the thermal history during fabrication. In our processes, it has been observed that a large tensile stress in AlN film has caused warps and cracks in membranes (as shown in Figure 7.22) when the Si substrate and the nitride layer underneath were removed, leading to an unbalance of internal stress distributions in different layers.

Figure 7.22: Fracture at joint of different shapes after backside opening

Generally, annealing is an effective way to remove a variety of stress gradients in thin films. In our study, using this process, intrinsic stress can be annealed out to some extent. However, high temperature annealing will damage Al metal because the melting point of this metal is only about 650°C, and the annealing is generally not capable of eliminating stresses due to thermal mismatch effect. Some amount of stress due to thermal mismatch is unavoidable when working with materials with different coefficients of thermal expansion. This means further optimization of fabrication process parameters for TFBAR devices is required and work in this direction is currently continuing at the Institute of Microelectronics, Singapore. Based on the achieved experiences and results, our solutions to stress problem have been to focus on the following:

- further optimization of AlN and Al films deposition conditions;
- optimization of processes for TFBAR device fabrication, including applications of new materials;
- adoption of new structural designs and optimizations of design parameters, such as the introduction of narrow trenches (as shown in Figure 7.23) to divide and isolate the stress effect in a membrane from one section to another.

Figure 7.23: Different designs to reduce the stress effect

7.4 Summary

In this part of work, development of high performance AlN piezoelectric material has been carried out firstly for high-Q TFBARs applications. Using newly developed pulsed DC reactive sputtering method, highly oriented AlN films have been grown on Si and Al/Si substrates. The effects of various influential factors on properties of AlN material have been analyzed systematically, and the deposition parameters have been optimized by trial and error for developing AlN film with preferred crystal orientation along c -axis, low growth temperature, fine grain size and low residual stress.

Successive work for the development of TFBAR devices designed earlier has also been carried out. It is found that the processes required for TFBARs fabrication have fewer fabrication steps and simpler layout designs, and much depend on the results of the AlN film grown. Although the optimal growth conditions for AlN development have been attained, many problems occurred when fabricating the device as a whole. Especially, the internal stress problem built in different film deposition history becomes severe due to thermal mismatch in different layers deposited, and leads to the crack of the final devices after the silicon substrate is removed. So far, no successfully completed device has been realized, while more in-depth research will be carried out to solve these problems in our future work.

Chapter 8

Conclusion and Recommendation

8.1 Conclusion

Aiming at the overall objective of using MEMS technologies to realize new microresonators with high frequency and high quality factor, extensive yet in-depth researches and developments have been carried out in the area of development of innovative solutions to the MEMS device design, fabrication, materials development, test and other relevant engineering approaches that directly or indirectly address the performance issues of high-Q MEMS resonators for RF applications. During the research and development, two different but interrelated types of microresonator have been identified to be the main focused area of research for this project. They are: (i) micromechanical resonators, and (ii) thin film bulk acoustic wave resonators. Around the work done on the development of these two types of resonator, achievements and conclusions can be summarized as follows.

I) Research and development of micromechanical resonator

This part of work is initiated based on the beam resonator to target at the investigation of fundamental issues and possible approaches that can be used to improve present resonant frequencies and performances of micromechanical resonators which can be realized by using the existing MEMS technology.

Through different mechanical and electrical modeling and simulations, extensive studies on areas such as the miniaturization of characteristic dimensions, the excitation of higher

order harmonic frequencies as well as the reduction of effective mass, have been analyzed and discussed. Within the conventional dimension limitation of microfabrication, beam resonator structures with various geometrical configurations which are extensions of current designs for higher frequencies have been designed and simulated. Resonator structures similar to disk-shape resonator and bar-type resonator with higher order vibration modes have also been designed and simulated. The simulation results have shown that these proposed resonators can achieve higher natural frequencies, but their small vibration amplitudes need to be improved so that they can be effectively detected using present electrical signal detection technology of small output current or voltage. Based on the simulation results, it is concluded that the achievable frequency application range of current micromechanical resonator falls within HF to VHF applications.

