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CONTROL SYSTEM FOR MASS SPECTROMETER

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CONTROL SYSTEM FOR MASS SPECTROMETER

A Thesis

Submitted to the Faculty

of

Purdue University

by

Jian Xu

In Partial Fulfillment of the

Requirements for the Degree

of

Master of Science

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Purdue University

West Lafayette, Indiana

To the Creator of the Universe and me

My dear Mother, Jinhua Liu

My dear wife, Yaguo Wang

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I would also like to thank my lab mates in Dr. Ouyang's lab in Weldon School of Biomedical Engineering, who have been constantly helping me on my research and life since Fall 2009. They gave me so many help and inspired discussions, without them I cannot finish my graduate study at Purdue.

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ABSTRACT

Xu, Jian. M.S., Purdue University, August, 2011. Control System for Mass Spectrometer.

Major Professor: Henry Zhang and Zheng Ouyang.

Mass spectrometry (MS) is a very popular analytical methodology that measures the mass of ions using a mass spectrometer. It is widely used for determining masses of chemicals, the elemental composition of a sample and molecule structure. The process of mass spectrometry normally consists of ionizing chemical compounds to ions and measuring their ratios of mass and charge for analysis.

MS instruments consist of three modules: Ionization, Analysis and detection. A LabVIEW system was developed to control the three modules of a mass spectrometer, giving the required signals in a right sequence. Experiments can be carried out by using the system very convenient since the software settings are very flexible.

Broadband radio frequency (RF) circuit was designed. Transformers were tested for the purpose of it, and a good one was chosen for further research. Frequency scan function will be enhanced which will significantly low down the necessary RF voltage within a mass spectrometer.

CHAPTER 1. INTRODUCTION

This chapter gives a basic overview of the research project, defining the research question and the scope and significance of the study. Assumptions, limitations and delimitations are also included to show a clear outline of the research.

1.1. Research Question

Can a mass spectrometry control system enable experiments in the lab be easier and help expand the imagination of researchers?

1.2. Scope

In the research, mass spectrometry system is well studied. It will focus on developing a modifiable control system for lab use. The scope of the research is to develop lab-use control system for recliner ion trap (RIT) based mass spectrometers. The performance testing is to check whether it can satisfy different kinds of experiments which will be carried out by the researchers in the lab. The goal of this research is to make lab experiments be easier, and give researchers more space to explore their imaginations.

1.3. Significance

There are many kinds of mass spectrometers which are widely used in companies, hospitals and labs. With the high safety requirements, and the development of analytical biology and chemistry, mass spectrometry will have big space to grow in the following several years, and it can even become home-use equipments as the size and price are reducing.

It is better that a mass spectrometer is like a black box for the user in companies, hospitals and institutions where people just take use of the function, people do not have to know anything inside it, but just take part in input and output processes. However, for researchers in the lab who are developing new mass spectrometry methodologies and trying to improve the functions, they need an open system to work on. Researchers have to know what is going on inside a mass spectrometer, and it better that they can design different kinds of experiments base on a mass spectrometry system. This research will focus on development of such a system, which can give researchers many options, the access to the inside of the system, and the freedom to modify the system.

1.4. Assumptions

The following assumptions are being made:

- The system can be transplanted to other kinds of mass spectrometers.
- The software and hardware can be upgraded in the future without big changes.
- Other similar sample can also be tested and give good results by using the system.
- Data formats and transmission methods of mass spectrometers which may connect to the system are the same with the requirements.

1.5. Limitations

The RF systems of mini equipments are quite different from those of big commercial equipments. The voltage can't be too high, or discharge will happen in the small spaces. The limitation of the voltage will affect the mass range we can get by mini mass spectrometers. So this project will not try to show a big range of mass range. The small sizes would not be allowed big pump system. So the sampling speed can't be too quick, or the vacuum can not be kept at a low pressure.

1.6. Delimitations

The research is about the control system of a mini mass spectrometer, it should cover every part which needs to be controlled. However, this project will focus on the design of RF signal output for ion trap. I will not do too much things on ionization part since we already have some good method to control this part. Also I may not do too much things about the control of pump system.

1.7. Chapter Summary

This chapter introduces the research that is encompassed in this thesis, outlining key aspects such as the research question, scope and assumptions. Also, this chapter notes the limitations and delimitations of the chosen scope and the contribution of this work to the existing body of knowledge by explaining its significance.

CHAPTER 2. LITERATURE REVIEW

This chapter gives an overview of a mass spectrometry system, the developing of mass spectrometry technology, the main types of mass spectrometry systems, and future directions. It then introduces the most important part of an ion trap based mass spectrometry system, ion trap. It talks about how to reduce the size of ion traps and how to improve its performance. Then it talks about the development of the whole mass spectrometry systems.

2.1. Overview of mass spectrometry

Research on mass spectrometry has been carried out all over the world for many years. It is a rich field includes Chemistry, Physics, Control, Mechanical and Electrical Engineering. Mass spectrometry labs of Purdue University have been the leaders in mass spectrometry instrumentation and analysis for many years. Purdue University focuses on developing simple methodologies and instruments to make mass spectrometry analysis be easier and more efficient. A great invention of Purdue Aston lab is a series of miniature mass spectrometers using ion traps(Ouyang 2009). Among different kinds of mass spectrometers, ion trap mass spectrometer is one of the best candidates due to its low vacuum

requirement, reasonable resolution, mass range and accuracy. An ion trap mass spectrometer system has three main processes:

1. Sources
2. MS analysis
3. Detection

More and more researchers and scientists are interested in developing miniature MS systems since they are convenient to use and energy save.

2.2. Mass spectrometry System

There are many kinds of commercial MS systems manufactured by Thermal, Agilent and other companies. Also there are some miniature MS systems have been demonstrated and commercialized.

There are many kinds of ion traps that are being used to analyze ions, and some labs at Purdue University use RIT(recliner ion trap) for mass analysis. RIT was invented in Aston Lab of Purdue university (Ouyang, 2004), and it becomes a good candidate for miniature ion traps because of its simple structure and high efficient. It has been used in a series of miniature mass spectrometers (Gao, 2008).

Future mass spectrometers will be smaller and smaller. "Mini 10" of Aston lab weighs only 10 kg and 32 by 22 by 19 cm in dimension. It consumes about 70 watt, but it very good resolution (Gao, 2006). A lot researches for future mass spectrometers are being done at Purdue and other mass spectrometry labs all

over the world. There will be more and more amazing works come out of the wisdoms and hard working of the researchers.

2.3. Chapter summary

This chapter talks about the researches on mass spectrometry currently. It started with an overview of the current research of mass spectrometry, the aspects development and emphasis. Then it focuses on the ion trap miniaturization. Several kinds of ion traps are introduced and compared, to give an introduction of research achievements. Finally, it gives some idea about the research on the system. It focus on the mini mass system, which is considered to be future research direction of mass spectrometry.

Nowhere in the literature is there any mention of research on development of lab use system. The next chapter will describe how to design a open system, which can make experiments in labs be easier.

CHAPTER 3. METHODOLOGY

This chapter will cover the research framework, instrumentation, data collection and data analysis.

3.1. Research Framework

The thesis is a quantitative study to analyze how to design a modifiable mass spectrometry control system which will be used by the researchers in labs who are going to develop new functions and improve the original functions, and it will also be used by researches who want to do special experiments. The research follows a well designed plan. Such methods require designing, instrumentation, coding, and many experiments.

The variables of the methodology are:

- Design tools of this research, including hardware, software, testing instruments.
- Mathematics model of the control system.
- The sample I choose to do experiments.
- Solutions of the problems during design and experiments, some of them are in expectation, while still many come up when really do something.

Hypotheses of the research are tested; these have been outlined below.

- Ho1 The open system can not help with many kinds of special experiments in the lab.
- Ho2 The modifiable system can not help with designing new experiments and offer more space of the imaginations of researchers.
- Ho3 There is no possibility to make improvement and upgrading on self developed system.
- Ha1 The open system can help with many kinds of special experiments in the lab.
- Ha2 The modifiable system can help with designing new experiments and offer more space of the imaginations of researchers.
- Ha3 There is possibility to make improvement and upgrading on self developed system.

This system will be used by different researchers in different ways to task its advantages comparing with the ones they always used in the labs.

3.2. Instrumentation

Four LabVIEW boards bought from National Instrument(NI) will be fixed together, to read the input signals and send output signals. After installing drivers for the four boards, computer can communicate with the four boards by using certain software from NI. This give accesses to test and read the status of the boards.

Inputs and outputs of RIT mass spectrometer can be connected with the ports on the LabVIEW boards, the amount of ports which will be use depends on

how many output and input signals the mass spectrometer needs. After the hardware is fixed, codes should be written using LabVIEW software. The program will define each of the four boards, and the signal types of each board as well.

Some normal chemical samples will be tested to see how the system works, whether any further steps to take to improve the hardware or the software. The goal is to enable its accurate and stable functions.

Transformers are chosen and tested to choose the best for us to design a new kind of RF circuit for mass spectrometers. We do experiments based on a simple and efficient way.

3.3. Data collection and analysis

Data of the LabVIEW boards can be collected by computer which has firm connection with them. The signals of mass spectrometry system will be collected by the LabVIEW boards, and send to computer. So the computer can collect most of signals. Other instruments also will be used to test signals directly from the mass spectrometry system, and these real data will be used to compare with the data collected by computer to see whether the control methodology works fine. There are also some meters which will be used to test high voltage signals, pressure of the vacuum system and other signals can not be collected by computer.

Data of testing of different transformers are recorded and put into excel form for statistical comparison.

3.4. Chapter Summary

This chapter covers the framework of the research, and the hypotheses that need to be tested. It also describes the instrumentation, data collection and data analysis.

CHAPTER 4. PROJECTS

This chapter will cover the introduction and details of my Master projects. It will follow the steps of how the ideas come from, and how to design and carry out experiments. Finally, I will give conclusion for each project.

The projects mainly focus on the development of a good control system for mass spectrometer. Here are some main challenges for mass spectrometer control system:

- The control system should cover many parts and give out many different signals, from source to MS analysis to Detection
- The precisely synchronization of different signals, the time differences between the signals are normally ~ms
- High precision requirements, radio frequency (RF) voltage could be as high as 5000V, however, the deviation should be controlled within 1V

A control system should first generate digital low voltage signals, and then amplify the voltage to a high RF voltage. LabVIEW system can generate the low voltage signals, and a transformer can amplify it to a high RF voltage. This chapter will discuss how the challenges be solved.

4.1. LabView System

4.1.1. Introduction

LabVIEW (Laboratory Virtual Instrumentation Engineering Workbench) by national instrument is a visual programming platform. It is stable, precise and flexible. It is very widely used in laboratories and industries because of its significant advantages.

A LabVIEW control system was built up with the goal to control ion trap mass spectrometers in the lab. The system can be used by researchers when they want to do experiments on prototype mass spectrometers. The LabVIEW system can provide different kind of signals as they need.

