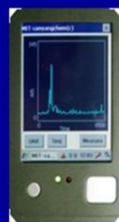
Design of Pocket Mass Spectrometer in a Mobile-Phone Size



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My name is Mo Yang from Korea Basic Science Institute.

Everybody here knows that a mass spectrometer is the most powerful analytical tool in chemistry. However, the target samples you want to analyze are very often not in the laboratory but in the field and often you have to detect them in real-time before the sample changes composition.

Then the mass spectrometer should go to the field, in your hand, small as possible, light as possible, and operated with light battery.

So I would like to discuss how small a portable mass spectrometer can be.

Outline

- Motivation for Pocket Mass Spectrometer
- Palm Portable MS Developed
- Further Shrinking-MS Technologies
  - Ionization, Ion Separation, Ion Detection
  - Vacuum System, Sample Concentration
  - Electronics, Power Supplies
- Custom-Made MS
  - Requirements for Pocket MS
  - MS in Harsh Environment
    (Sprite Discharge Environment)

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I would first talk shortly about what is driving interest in pocket mass spectrometers.

And I will show you a previously developed Palm Portable Mass Spectrometer. This PPMS was introduced 4 years ago in this HEMS workshop. After that I received dozens of emails, asking me whether a commercial PPMS would be available. Some of them were asking for just a couple of prototype PPMS. But I am sorry that I could not reply yet because of some reasons.

Anyway we are now implementing a new project that reduces the size of the PPMS again, this time in a mobile phone size. So the shrinking technology should be discussed today, and compared with the PPMS. The shrinking technologies include the tiny ion trap, vacuum and sampling system, and control electronics with various power supplies.

The next problem for the commercial product of portable MS is that every application has different target samples and requires specific capabilities for their own purpose.

If a portable MS could have all universal capabilities, then it would be fancy but I would say that it is not real.

And more functions the portable MS has, then it becomes larger and heavier.

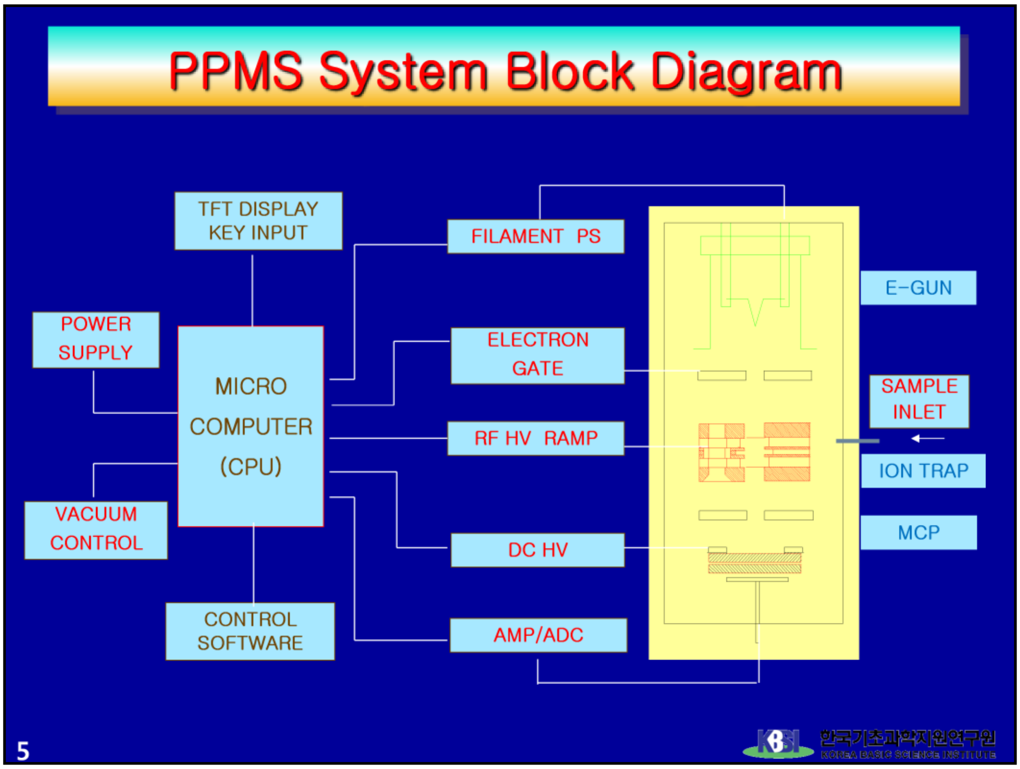
But in the field, you do not want to carry unnecessary functions all the time without use.