A new equivalent electrical model has also been developed to eliminate the antiresonance effect by subtracting the static capacitance from the equivalent oscillation system of μ -mechanical resonator, and the relevant simulation result has demonstrated its workability. Further research on this proposal will be carried out to realize better electrical performance of devices through system-on-chip technology.

The development of micromechanical resonators designed has been achieved by using conventional poly-Si micromachining technology and the state-of-the-art SOI technology respectively. Firstly, a new polysilicon surface micromachining process has been researched and developed successfully to fabricate various μ -mechanical resonators designed early in batches. This process is compatible with current CMOS technology and is available for future industrial development.

To improve the performance of polysilicon based resonators, SOI based resonators and related fabrication processes have been developed subsequently. Preliminary results have revealed that our method is feasible and can achieve better device performances in design, fabrication and dynamic responses, while further improvement in micromachining and packaging need to be carried out to make this technology a mature one for commercialization.

Experimental studies on various resonator designs, fabrications and correlation with simulation results have been carried out using typical RF measurement set-up in vacuum environment. The measured 1st natural frequencies of the clamped-clamped beam resonator range from several megahertz to hundreds of megahertz, and the measured Q-factors change from several hundreds in atmospheric condition to several thousands in vacuum condition.

Alongside with those studies, a new image measurement method and system for 3D microstructure inspection has also been developed and applied in our work, which shows the characteristics of adequate accuracy, high reliability and convenient measurement requirements.

According to achieved results of design, fabrication and measurement, the advantages of micromechanical resonators can be summarized as follows,

- simple and multiform structural configurations, and orders of magnitude smaller in geometrical size;
- conventional and batch fabrication capacity, and IC-compatible micromachining processes;

- electrostatic actuation with low power consumption;
- the range of the achieved 1st natural frequency is from several megahertz to hundreds of megahertz, leading to potential applications for HF (3MHz–30MHz) and VHF (30MHz–300MHz) bandwidth devices such as resonators and filters.

However, being limited to our present capabilities of fabrication, RF signal detection and packaging, other important characteristics such as possible large reduction in power consumption and potentially higher quality factor have not yet been tested and verified. By improving the design of structural and electrical components, optimizing the microfabrication process and employing new micro-detection technology, the performance of μ -mechanical resonators in frequency response and loss dissipation can be enhanced in future work.

II) Research and development on TFBAR technology

Considering the limitation of achievable frequency range of foregoing μ -mechanical resonators, and the good characteristics and potential commercialization of TFBARs, applicable researches in this field have also been carried out. The work on TFBAR devices begins with the improvement of quality factor of similar devices at high frequencies. Extensive simulations have been carried out and analyzed based on FEM and characteristic impedance analysis using equivalent Mason model and our developed software program. It has been found that characterized by the thin film thickness, high acoustic velocity and low Q-factor of piezoelectric material, TFBAR devices can have high operating frequencies up to GHzs, but low quality factors in the range of hundreds to thousands. At such high frequency applications, the metal loading effect becomes one of the main Q-detractors in the overall device design, and thus influences the frequency responses and the equivalent impedance characteristics of devices designed to a great

extent.

Based on simulation results, two newly developed designs, namely, serial-resonator configuration and electrode-isolation structure, have been proposed from the point of view of improving the processability and the Q-factor of current devices. The simulation results have demonstrated that these designs have better performance than the conventional TFBAR devices.

Development of high performance AlN piezoelectric material has been carried out firstly for high-Q TFBARs applications. Using newly developed pulsed DC reactive sputtering method, highly oriented AlN films have been grown on different substrates. The effects of various influential factors on properties of AlN material have been analyzed systematically, and the deposition parameters have been optimized by trial and error for developing AlN film with preferred crystal orientation along *c*-axis, low growth temperature, tiny grain size and low residual stress.

Successive work for the development of TFBAR devices designed earlier has also been carried out. It is found that, although the optimal growth conditions for AlN development have been attained, many problems still exist when fabricating the device as a whole, especially, the problem of internal stress. So far, successfully completed devices have yet to be realized, while more in-depth research will be carried out to solve these problems in our future work.