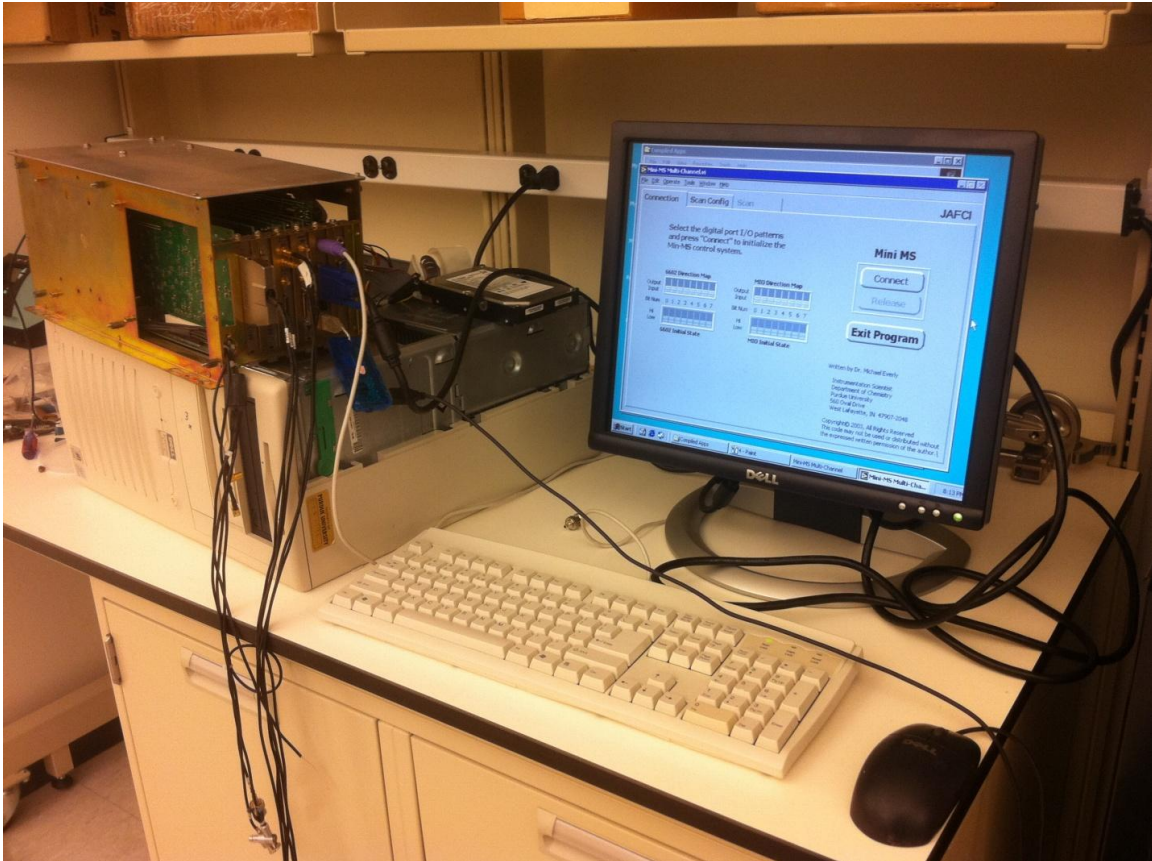


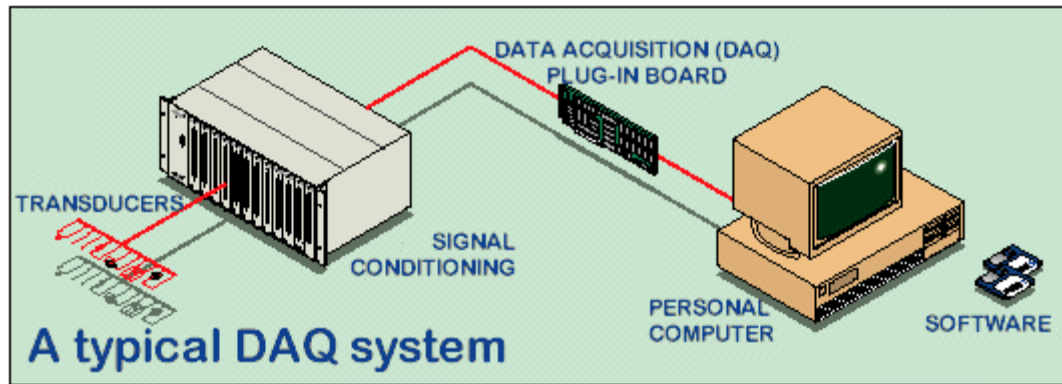
Figure 4.1. LabVIEW system

4.1.2. Hardware and software of the system

The system includes 6 boards, 4 boards from National Instruments (NI), a CPU board and a communication board. The system works like a small computer, while the main purpose is to control a mass spectrometer through the 4 NI boards by sending and reading signals and information.

LabVIEW is a very good candidate for developing automated instrumentation systems using the PC plug-in Data Acquisition (DAQ) boards. It is very efficient for engineering data acquisition, analysis, and presentation. The plug-in DAQ is flexible, computerized measurement of real world analog signals and generation

of analog signals. A typical DAQ system may consist of transducers, signal conditioning hardware, plug-in DAQ boards, and LabVIEW application software.



[HTTP://WWW.NIU.EDU/ME/LABS/COMPUTERIZED_DATA.SHTML](http://www.niu.edu/me/labs/computerized_data.shtml)

Figure 4.2. DAQ system

The NI boards are: PCI-5411x2, 6602x2.

PCI-5411 is DAQ board, which is translator between computer and transducers. The two signal conditional boards (6602) can give up to tens of input and output signals, which can provide different kind of signals for mass spectrometry experiments. The software can read and edit the commends in the configuration files which will be saved in the hard drive, so if different signals of different sequences are saved in different configuration files, that would be very helpful for researchers to repeat and explore experiments.

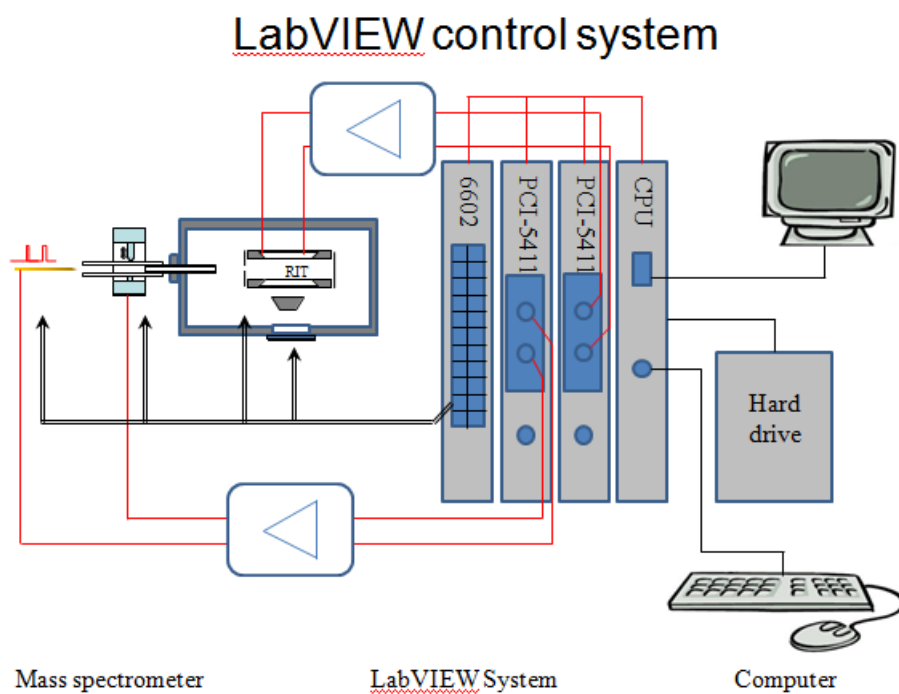


Figure 4.3. Structure of LabVIEW system

The hardware is like following:

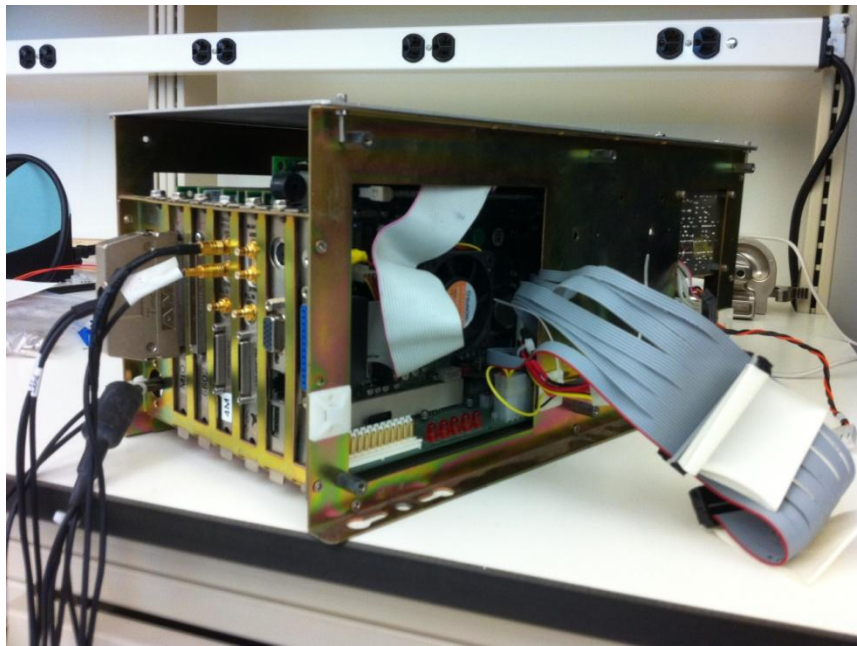


Figure 4.4. LabVIEW system

The system can connect to a monitor and can be operated by using mouse and keyboard. We have a hard drive connecting with the CPU board, which can be used to save software and data of experiments.



Figure 4.5. Input and output

The software to control the hardware was programmed using G language, which is a visual language. So it is easy to read and modify the software even if you are not well trained. Users of the system can either type in a new configuration file or modify a saved one, which enhance very convenient platform for researchers.

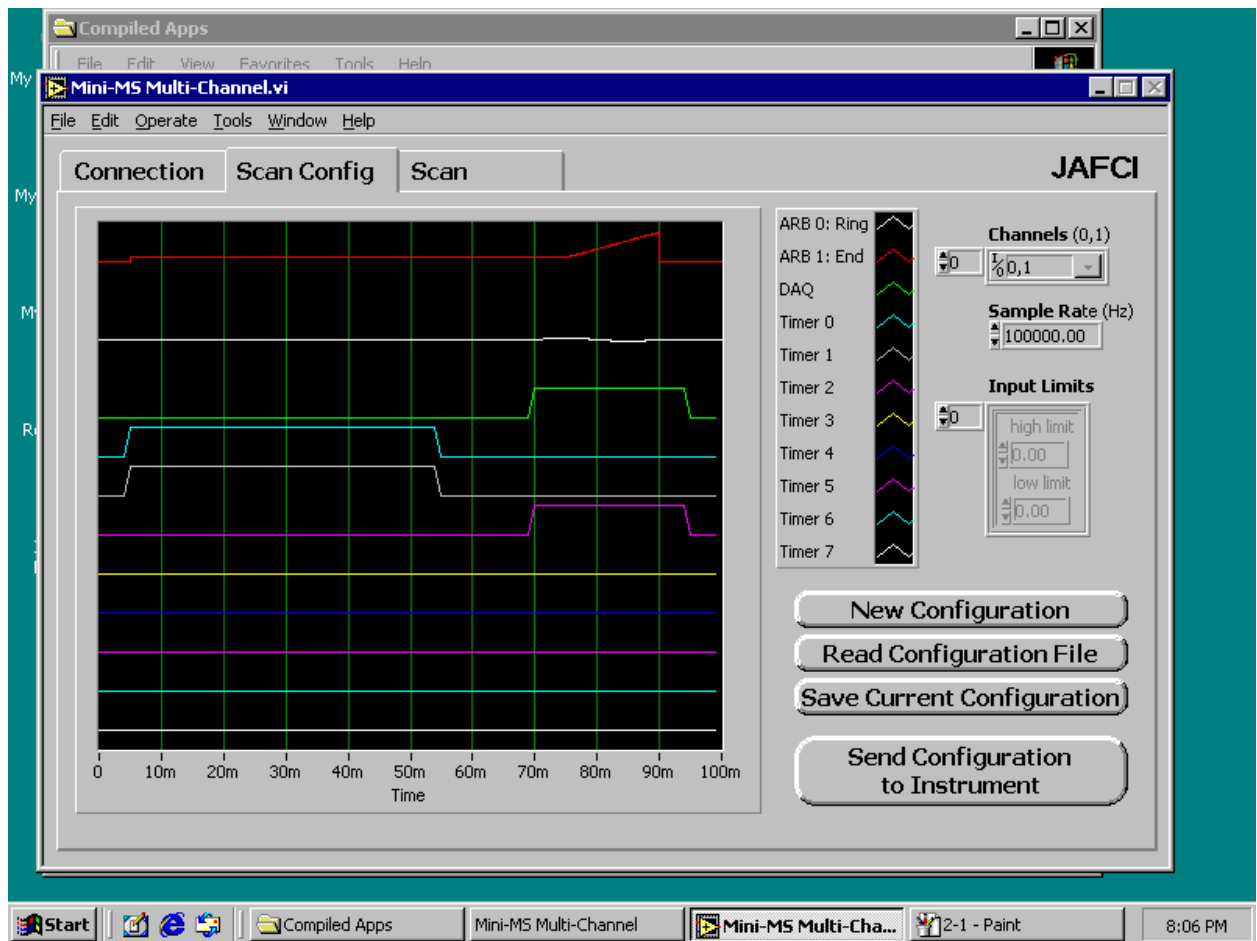


Figure 4.6. Software

4.1.3. Application of the system

The LabVIEW system was used in the project: Sampling Wand for an Ion Trap Mass Spectrometer. In this project, we want to design a special prototype mass spectrometer. So we are not going to use a commercial mass spectrometer to work with the project, instead, we need to build up a new system. From this point, a LabVIEW control system is of great advantage and can be used to control the prototype mass spectrometer. We can edit the configuration file in the

software to provide any kind of signals in any sequences as we want, which can enhance great space for the development of prototype mass spectrometers.