So a reasonable solution should be a custom made mass spectrometer, designed compact for your own purpose only.

Sometimes you also need a MS that is able to operate in a very harsh environment. I will talk some about that at the end.

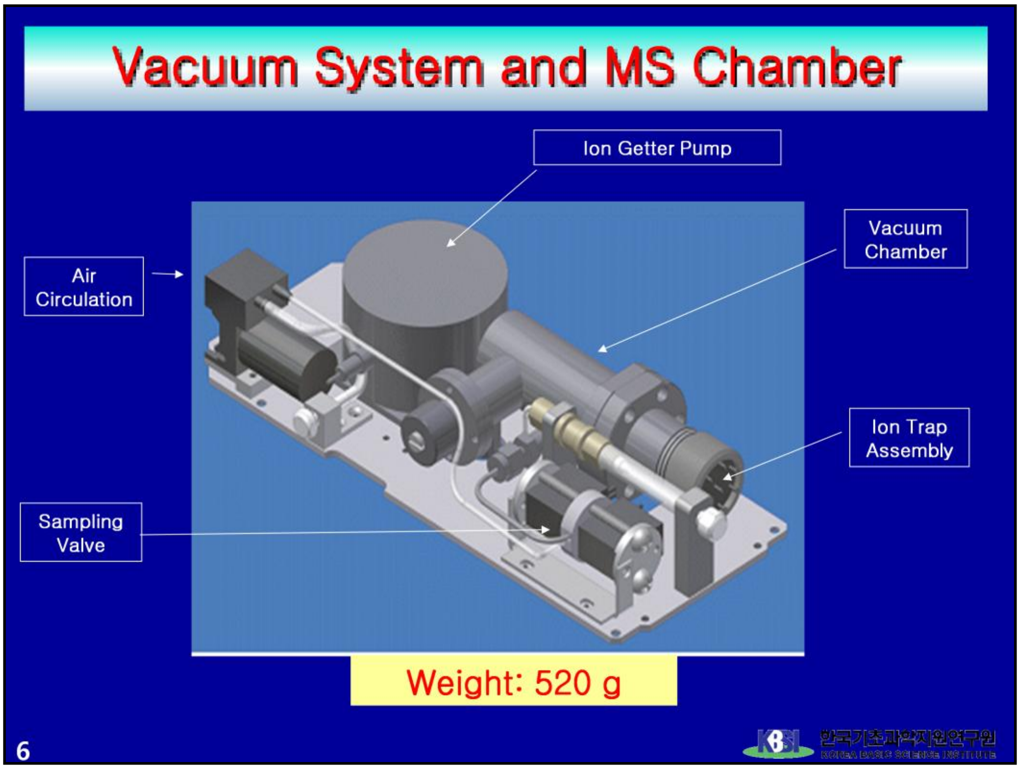
A portable mass spectrometer is needed in various application such as military use for CWA detection/identification, environmental monitoring of air pollution, homeland security for explosives/drug inspection, rapid food screening for perishable foods, and space exploration for gas analysis on a planet surface.

This Palm Portable Mass Spectrometer was developed years ago initiated by a military interest. So far this is the world's smallest mass spectrometer yet as far as I know.



This is the basic system block diagram of the PPMS.