8.2 Recommendation

According to current research and development of different types of microresonator, the micromechanical resonator has relatively high quality factor but limited operating

frequency. On the other hand, the main problem of high frequency TFBAR device is its low Q-value. Aiming at these different problems associated with each of these devices, our future work would have different emphases.

- i) research on further improving the performance of the micromechanical resonators, which includes,
 - further improving the design of structural and electrical components to reduce mechanical and electrical losses;
 - further optimizing microfabrication processes for both polysilicon and SOI based technologies, and improving the related packaging technology;
 - development of advanced integrated measurement technology, such as STM technology, for tiny signal detection, and further improvement of image measurement system to enhance its applicable range and accuracy;
 - practical realization of the proposal tactic for eliminating antiresonance effect through integrating MEMS devices with corresponding tuning circuit.
- ii) research on TFBAR resonators for enhancing the quality factor, which includes,
 - improving current 1D Mason model to 3D model combined with more accurate loss mechanism such as lateral field dissipation of acoustic energy, dielectric loss in substrate and microwave transmission line loss, to provide guidelines for the fabrication of high performance devices;
 - further researches on fabrication and measurement techniques for development and evaluation of high performance AlN materials;
 - consummation of present process for serial-resonator structure fabrication and further development of electrode-isolation structure.

References

- A. N. Cleland and M. L. Roukes, 1996, 'Fabrication of High Frequency Nanometer Scale Mechanical Resonators from Bulk Si Crystals', *Applied Physics Letters*, 69(18), pp. 2653-2655.
- A. P. French, 1971, *Vibrations and Waves – The MIT Introductory Physics Series*, W. W. Norton & Company.
- Adolfo C. Reyes, Samir M. El-Ghazaly, Steve Dorm *et al*, 1994, "Silicon as a microwave substrate", *Dig. IEEE Microwave Theory Technical Symp. (San Diego, CA, May 1994)*, pp. 1759–1762.
- Agilent products report, 2004, "5 x 5 mm FBAR Duplexer for US PCS Band", from www.agilent.com, released by Agilent Technologies.
- ANSYS user manual, 2002, "Coupled-Field Analysis Guide", released by ANSYS Inc.
- ANT technical report, 2004, "Film bulk acoustic resonator fabrication for RF filter applications", from <http://www.antechnology.com/>, released by ANT Co., Ltd.
- B. Auld, 1973, *Acoustic Fields and Waves in Solids*, John Wiley and Sons, NY.
- Brian C. Wadell, 1991, *Transmission Line Design Handbook*, Artech House Boston, London.
- C. Caliendo, G. Saggio, P. Verardi and E. Verona, 1993, "Piezoelectric AlN film for SAW devices applications", *Proc. of 1993 IEEE Ultrasonic Symposium (Baltimore, USA, 1993)*, pp. 249-252.
- C. F. Beards, 1981, *Vibration Analysis and Control System Dynamics*, Ellis Horwood Limited, pp. 82-86.
- Clark T.-C. Nguyen, 1998, "Microelectromechanical Devices for Wireless Communications", *Proc. of 11th IEEE International Conf. MEMS Workshop (Heidelberg, Germany, January 1998)*, pp. 1-7.
- Clark T.-C. Nguyen, 1999, "Microelectromechanical Components for Miniaturized Low-Power Communications", *Proc. of 1999 IEEE MTT-S International Microwave Symposium RF MEMS Workshop (Anaheim, Calif., June 1999)*, pp. 48-53.
- Clark T. -C. Nguyen, 1999, "Micromechanical filters for miniaturized low-power communications", *Proc. of SPIE: Smart Structures and Materials (Smart Electronics and MEMS) (Newport Beach, CA, March 1999)*, pp. 55-66.
- D. J. Young, V. Malba, J. J. Ou, A. F. Bernhardt and B. E. Boser, 1997, "Monolithic High Performance Three-Dimensional Coil Inductors for Wireless Communications

References

Applications”, *Technical Digest, International Electron Devices Meeting (Washington, December 1997)*, pp. 67-70.