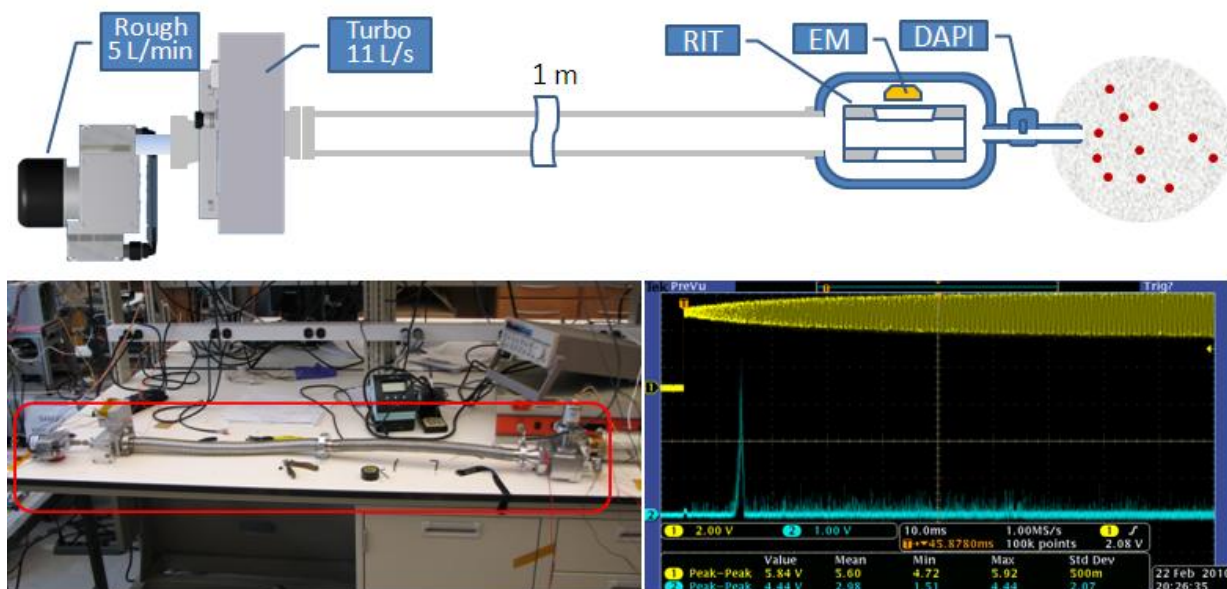
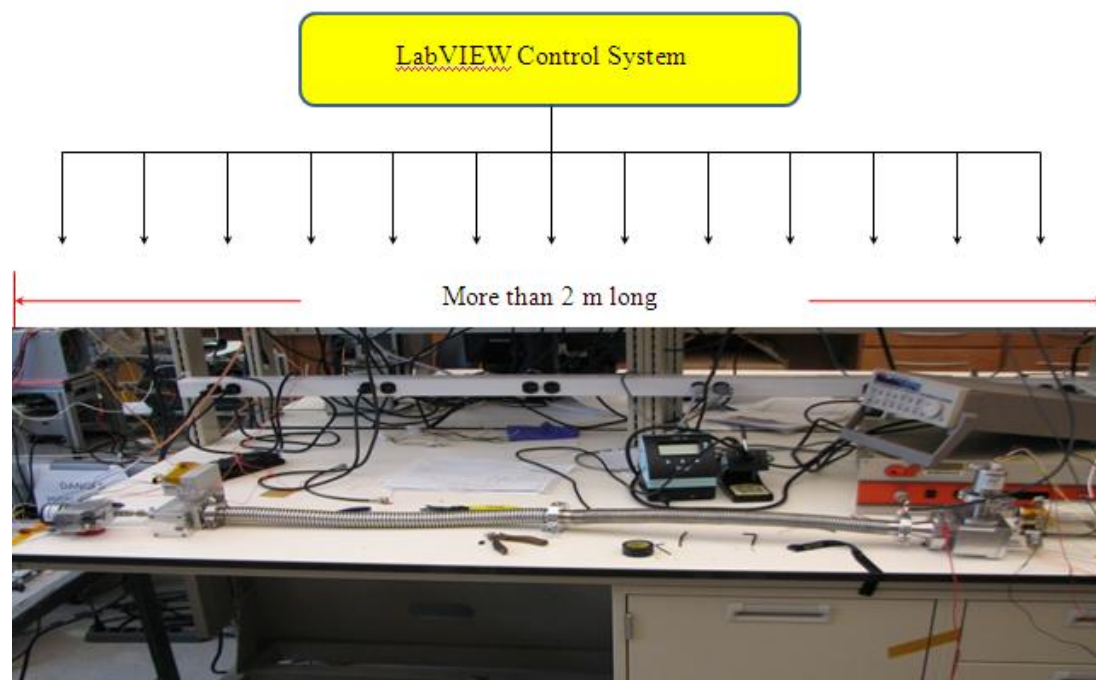
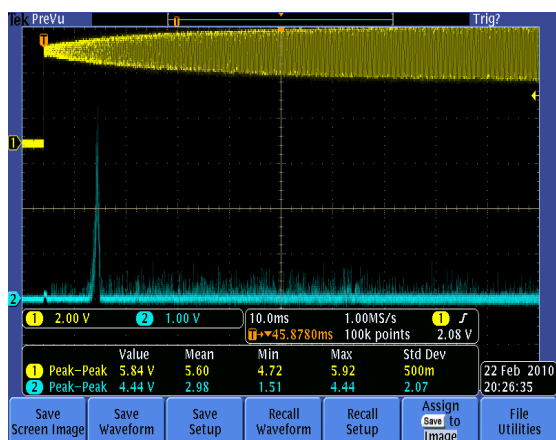


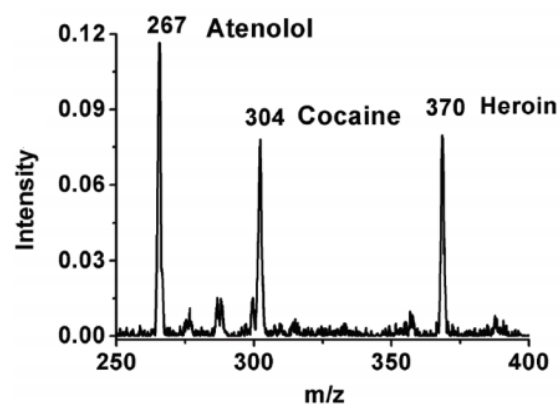
Figure 4.7. A prototype mass spectrometer



(a)



(b)



(c)

Figure 4.8. (a) Flexility of the LabVIEW control system, (b) Signals detected by oscilloscope, (c) Mass spectra of a mixture of atenolol, cocaine, and heroin (Hou, 2011)

4.2. Broadband RF Circuit

4.2.1. Mass Spectrometer RF circuits

Normally, people use LC circuit to amplify the RF voltage for ion trap in mass spectrometer. However, LC (inductance and capacitance in series) RF amplifier circuit is very complex and big, and it can only work at narrow band frequency. An idea of using a small transformer as amplifier to design a broadband RF circuit was tried. The first step of this project is to find out a good transformer that can work well in both high voltage and long-range frequency. This idea is possible based on the new technology of making small size and better characteristics transformers.

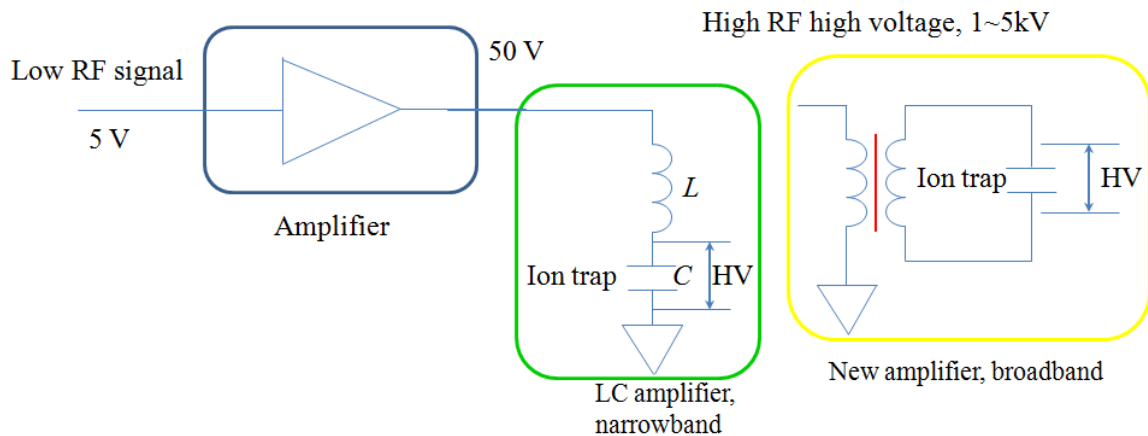


Figure 4.9. Narrowband and broadband RF circuit

4.2.2. Idea of broadband RF circuit

Use a transformer to generate high RF voltage for ion trap, which can not only simplify the RF circuits, but also enhance the automatic frequency adjustment ability. The most important thing is that, it may enhance frequency scan function rather than voltage scan which would significantly low down the RF voltage level. This is especially good for miniaturization of mass spectrometer.

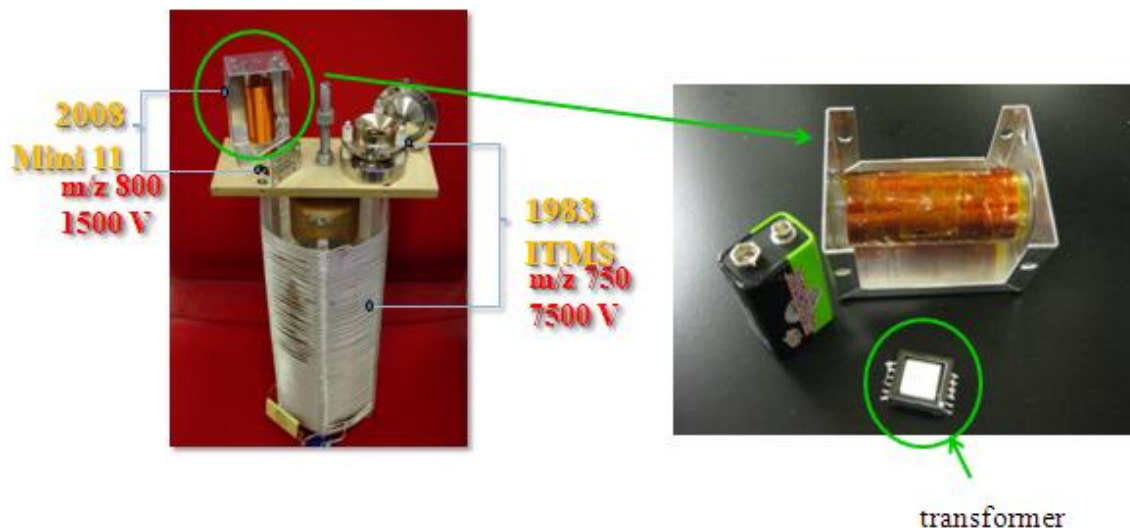


Figure 4.10. Comparison of transformer and LC coils

4.2.3. Transformer testing

The first step of this project is to find a good transformer which can work well at both high voltage and long frequency range.

4.2.3.1 Preparation

We want to build a new RF voltage generating circuit for a smaller vacuum chamber. Smaller chamber and ion trap make a low RF signal be possible. Low RF voltage has many advantages, it enable low discharge possibilities and can be easily controlled.

4.2.3.1.1 Fourier Transformation

At the very beginning, we wanted to try square wave input. Fourier equation was studied and used to help analyze the output signals.

The period of the square wave is τ and the amplitude is E .

$$f_1(t) = \begin{cases} E & (|t| \leq \frac{\tau}{2}) \\ 0 & (|t| > \frac{\tau}{2}) \end{cases} \quad (4.1)$$

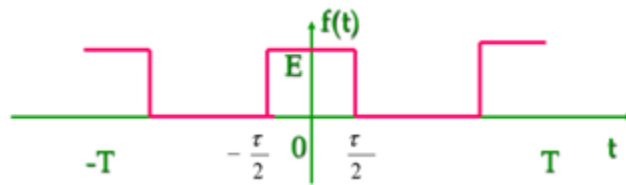


Figure 4.11. Square wave input

Do Fourier transformation:

$$\begin{aligned} F_n &= \frac{1}{T_1} \int_{-\frac{\tau}{2}}^{\frac{\tau}{2}} E e^{-jn\omega_1 t} dt \\ &= \frac{E}{T_1(-jn\omega_1)} (e^{-jn\omega_1 \tau/2} - e^{jn\omega_1 \tau/2}) \\ &= \frac{E\tau}{T_1} \frac{\sin(\frac{n\omega_1 \tau}{2})}{\left(\frac{n\omega_1 \tau}{2}\right)} \end{aligned} \quad (4.2)$$

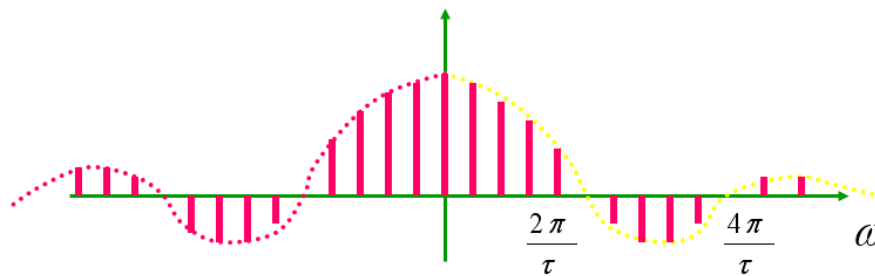


Figure 4.12. Fourier wave

$$F_0 = \frac{E\tau}{T_1}, \quad F_n = \frac{E\tau}{T_1} Sa\left(\frac{n\pi\tau}{T_1}\right) \quad (4.3)$$

4.2.3.1.2 LC Circuit

We want to do some experiments on LC Circuit for comparison. LC Circuit is the main methodology to amplify the low signal to a high RF voltage. We had a plan to find ways to generate stable lower voltage RF signal by working on a LC circuit.

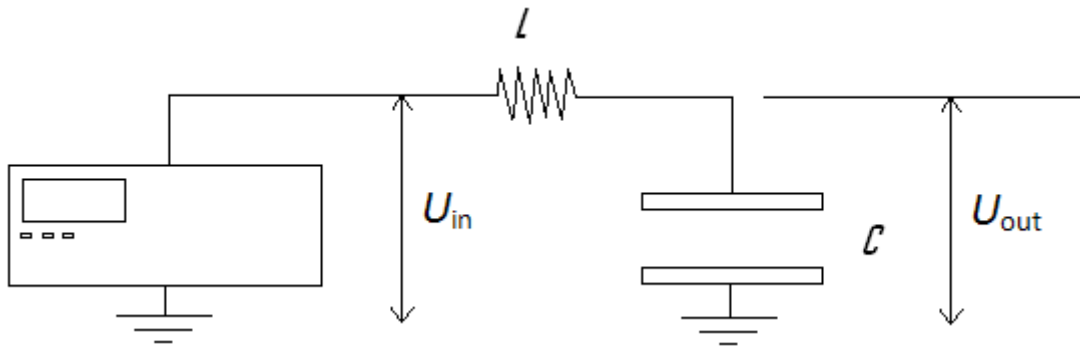


Figure 4.13. LC Circuit

$$Q = U_{out}/U_{in} = \omega L/r = 1/\omega cr \quad (4.4)$$

4.2.3.2 Experiments

We designed and did experiments with the circuits. First we tested the LC circuit with square wave input, the output signals were just as what we expected. Then we tried using high frequency transformers to substitute the coil and did some corresponding experiments.

4.2.3.2.1 LC Circuit Test

Square wave was applied to the LC circuit, and we got output data. We tried to find out how the amplitude and the period affect the output signal.

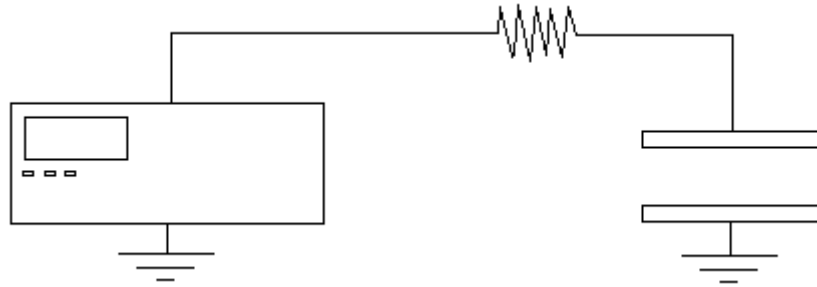


Figure 4.14. LC circuit testing

First, we fixed the period to get the input and output data.

Table 4.1. *LC data with period fixed*

$T=1.22\mu\text{S}$,
 $\tau=600\text{nS}$

E(V)	Amp(V)
0.5	140
1	180
1.5	220
2	270
2.5	300
3	350
3.5	380
4	420
4.5	460
5	500

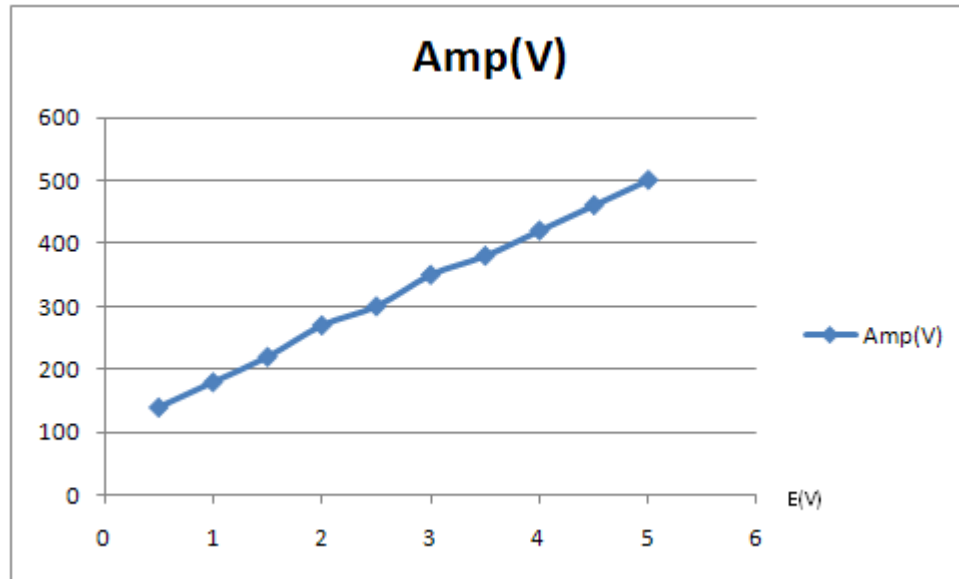


Figure 4.15. Scatter chart of the period fixed test

Then, we fixed the amplitude to get the input and output data.

Table 4.2. LC data with amplitude fixed

$T=1.22\mu S$,
 $E=5V$

$\tau(ns)$	Amp(V)
100	150
200	260
300	360
400	440
500	480
600	500
700	490
800	450
900	380
1000	280
1100	170
1200	170

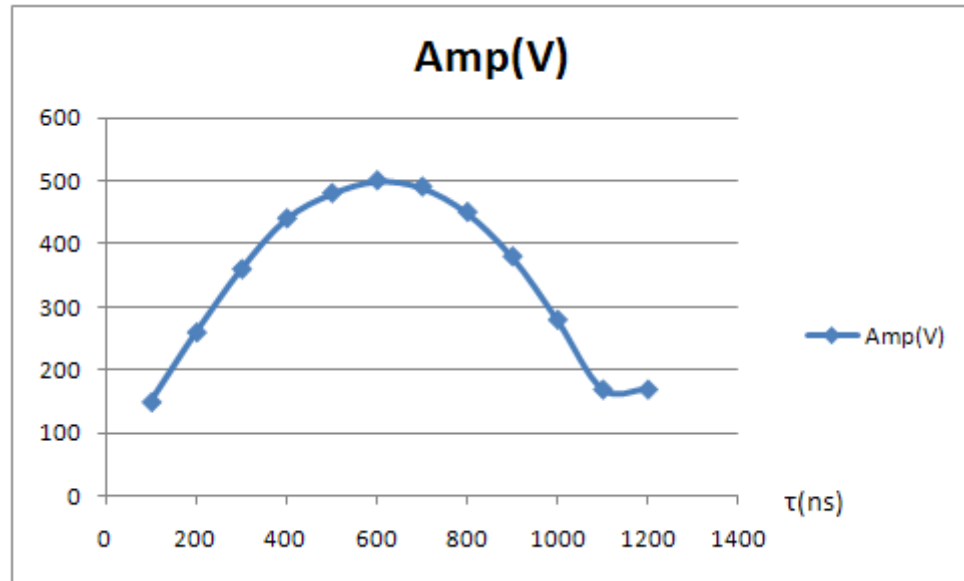


Figure 4.16. Scatter chart of the amplitude fixed test

When $E=5V$, $\tau=600ns$, $T_1=1.22 \mu s$,

$$F_0 = \frac{E\tau}{T_1} = \frac{5 * 600ns}{1.22\mu s} = 2.46 \quad (4.5)$$

4.2.3.2.2 Transformer Circuit Test

Then we used transformers to substitute the coil, and did some tests. We tried to find out a good transformer which can be used to generate stable RF voltage across quite a wide frequency range. To simulate the real situation, I connected the transformer to a real rectilinear ion trap (RIT).

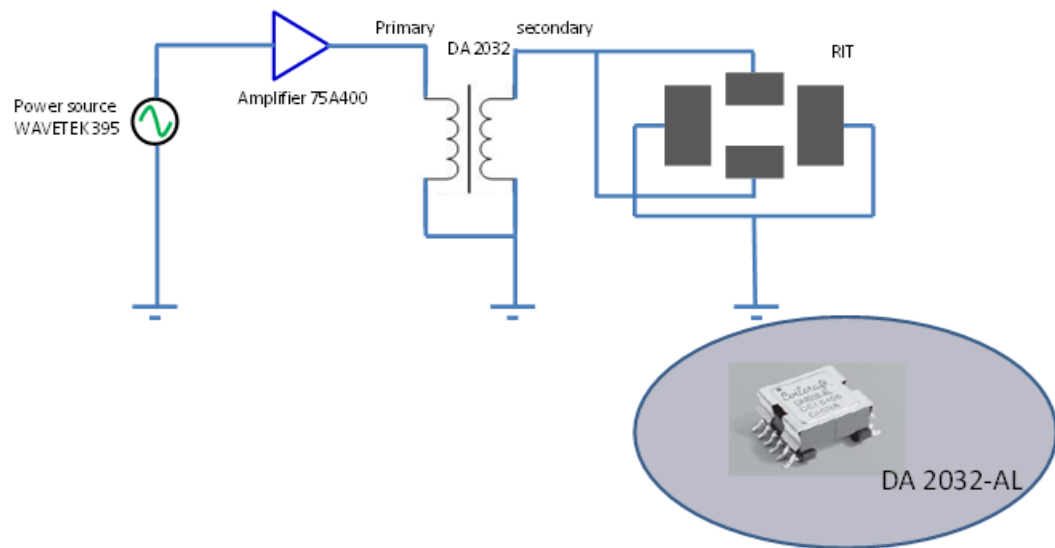


Figure 4.17. Test circuit

We spent quite a long time to look for good high frequency transformers. Many transformers were collected and tested.

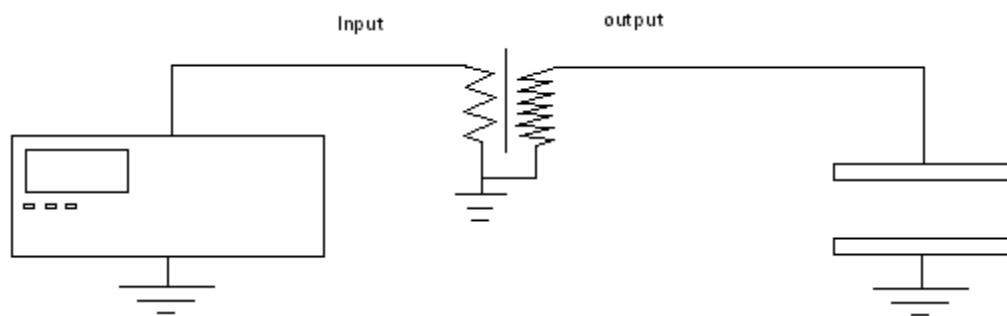


Figure 4.18. Transformer circuit testing

After we find out a good transformer, we can design a new RF circuit with it. There will be a preamplifier before the transformer to amplify the digital signal to a higher voltage before the transformer. Furthermore, a good feedback circuit is needed to give stable RF output.