D. J. Young, V. Malba, J. J. Ou, A. F. Bernhardt and B. E. Boser, 1998, “A Low-Noise RF Voltage-Controlled Oscillator Using On-Chip High-Q Three Dimensional Coil Inductor and Micromachined Variable Capacitor”, *Technical Digest, IEEE Solid-State Sensor and Actuator Workshop (South Carolina, June 1998)*, pp. 128-131.

Dan McNamara, 2000, “FBAR Technology Shrinks CDMA Handset Duplexers”, *Microwaves & RF*, pp. 71-79.

David A. Koester, Ramaswamy Mahadevan, Buzz Hardy and Karen W. Markus, 2000, MUMPs Design Handbook Revision 5.0, released by Cronos Integrated Microsystems.

David M. Pozar, 1990, Microwave engineering, Addison-Wesley Publishing Company, pp. 185.

David P. Morgen, 1998, “History of SAW Devices”, *IEEE International Frequency Control Symposium (Pasadena, May 1998)*, pp. 439-460.

David Salt, 1987, High-Q Handbook of Quartz Crystal Devices, Van Nostrand Reinhold (UK) Co. Ltd.

Dimitri Galayko, Andreas Kaiser, Lionel Buchaillet *et al*, 2003, “Design, realization and testing of micro-mechanical resonators in thick-film silicon technology with postprocess electrode-to-resonator gap reduction”, *Journal of Micromechanics and Microengineering*, vol. 13, pp. 134-140.

Dubravka Bilic, 2001, “Micromachined Resonators”, Ph.D. dissertation of University of California at Berkeley.

EM3DS user manual, 2003, from <http://www.memresearch.com>.

Ewald Benes, Martin Groschl, Franz Seifert and Alfred Pohl, 1998, “Comparison Between BAW and SAW Sensor Principles”, *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, vol. 45(5), pp. 1314-1330.

Fred L. Walls and John R. Vig, 1995, “Fundamental Limits on the Frequency Stabilities of Crystal Oscillators”, *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, vol. 42 (4), pp. 576-589.

G. Carlotti, F. S. Hickerness, H. M. Liaw *et al.*, 1995, “The Elastic Constants of Sputtered Aluminum Nitride Films”, *Proc. 1995 IEEE Ultrasonics Sym. (Seattle, USA, 1995)*, pp. 353-356.

G. K. Grover, 1977, Mechanical Vibrations, Roorkee: Nem Chand, pp. 435-437.

Giwan Yoon, Jae-Don Park and Hee-Dae Park, 2000, “Characterization of ZnO-Based FBAR Devices for RF Applications”, *Proc. of 2nd International Conferences on Microwave and Millimeter Wave Technology (Beijing, Sep 2000)*, pp. 192-195.