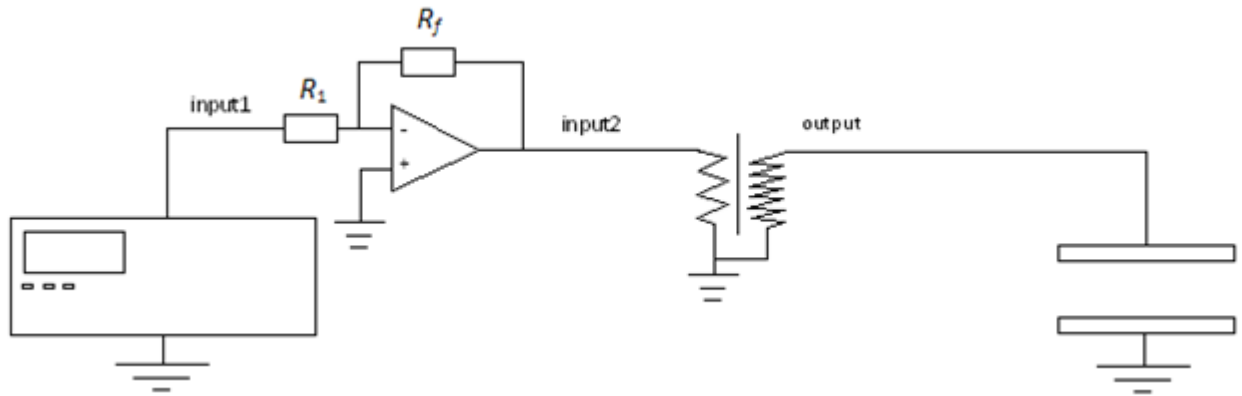


Figure 4.19. RF circuit design

Hundreds of transformers were collected and tested. Some of them cannot work at high voltage (>600V), while some of them can only work well at certain or quite short frequency range. What we need is a transformer which can work well at quite high voltage, and also at quite a long frequency range.

4.2.3.2.2.1 Test of transformer DA2033

Amplitude fixed test:

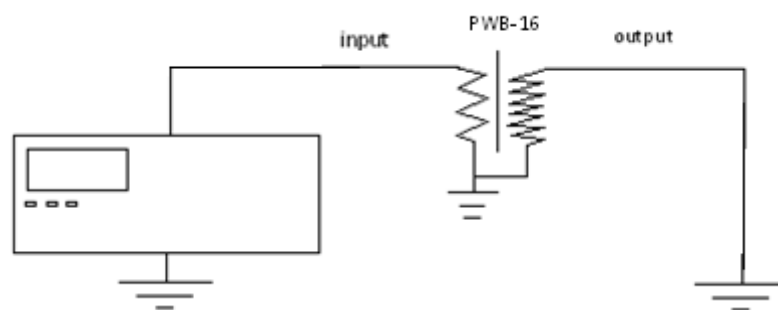


Figure 4.20. Test circuit

Table 4.3. *Amplitude fixed test data*

Vp=1.00	PRIM	SECOND
100kHz	0.54	4.7
200kHz	1.3	10
300kHz	2	16
400kHz	2.8	23
500kHz	3.6	31
600kHz	3.9	36
700kHz	3.5	34
800kHz	2.9	30
900kHz	2.3	26
1MHZ	1.7	22
1.1MHZ	1.3	20
1.2MHZ	0.9	17
1.3MHZ	0.6	15
1.4MHZ	0.4	14
1.5MHZ	0.15	13
1.6MHZ	0.13	12
1.7MHZ	0.26	11
1.8MHZ	0.4	10
1.9MHZ	0.56	9
2MHZ	0.72	9

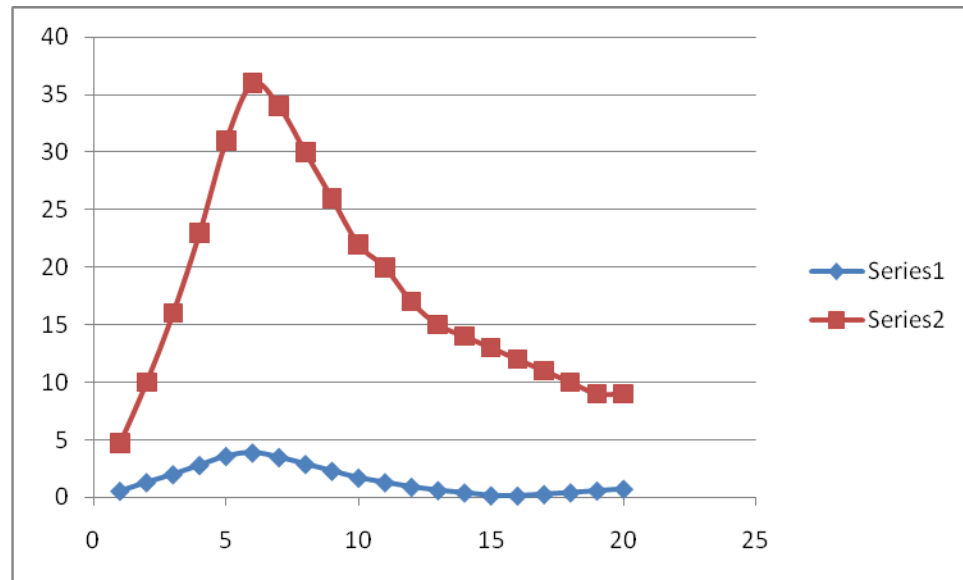


Figure 4.21. Scatter chart, where Series1 is primary side signal, and Series2 is secondary side signal.

We tried two transformers in series to see whether the amplification would be doubled.

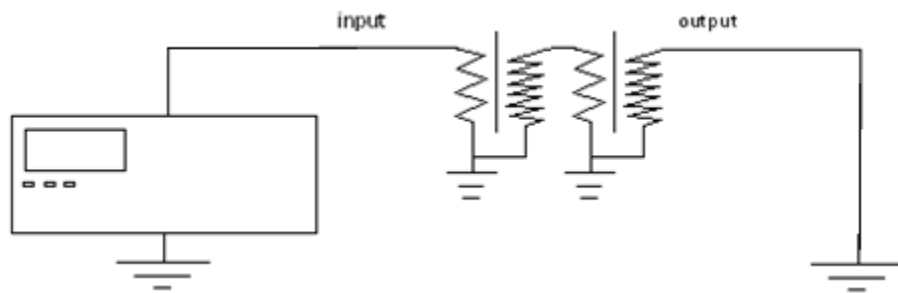


Figure 4.22. Two transformers test

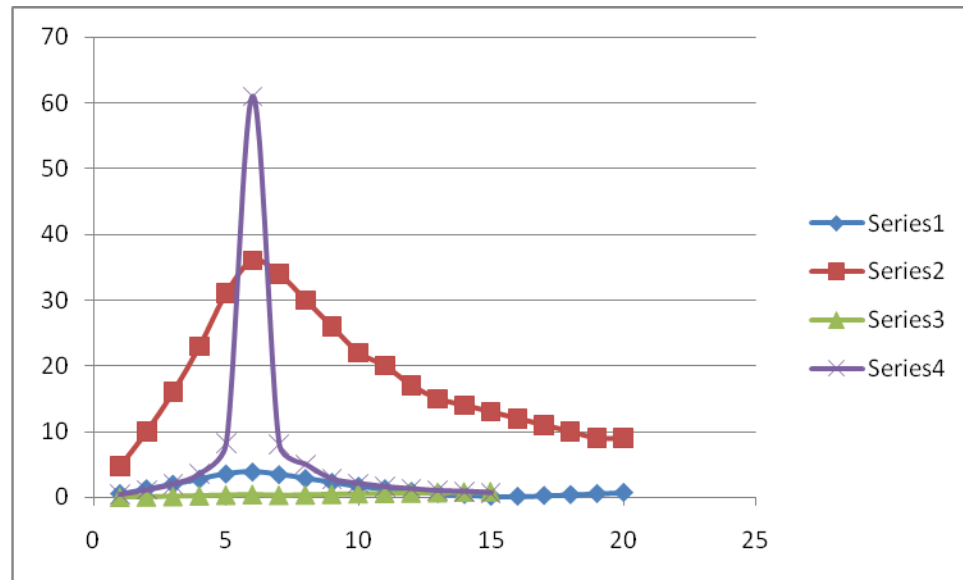


Figure 4.23. Scatter chart

Series 3 and Series 4 are got when two transformers are combined in series

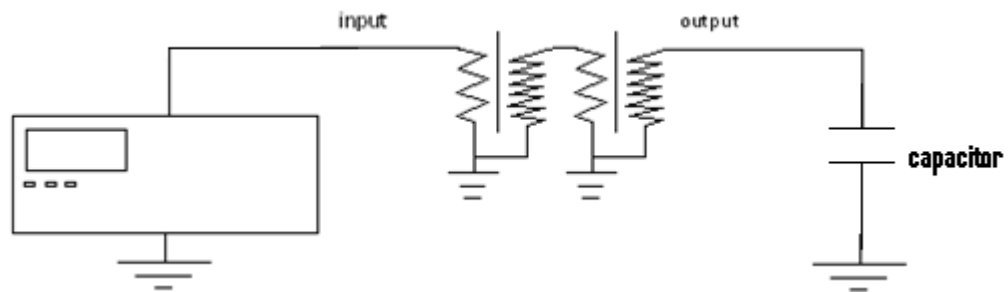


Figure 4.24. Circuit with capacitor

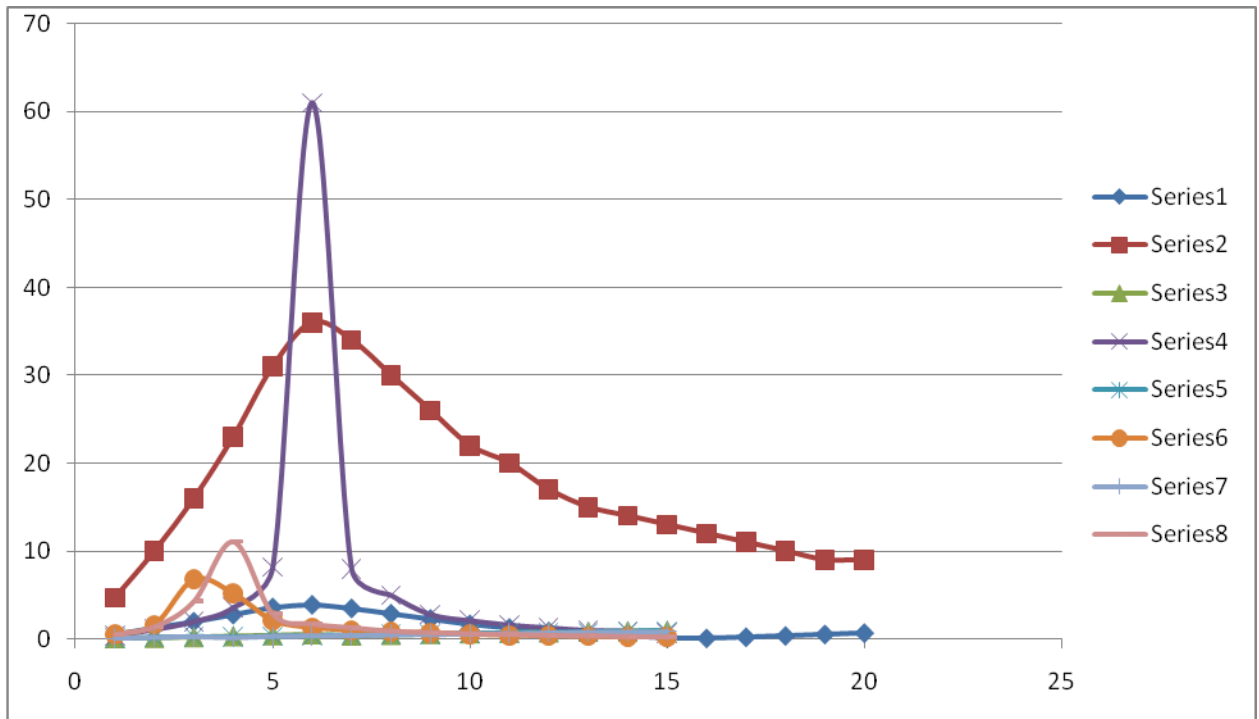


Figure 4.25. Scatter chart, where Series 5&6 are got at a certain capacitor, and Series7&8 are got at another capacitor value