References

- Gregory T. A. Kovacs, 2000, *Micromachined Transducers Sourcebook*, McGraw-Hill Book Company.
- H. Okano, Y. Takahashi, T. Tanaka, K. Shibata and S. Nakano, 1992, "Preparation of *c*-Axis Oriented AlN Thin Films by Low-Temperature Reactive Sputtering", *Jpn. J. Appl. Phys.*, vol. 31, pp. 3446-3451.
- H. P. Löbl, M. Klee, O. Wunnicke, R. Kiewitt *et al.*, 1999, "Piezo-electric AlN and PZT films for micro-electronic applications", *Proc. of 1999 IEEE Ultrasonic Symp. (Lake Tahoe, USA, 1999)*, pp. 1031-1036.
- H. P. Löbl, M. Klee, C. Metzmacher, W. Brand, R. Milsom *et al.*, 2001, "Piezoelectric Materials for BAW Resonators and Filters", *Proc. of 2001 IEEE Ultrasonic Symp. (Atlanta, Georgia, 2001)*, pp. 807-811.
- H. Windishmann, 1991, "Intrinsic Stress in Sputtered Thin Films", *J. Vac. Sci. Technol. A.*, vol. 9, pp. 2431-2435.
- H. Y. Joo, H. J. Kim, S. J. Kim and S. Y. Kim, 2000, "The Optical and Structural Properties of AlN Thin Films Characterized by Spectroscopic Ellipsometry", *Thin Solid Films*, vol. 368, pp.67-73.
- Henrik Morkner, Rich Ruby, Mike Frank and Domingo Figuerdo, 1999, "An Integrated FBAR Filter and PHEMT Switched-Amp for Wireless Applications", *Digest of 1999 IEEE MTT-S International Microwave Symposium (CA, 1999)*, pp. 1393-1396.
- H. Kim and S. H. Kim, 1995, "Effect of N ion bombardment on the compositional change and residual stress of AlN film synthesized by ion beam assisted deposition", *J. Vac. Sci. Technol. A*, vol. 13, pp. 2814-2818.
- J. B. Starr, 1990, "Squeeze Film Damping in Solid State Accelerometer", *Technical Digest, IEEE Solid State Sensor and Actuator Workshop (SC USA, June 1990)*, pp. 44-47.
- J. S. Kim, K. Choi and I. Yu, 1993, "A New Method of Determining the Equivalent Circuit Parameters of Piezoelectric Resonators and Analysis of the Piezoelectric Loading Effect", *IEEE Trans on Ultrasonics, Ferroelectrics, and Frequency Control*, vol. 40(4), pp. 424-426.
- Jacob Fraden, 1993, *AIP Handbook of modern sensors: physics, designs and applications*, American Institute of Physics, New York.
- Jerry R. Norton and Raymond J. Besson, 1993, "Tactical BVA Quartz Resonator Performance", *Proc. of IEEE International Frequency Control Symposium (Salt Lake City, USA, June 1993)*, pp. 609-613.
- Joel F. Rosenbaum, 1988, *Bulk Acoustic Wave Theory and Devices*, Artech House Inc.
- Joachim N. Burghartz, 1999, "Status and trends of silicon RF technology", *Technical Digest ESSDERC 99*, pp. 56-63.

References

- John E. Vig and Yoonkee Kim, 1999, "Noise in Microelectromechanical System Resonators", *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, vol. 46, pp. 1558-1565.
- John R.Clark, Frank D. Bannon III, Ark-Chew Wong and Clark T.-C. Nguyen, 1997, "Parallel-Resonator HF Micromechanical Bandpass Filters", *Proc. of 1997 International Conference on Solid-State Sensors and Actuators (Chicago, June 1997)*, pp. 1161-1164.
- John R.Clark, Wan-Thai Hsu and Clark T.-C. Nguyen, 2000, "High-Q VHF Micromechanical Contour-Mode Disk Resonators", *Technical Digest, IEEE International Electron Devices Meeting (San Francisco, Dec. 2000)*, pp. 399-402.
- K. Grenier, L. Rabbia, A.Tackacs *et al*, 2001, "MEMS technology as a contender for the future wireless applications", *2001 International Semiconductor Conference (Sinaia, Roumania, Oct.)*, pp.101-110.
- K. Kusaka, D. Taniguchi, T. Hanabusa and K. Tominaga, 2000, "Effect of Input Power on Crystal Orientation and Residual Stress in AlN Film Deposited by dc Sputtering", *Vacuum*, vol. 59, pp. 806-813.
- K.M. Lakin, 2001, "Thin Film Resonators and High Frequency Filters", Report of TFR Technologies.
- Karl S. Van Dyke, 1925, "The Electric Network Equivalent of A Piezoelectric Resonators", *Physical Review*, vol. 25, pp. 895-860.
- Kun Wang, Ark-Chew Wong, Wan-Thai Hsu and Clark T.-C. Nguyen, 1997, "Frequency Trimming and Q-Factor Enhancement of Micromechanical Resonators Via Localized Filament Annealing", *Technical Digest, The 9th International Conference on Solid-State Sensors and Actuators(Chicago, June 1997)*, pp. 109-112.
- Kun Wang, Yinglei Yu, Ark-Chew Wong and Clark T.-C. Nguyen, 1999, "VHF Free-Free Beam High-Q Micromechanical Resonators", *Technical Digest, 12th IEEE on MEMS (Orlando, Jan. 1999)*, pp. 453-458.
- Kurt E. Petersen, 1991, "Silicon as a Mechanical Material", *Microsensors* (Reprinted from Proc. IEEE, vol. 70 (5), pp. 420-457, 1982.), IEEE Press Inc, New York.
- Levinshstein, Rumyantsev and Shur, 2001, *Properties of Advanced Semiconductor Materials*, John Wiley & Sons Inc, New York.
- Liu Xunliang, 1998, *Optical Visual Sensing*, Science & Technology Press House, Beijing.
- M. -A. Dubois, P. Muralt, H. Matsumoto and V. Plessky, 1998, "Solidly mounted resonator based on aluminum nitride thin film", *Proceeding of 1998 IEEE Ultrasonic Symposium*, pp. 909-912.
- M. -A. Dubois, P. Muralt and V. Plessky, 1999, "BAW resonators based on aluminum nitride thin films", *Proceedings of 1999 IEEE Ultrasonic Symposium*, pp. 907-910.