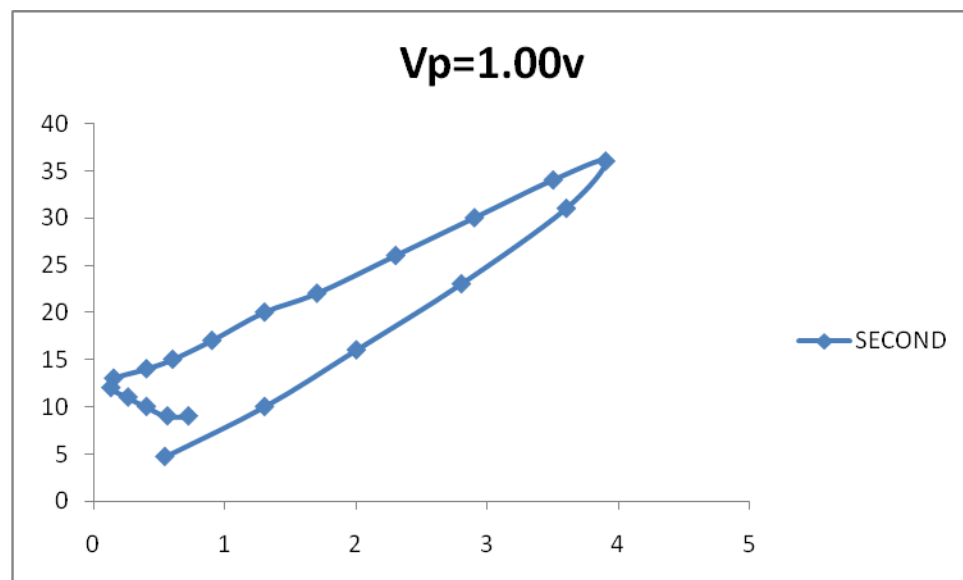


Figure 4.26. Output linear check

Table 4.4. 800KHZ Linear test

800kHz	PRIM	SECOND
Vp=1	2.7	31
Vp=2	5.7	60
Vp=3	8.6	91
Vp=4	11.4	120
Vp=5	14.3	151

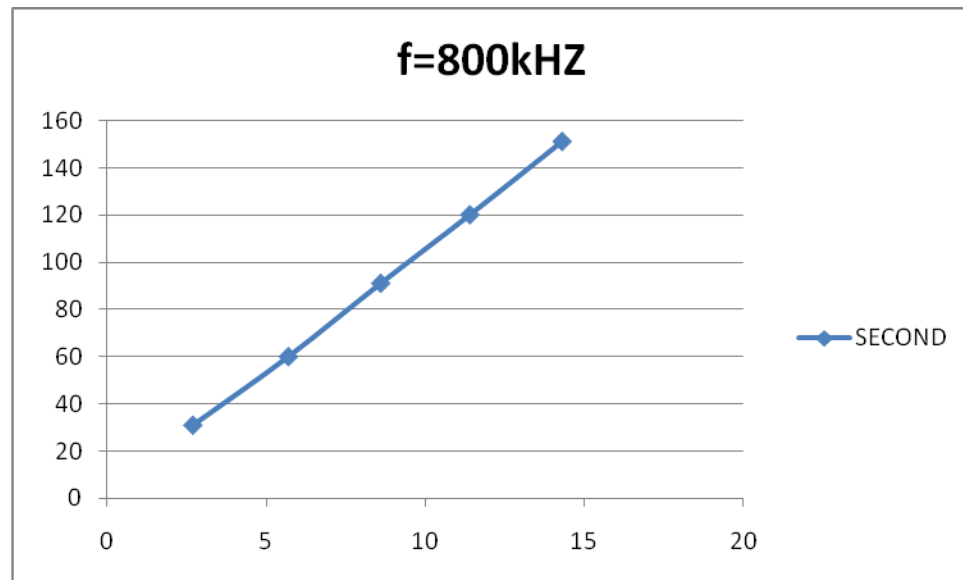


Figure 4.27. Scatter chart

Table4.5. 900KHZ Linear test

900kHz	PRIM	SECOND
Vp=1	2.2	24
Vp=2	4.4	52
Vp=3	6.7	78
Vp=4	9	104
Vp=5	11.1	131

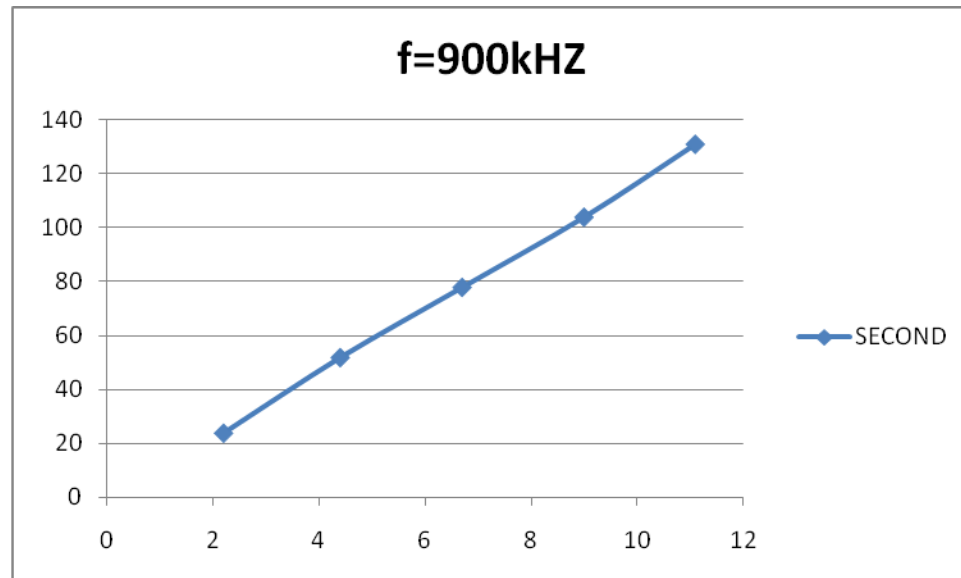


Figure 4.28. Scatter chart

Table 4.6. 1MHZ linear test

1000kHz	PRIM	SECOND
Vp=1	1.7	21
Vp=2	3.3	44
Vp=3	5.1	68
Vp=4	6.8	90
Vp=5	8.4	113

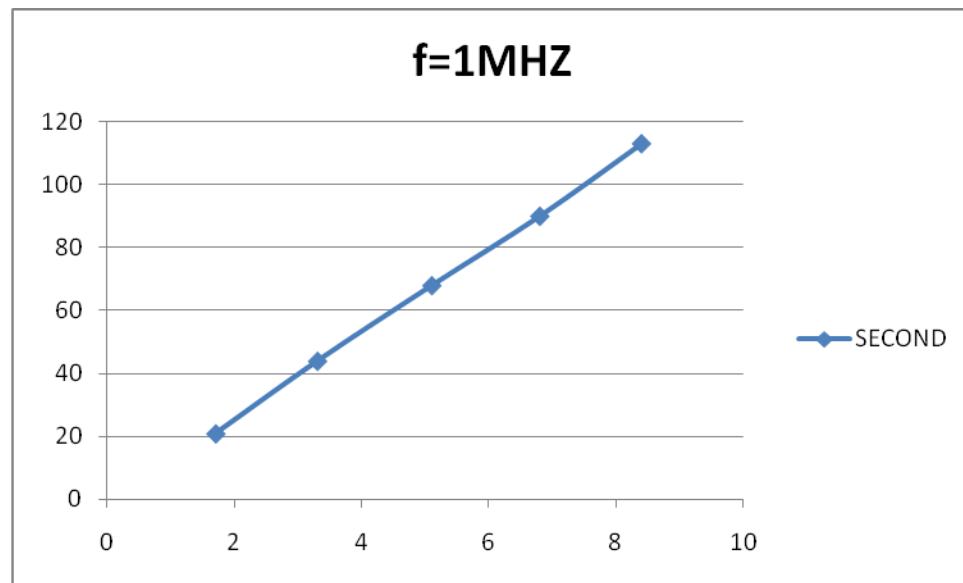


Figure 4.29. Scatter chart

4.2.3.2.2.2 Test of transformer CJ5143

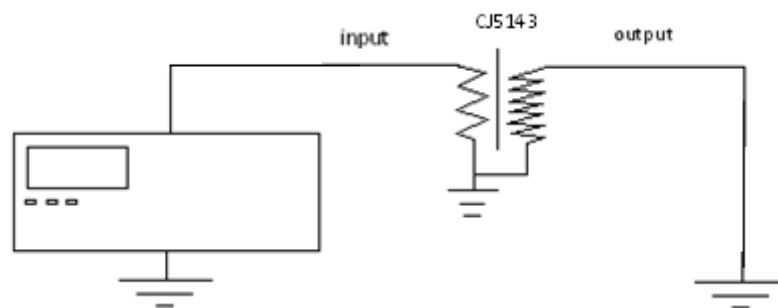


Figure 4.30. Test circuit

Table 4.7. *Amplitude fixed test*

V _p =1.00	PRIM	SECOND
100kHz	0.8	11
200kHz	1.7	23
300kHz	2.7	38
400kHz	3.6	50
500kHz	3.6	53
600kHz	3.1	48
700kHz	2.5	41
800kHz	1.9	35
900kHz	1.6	30
1MHZ	1.2	26
1.1MHZ	0.9	23
1.2MHZ	0.7	21
1.3MHZ	0.6	19
1.4MHZ	0.4	18
1.5MHZ	0.21	16
1.6MHZ	0.19	14.6
1.7MHZ	0.28	13.8
1.8MHZ	0.38	12.7
1.9MHZ	0.54	11.8
2MHZ	0.6	11.1
2.1MHZ	0.71	10.3
2.2MHZ	0.82	9.7
2.3MHZ	0.89	9.1
2.4MHZ	0.99	8.7
2.5MHZ	1.09	8.3
2.6MHZ	1.17	7.8
2.7MHZ	1.27	7.4
2.8MHZ	1.3	7
2.9MHZ	1.38	6.7
3MHZ	1.47	6.4

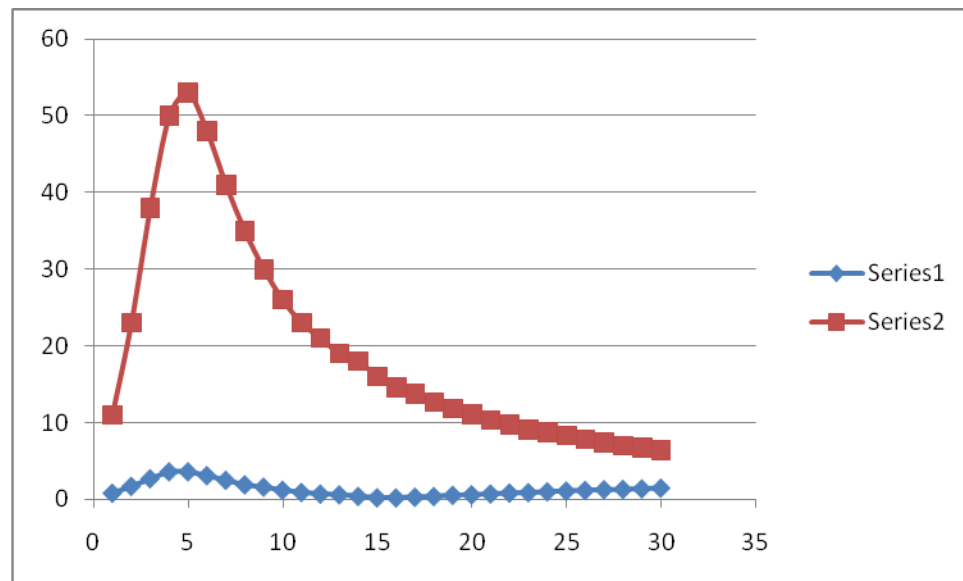


Figure 4.31. Scatter chart, where Series1 is primary side signal and Series2 is secondary side signal

Table 4.8. *HV test with ion trap in the circuit*

with trap

V _p =0.5	PRIM	SECOND	PRIM	SECOND
100kHz	6	74	7	76
200kHz	13	160	19	247
300kHz	23	294	39	550
400kHz	37	490	17	258
500kHz	43	590	10	160
600kHz	33	470	6	119
700kHz	24	360	4	96
800kHz	18	290	2	80
900kHz	14	242	1.1	69
1MHZ	11	208	1.3	61
1.1MHZ	9	180	2.3	55
1.2MHZ	7	162	3.1	48
1.3MHZ	5	148	4	44
1.4MHZ	4	136	4.8	42
1.5MHZ	2	125	5.5	38
1.6MHZ			6.3	35
1.7MHZ			7	32
1.8MHZ			7.8	30
1.9MHZ			8.6	28
2MHZ			9.2	26
2.1MHZ			10	25
2.2MHZ			10.6	24
2.3MHZ			11.4	22
2.4MHZ			12.2	20
2.5MHZ			12.9	18
2.6MHZ			13.5	17
2.7MHZ			14.1	16
2.8MHZ			14.9	15
2.9MHZ			15.6	14
3MHZ			16.4	12

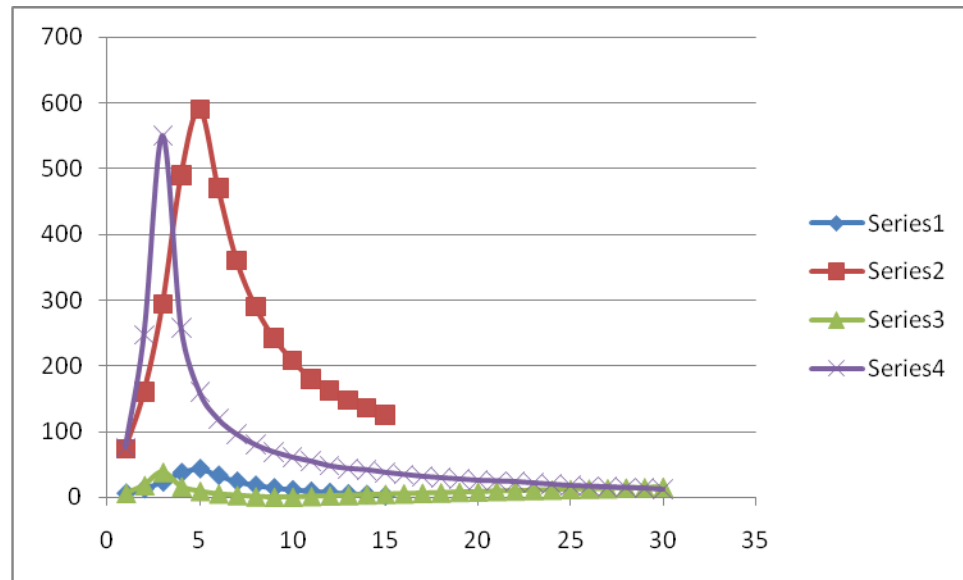


Figure 4.32. Scatter chart, where Series3 is primary side signal with trap and Series4 is secondary side signal with trap

Table 4.9. Limitation test (regular wave shape)

	PRIM	SECOND
100kHz	22	270
200kHz	31	390
300kHz	51	640
400kHz	61	800
500kHz	66	910
600kHz	62	840
700kHz	76	1000
800kHz	55	930

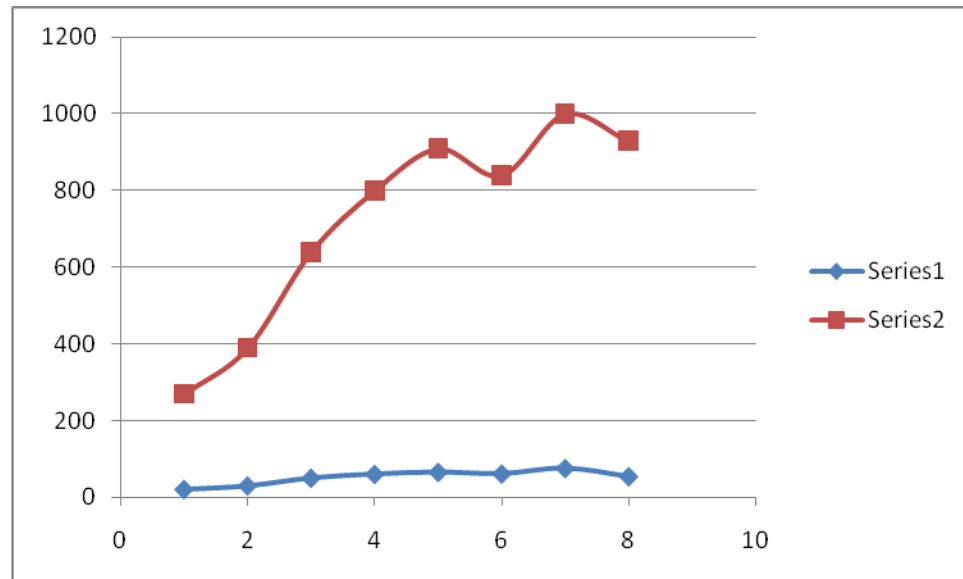


Figure 4.33. Scatter chart, where Series1 is primary side, and Series2 is secondary side

4.2.3.2.2.3 Test of transformer DA2032



Figure 4.34. Test circuits

Table 4.10. *Amplitude fixed test*Input $V_p=1V$ without trap with trap

Fre	First	Second	First	Second
100k	8	75	8	76
200k	17	160	19	180
300k	28	275	38	380
400k	48	475	75	770
500k	74	750	51	550
600k	69	710	31	350
700k	49	530	22	260
800k	37	400	16	210
900k	27.5	320	12.5	175
1M	22.5	275	10	160
1.1M	18	240	7.6	140
1.2M	15	210	6	125
1.3M	12.5	190	3.8	110
1.4M	11	175	2.7	105
1.5M	8	160	1.75	100
1.6M	7	150	1.6	95
1.7M	5	140	2.3	90
1.8M	3.75	130	3.3	85
1.9M	3.7	128	4.2	80
2M	2	125	5.2	76

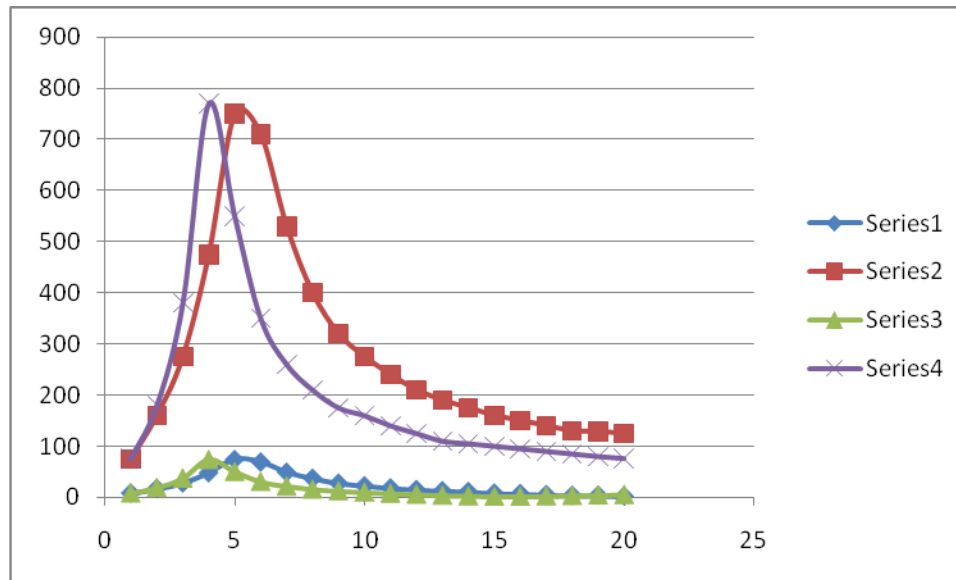


Figure 4.35. Scatter chart, where Series1 is primary side signal, Series2 is secondary side signal, Series3 is primary side signal with trap, and Series4 is secondary side signal with trap

Table 4.11. *Output fixed test*

	Input Vp	PRIM	SECOND
100k	5	45	400
200k	3.7	72	700
300k	1.7	70	700
400k	0.85	67	700
500k	1.3	65	700
600k	2.04	62	700
700k	2.78	58	700
800k	3.53	53	700
900k	4.34	47	700
1M	5.2	38	700

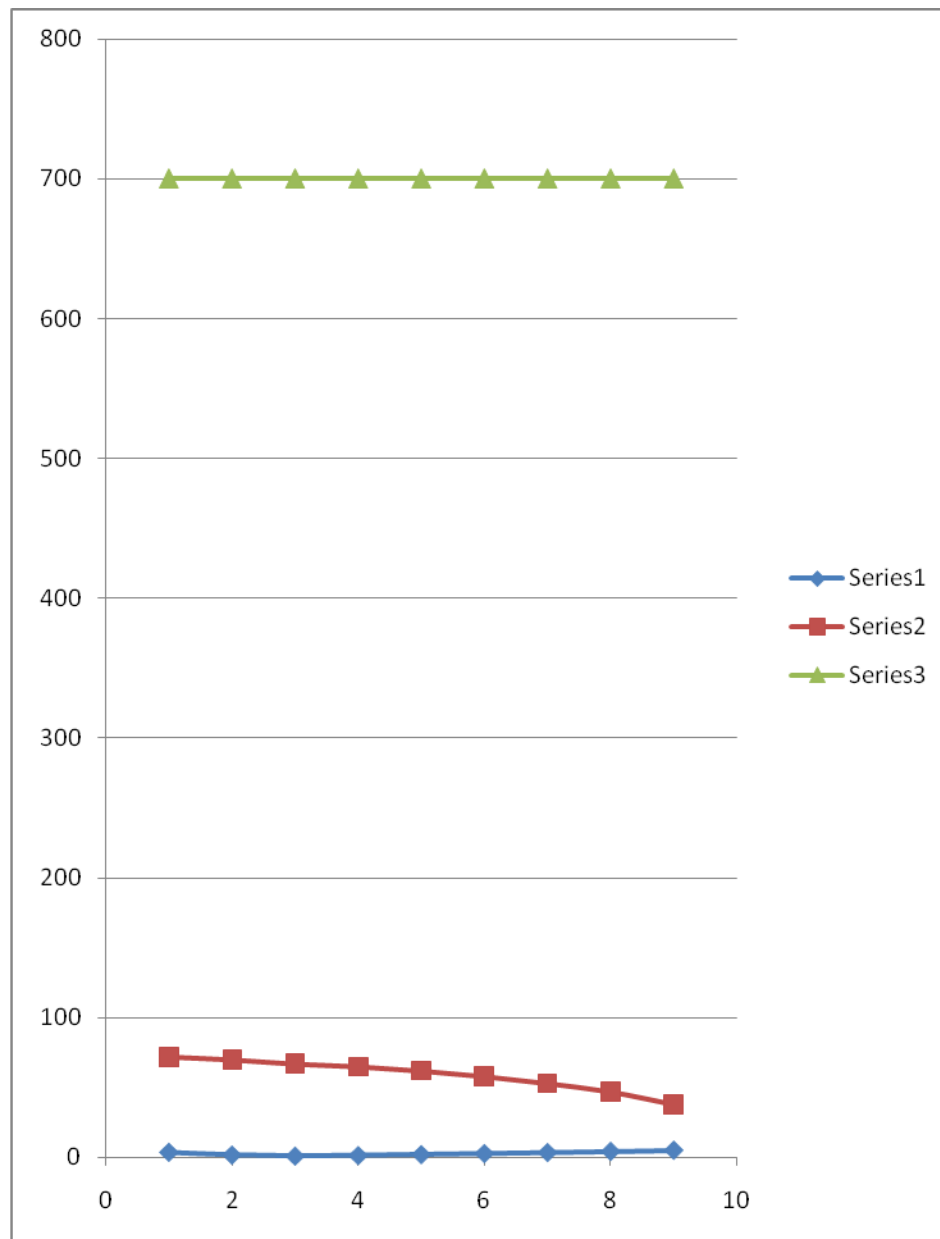


Figure 4.36. Scatter chart, where Series1 is pre-amplified input signal, Series2 is Primary side signal with trap, and Series3 is Secondary side signal with trap

4.2.3.2.2.4 Test of transformer DA2034



Figure 4.37. Test circuits

Table 4.12. *Amplitude fixed test*

Input $V_p=1V$ without trap with trap

Fre	First	Second	First	Second
100k	9	90	9	90
200k	18	175	21	200
300k	35	330	48	475
400k	75	700	75	760
500k	75	700	36	380
600k	45	450	22	260
700k	35	340	16	200
800k	25	260	11	160
900k	16	200	8	140
1M	12	175	6.5	120
1.1M	9	160	3.7	110
1.2M	7.5	140	2.3	100
1.3M	6	130	1.6	90
1.4M	3.5	120	2	80
1.5M	2.5	110	3	75
1.6M	1.8	105	4.2	75
1.7M	2.3	100	5	74
1.8M	3.3	95	6	70
1.9M	4.3	90	7	69
2M	5.2	85	7.8	69