References

- M. -A. Dubois and P. Muralt, 1999, "Properties of aluminum nitride thin films for piezoelectric transducers and microwave filter applications", *Applied Physics Letters*, vol. 74(20), pp. 3032-3034.
- M. Elwenspoek and R. Wiegerink, 2001, *Mechanical Microsensors*, New York: Springer.
- M. L. Roukes, 2000, "Nanoelectromechanical Systems", *Technical Digest, IEEE Solid-State Sensor and Actuator Workshop (Hilton Head Island, SC)*, pp. 367-376.
- M. Stickel, G. V. Eleftheriades and P. Kremer, 2001, "High-Q Bulk Micromachined Silicon Cavity Resonator at K-Band", *Electronics Letters*, vol. 37 (7).
- M. T. Duffy, C. C. Wang, G. D. O'Clock Jr., S. H. McFarlane III, and P. J. Zanzucchi, 1973, "Epitaxial growth and piezoelectric properties of AlN, GaN, and GaAs on sapphire or spinel", *J. Electronics Materials*, vol. 2, pp. 359.
- Ma Songde and Zhang Zhengyou, 1998, *Computer Vision-Computing Theory and Algorithm Foundation*, Science Press House, Beijing.
- Marc Madou, 1997, *Fundamentals of Microfabrication*, CRC Press, New York.
- MATLAB, 1998, *Signal Processing Toolbox, User's Guide*, released by Mathworks Inc.
- Matthew R. Hart, Robert A. Connant, Kam Y. Lau and Richard S. Muller, 2000, "Stroboscopic Interferometer System for Dynamic MEMS Characterization", *Journal of Microelectromechanical Systems*, vol. 9, pp. 409-418.
- Michael Warren Judy, 1994, *Micromechanisms Using Sidewall Beams*, Ph.D thesis of University of California.
- N. Fujimura, T. Nishihara, S. Goto, J. Xu and T. Ito, 1993, "Control of preferred orientation for ZnO films: control of self-texture", *J. Cryst. Growth*, vol. 130, pp. 269.
- N. Jiang, R. K. Sharma, Z. Wang and Wang Xiaowei, 2003, "Impact of Deposition Parameters on the Characterizations of Highly Orientated Aluminum Nitride for Film Bulk Acoustic Resonator Device", *International Journal of Computational Engineering Science*, vol. 4(3), pp. 547-550.
- Murata Report, 2003, "Ceramic Resonator Application Manual", from <http://www.murata.com/>, released by Murata Manufacturing Co., Ltd.
- NSM Archive, 2003, "New Semiconductor Materials. Characteristics and Properties", from <http://www.ioffe.rssi.ru/SVA/NSM/Semicond/AlN/>.
- Ni Zhenghua, 1989, *Mechanics of Vibration*, Xi'an JiaoTong University Publishing House, Xi'an, pp. 378-382.
- P. B. Kirby, Q. X. Su, E. Komuro, Q. Zhang *et al.*, 2001, "PZT thin film bulk acoustic wave resonators and filters", *Proc. of 2001 IEEE International Freq. Control Sym. and PDA Exhibition (Seattle)*, pp. 687-694.