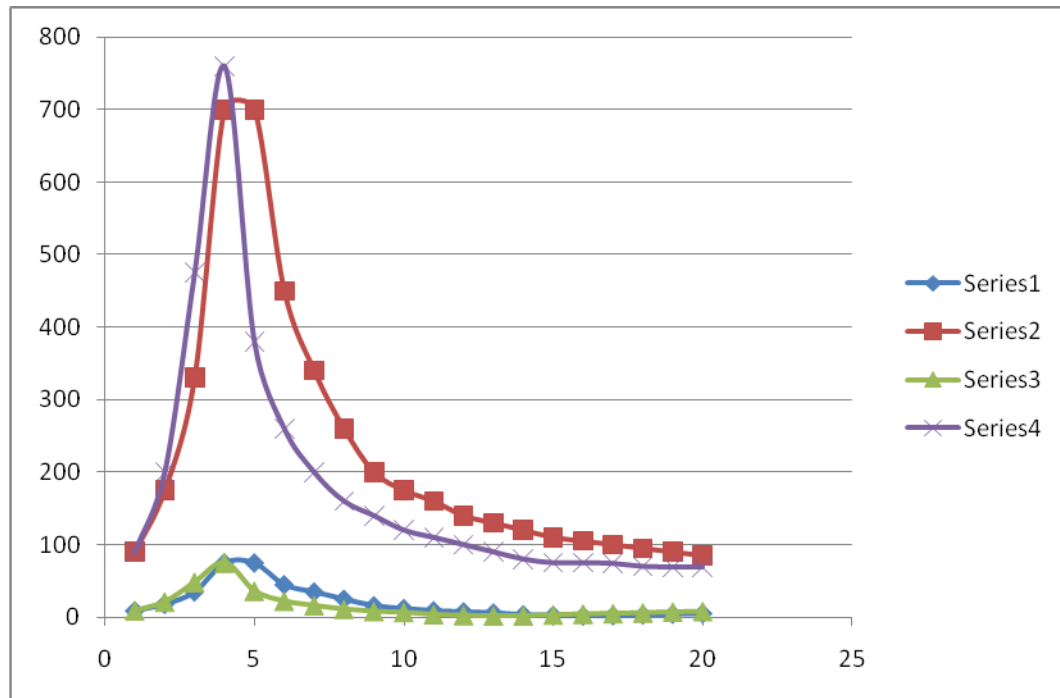


Figure 4.38. Scatter chart, where Series1 is primary side signal, Series2 is secondary side signal, Series3 is primary side signal with trap, Series4 is secondary side signal with trap

We have tested many kinds of transformers. WBC16-1TLB, GA3460-BL, PWB-16-BL, CJ5143-ALB, DA2032, DA2033, DA2034, etc, were all carefully tested.

From the experiments, we found that some transformers have very good frequency response, like CJ5143. However, they could not bear very high voltage. Some transformers could work well at very high voltage envelopment, but they do not have very good frequency response, like DA 2034. Comparing different transformers, DA2032 is a better one. Certainly it is not perfect. However, it can work at very high voltage, and also has quite stable frequency

response. That is, the high voltage amplification is stable at quite a long range frequency.

In order to make clear the response of the transformer at high frequency and high voltage, the relationship between input (primary side) and output (secondary side) signals of transformer DA2032 (1:10 ratio) was carefully tested. When the output of the power resource was fixed at $V_{p-p}=2V$, signals at both primary and secondary sides were collected. From the log chart of the data, we can see that resonance happened at the frequency around 400 kHz.

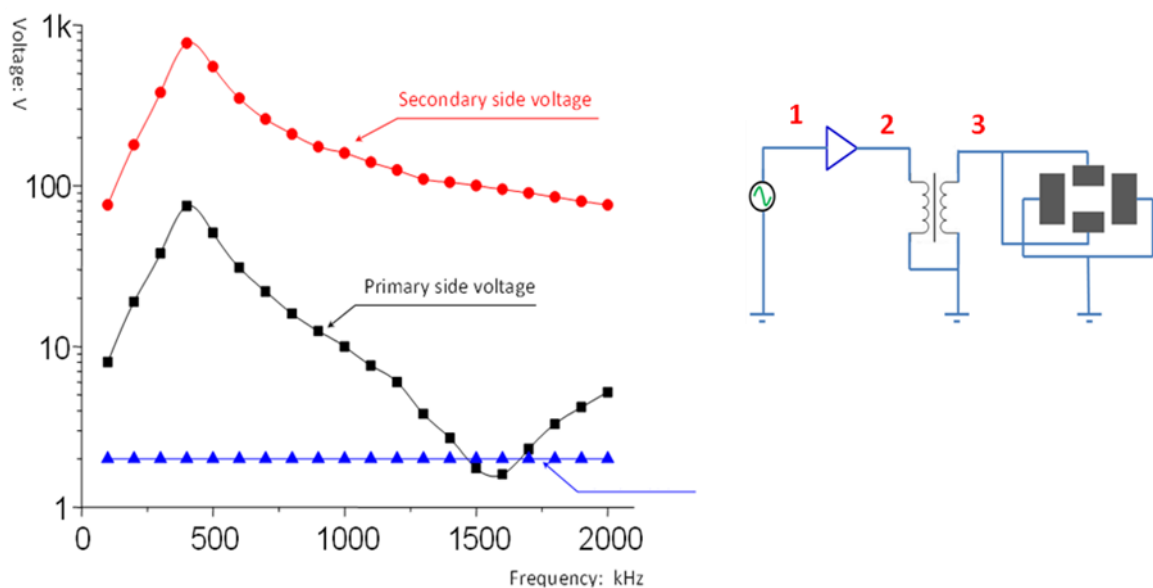


Figure 4.39. Relationship between primary and secondary signals of transformer DA2032

When the transformer is used to generate RF signal for RIT, an output signal with constant amplitude but tunable within a relatively wide frequency range is desired. Feedback circuits can be designed to compensate the resonance effect. The next experiment was designed to test the input signals

when the output (secondary side) voltage of the transformer was fixed at $V_{p-p}=700V$. The input (primary side) voltage of the transformer and the output voltage of the power resource were monitored.

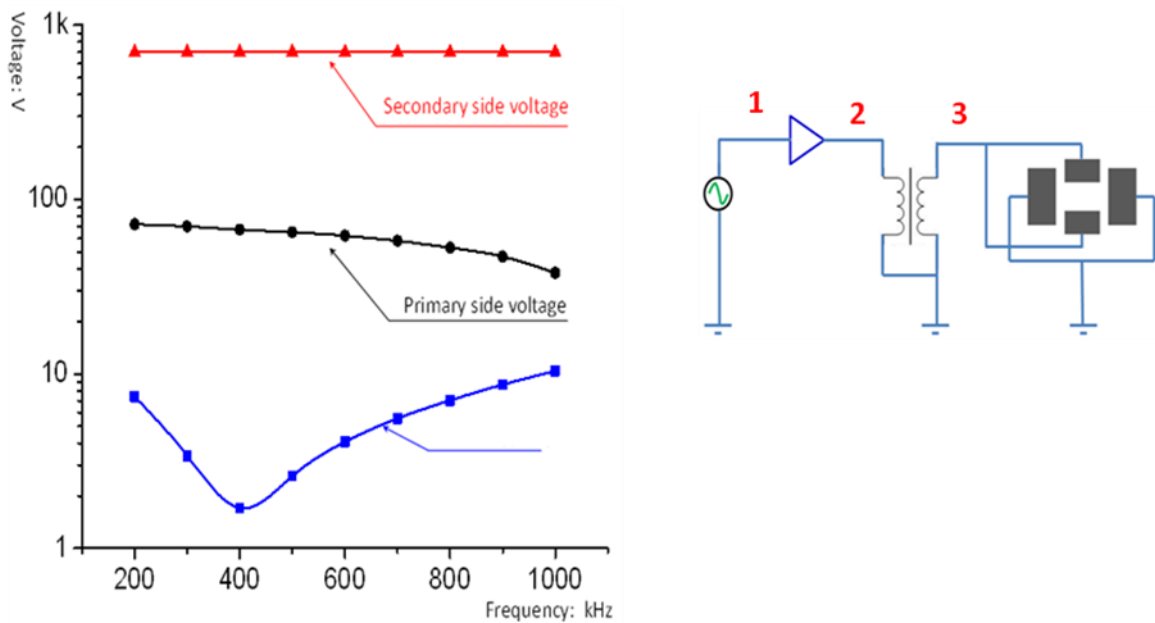


Figure 4.40. Signals of the primary side and power resource when the secondary voltage $V_{p-p}=700V$

From the carefully retest of DA2032, we can see that this transformer has very good frequency response below 1MHz and voltage handling capability.

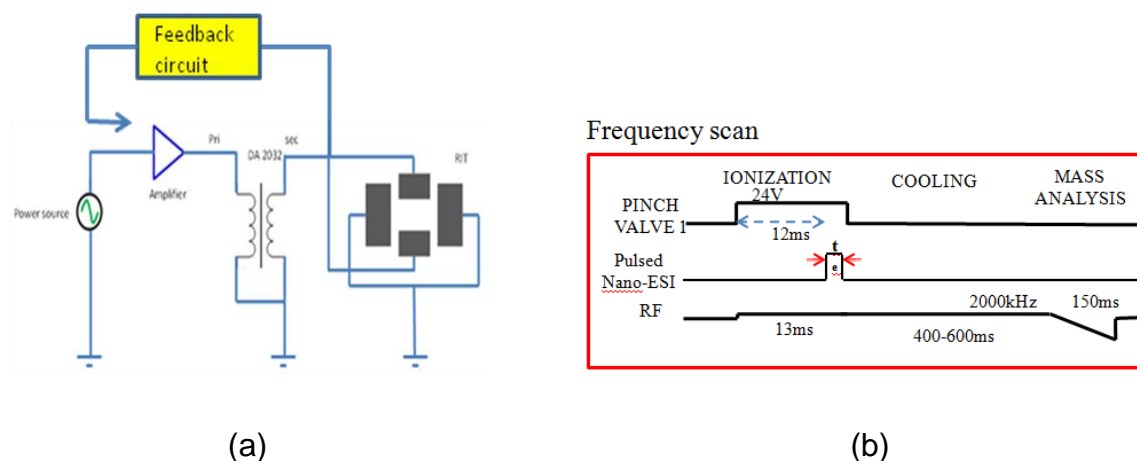


Figure 4.41. (a) Future design on feedback, (b) Frequency scan

Feedback circuit will be designed so that the output RF voltage can be adjusted and fixed at certain amount to do frequency scan analysis.

$$q = \frac{2Z|e|\tilde{U}}{m\omega_{rf}^2} \quad (4.6)$$

From the equation 4.6, due to the square of frequency at the denominator part, we can see that frequency scan will have more efficiency and speed. RF voltage can be very low and it will open a new era of mass spectrometry instrumentation, especially for miniature of mass spectrometers. Comparing to digital methodologies to apply frequency scan, a transformer has advantage that it can take in any form of sinusoidal wave or the combine of sinusoidal waves. So it is possible to optimize the scan function by trying different kinds of waves to find the best one which can enhance the highest efficiency and resolution mass spectrometry.

There are still some problems with transformer comparing with LC, such as noises, energy consumption. However, it is really a meaningful try and could lead to a evolution of mass spectrometer control system.

4.3. Chapter Summary

This chapter covers the main research works, including the processes and data from the experiments. It gives an overview of the research and the possible future applications of the research achievements.

CHAPTER 5. CONCLUSION

Control system of ion trap mass spectrometer was studied. With the goal to develop a noble control system for lab-use mass spectrometer, a LabVIEW system was designed and built. The LabVIEW system was used as control system in some projects, and the results show its advantages. Transformers were tested and a good one was chosen from them. A broadband RF circuit will be developed based on its advanced characteristics both in high voltage and long-range frequencies. Due to the higher efficiency and low voltage level, frequency scan will open a new era of miniaturization of mass spectrometer.

A lot further work should be done to revise the system and develop a good broadband RF circuit for mass spectrometer. Some very new ideas were tried in my projects, which are good beginnings of seeking for solutions and bottleneck.

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