References

- Qing-Xin Su, Paul Kirby, Eiju Komuro, Masaaki Imura *et al.*, 2001, "Thin-Film Bulk Acoustic Resonators and Filters Using ZnO and Lead–Zirconium–Titanate Thin Films", *IEEE Transactions on Microwave Theory and Techniques*, vol. 49(4), pp. 769-778.
- Philippe Jacot, Christian Lambert and Philippe Krebs, 2002, "Wireless Future with BAW", *Chip Unaxis Company Technique Report*, pp. 22-26.
- R. Besson and U. Peier, 1980, "Further Advances on B.V.A. Quartz Resonators", *Proc. 34th Annual Frequency Control Symp*, pp. 175-182.
- R. Lerch, 1990, "Simulation of piezoelectric devices by two and three dimensional finite element", *IEEE trans. Ultrason. Freq. Contr.*, vol. 37, pp. 233-247.
- R. Ruby, 1996, "Micromachined cellular filters", *IEEE MTT-S International Microwave Symposium Digest*, vol. 2, pp. 1149-1152.
- R. Ruby and P. Merchant, 1994, "Micromachined Thin Film Bulk Acoustic Resonators", *Proc. of 48th IEEE International Frequency Control Symposium (Piscataway, NY)*, pp. 135-138.
- Randy J. Richards and Hector J. De Los Santos, 2001, "MEMS for RF/Microwave Wireless Applications: The Next Wave", *Tutorial of Coventor Inc.*
- Richard C. Jaeger, 1993, "Modular Series of Solid State Devices: Introduction to Microelectronic Fabrication", (vol. V), Addison-Wesley Publishing Company.
- Richard Ruby, Paul Bradley, John Larson III, Yury Oshmansky and Domingo Figuerdo, 2001, "Ultra-Miniature High-Q Filters and Duplexers Using FBAR Technology", *IEEE International Solid-State Circuits Conference (San Francisco, Feb. 2001)*, pp. 120-121.
- Richard S. Muller, Roger T. Howe, Stephen D. Senturia, Rosemary L. Smith, and Richard M. White, 1991, "Resonant Microsensors", *Microsensors*, IEEE Press Inc, New York.
- Richard S. Muller and Theodore I. Kamins, 1986, *Device Electronics for Integrated Circuits*, John Wiley & Sons, Inc., Second Edition.
- S. V. Krishnaswamy, J. Rosenbaum, S. Horitz, C. Vale and R. A. Moore, 1990, "Film Bulk Acoustic Wave Resonator Technology", *Proc. of IEEE Ultrasonics Symposium (Honolulu, USA, Dec. 1990)*, pp. 529-536.
- S. Wolf and R. N. Tauber, 2000, *Silicon Processing for the VLSI Era*, Lattice Press, vol. 1, pp. 110.
- Satoru Fujishima, 2000, "The History of Ceramic Filters", *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, vol. 47(1), pp. 1-7.
- Siavash Pourkamali and Farrokh Ayazi, 2003, "SOI-Based HF and VHF Single-Crystal Silicon Resonators with Sub-100 Nanometer Vertical Capacitive Gaps", *Digest of the 12th International Conference on Solid State Sensors, Actuators and Microsystems (Boston, June 2003)*, pp. 837-840.

References

- Stephen. D. Senturia, 2001, *Microsystem Design*, Boston: Kluwer Academic Publisher.
- T. Lamminmäki, K. Ruokonen, I. Tittonen and T. Mattila, 2000, “Electromechanical analysis of micromechanical SOI-fabricated RF resonators”, *Proceedings of MSM’ 2000*, pp. 217-220.
- T. Mattila, J. Kiihamaki and T.Lamminmaki, 2002, “A 12MHz micromechanical bulk acoustic mode oscillator”, *Sensors and Actuators (A)*, pp. 1-9.
- T. Mukherjee and G. K. Fedder, 1997, “Structured Design of Microelectromechanical Systems”, *Proceedings of the 34th Design Automation Conference*, pp. 680-685.
- Tapani Makkonen, Antti Holappa and Martti M. Salomaa, 2000, “3D FEM Modeling of Composite BAW Resonators”, *Proc. of IEEE Ultrasonics Symposium (San Juan, Puerto Rico (USA))*, pp. 893-896.
- Tapani Makkonen, Antti Holappa, Juha Ella and Martti M. Salomaa, 2001, “Finite Element Simulations of Thin-Film Composite BAW Resonators”, *IEEE Trans on Ultrasonics, Ferroelectrics and Frequency Control*, vol. 48 (5), pp. 1241-1258.
- Terry V. Roszhart, 1990, “The Effect of Thermoelastic Internal Friction on the Q of Micromachined Silicon Resonators”, *In Technical Digest, IEEE Solid-State Sensor and Actuator Workshop*, pp. 13–16.
- Trey A. Roessig, Roger T. Howe, Albert P. Pisano and James H. Smith, 1998, “Surface-Micromachined 1MHz Oscillator with Low-Noise Pierce Configuration”, *In Technical Digest, IEEE Solid-State Sensor and Actuator Workshop*, pp. 328-332.
- V. B. Braginsky, V. P. Mitorfanov and V. I. Panov, 1985, *Systems with Small Dissipation*, The University of Chicago Press, Chicago.
- Ville Kaajakari, Tomi Mattila, Aarne Oja, Jyrki Kiihamaki, Hannu Kattelus *et al*, 2003, “Square-extensional mode single-crystal silicon micromechanical RF-resonator”, *the 12th Internal Conference on Solid State Sensors and Actuators (Boston, June 2003)*, pp. 425-432.
- Velimir M. Ristic, 1983, *Principles of Acoustic Devices*, John Wiley & Sons, Inc.
- W. Y. Chiu, C. H. Wu, H. L. Kao, Erik S. Jeng, Jyh S. Chen and C. C. Jaing, 2002, “The optical properties and applications of AlN thin films prepared by a helicon sputtering system”, *J. Vac. Sci. Technol. A*, vol. 20, pp. 843-847.
- Wan-Thai Hsu, John R. Clark, and Clark T.-C. Nguyen, 2001, “A Sub-Micron Capacitive Gap Process for Multiple-Metal-Electrode Lateral Micromechanical Resonators”, *Technical Digest, The 14th IEEE International MEMS Conference (Interlaken, Switzerland, Jan. 2001.)*, pp. 349-352.
- Wang Jingyi, 1993, *Theory of Thin Film Growth*, Wu Han: Huazhong Science and Technology University Publisher.

References

- Wang Xiaowei, Lin Rongming and Wang Zhe, 2003, "Image measurement of geometrical size for three-dimensional microstructure of MEMS", *Journal of Micromechanics and Microengineering*, vol. 13, pp. 300-306.
- Wang Xiaowei, Wang Zhe and Lin Rongming, 2003, "Design and Realization of Micromechanical Resonator", *Technical Digest, Symposium on Microelectronics (Singapore, 2003)*, pp. 30-32.
- X W Wang, R M Lin, Z Wang and W J Wang, 2005, "Development of micromechanical resonator using a new process flow based upon SOI technology", *Journal of Micromechanics and Microengineering*, vol. 15, pp. 557-563.
- X. Wang, Y. P. Xu, Z. Wang, S. Liw *et al.*, 2003, "A Bandpass sigma-delta modulator employing micron-mechanical resonator", *Proceedings of IEEE ISCA'03*, vol. 1, pp. 1041-1044.
- William Mueller, 2002, A Brief Overview of FBAR Technology, *Agilent Technologies White Paper*.
- Y. He, J. Marchetti, C. Gallegos and F. Maseeh, 1999, "Accurate Fully-coupled Natural Frequency Shift of MEMS Actuators due to Voltage Bias and Other External Forces", *Proc. of the 12th IEEE International MEMS Conference*, pp. 321-325.