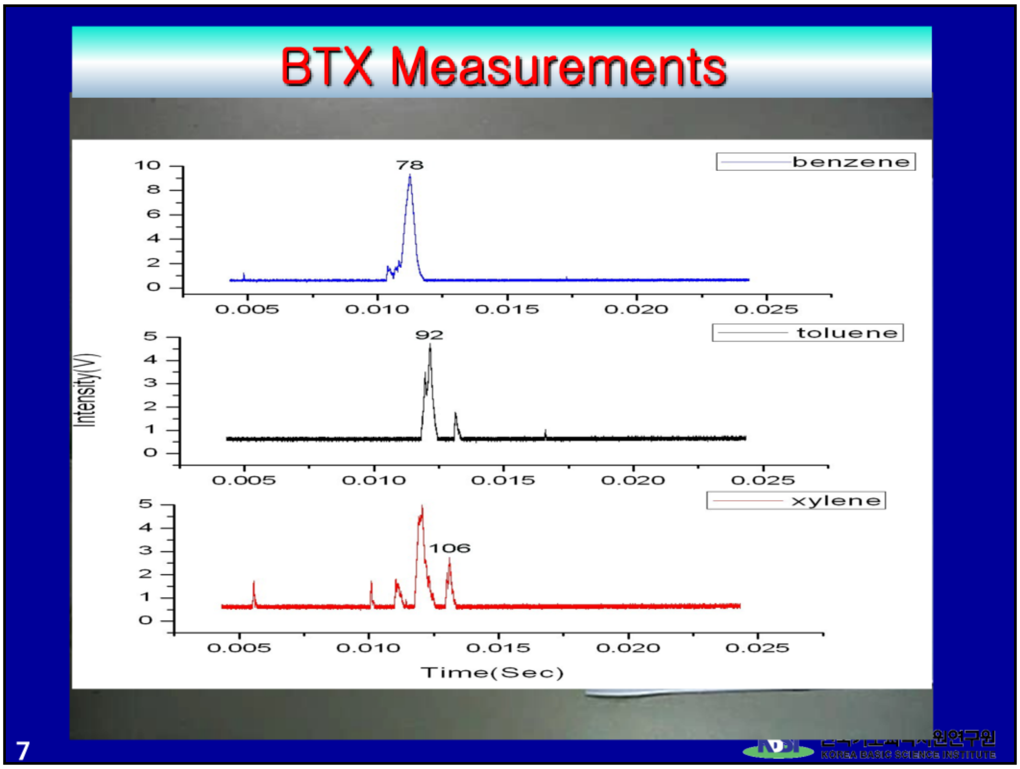
Here is the electron gun, ion trap, MCP ion detector, and control electronics, just as usual ion trap MS.



This is the vacuum and gas sampling system.

The tiny ion trap can be found in this chamber, here is the ion getter pump, and here the gas sampling system.

It weighs total 520 g but it can be much lighter by cutting off the unnecessary metal flanges and chamber.



People say that proof of pudding is in the eating. Let's take a look at how it works.

(demonstration video)

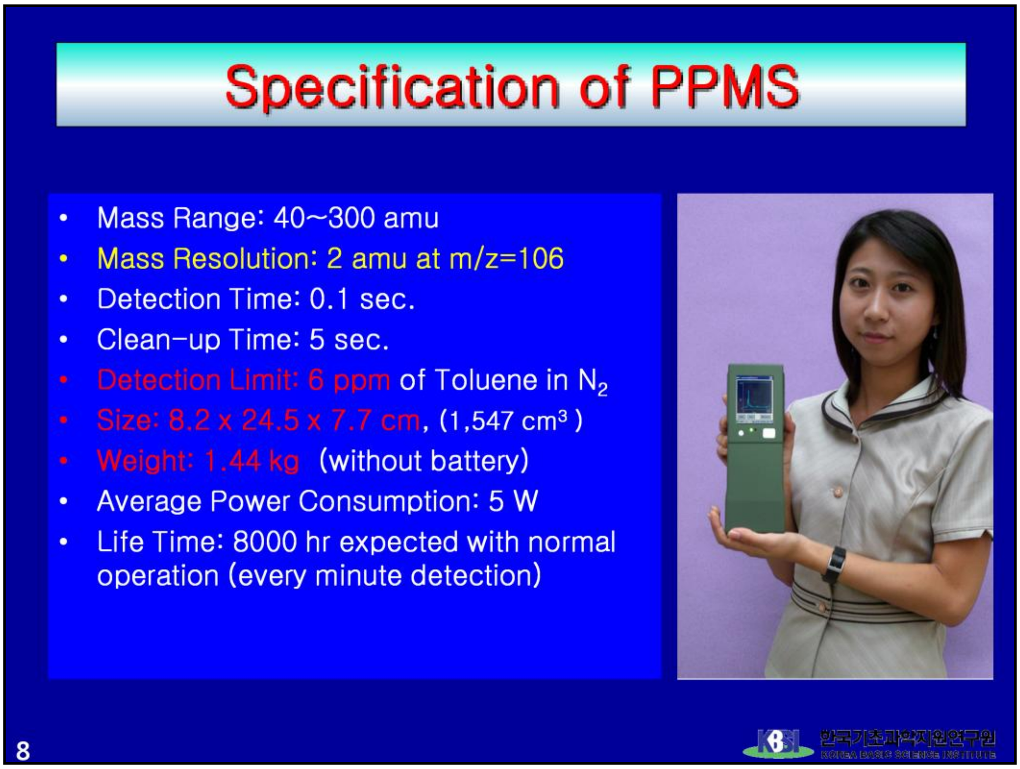
When you turn on the power, the software checks every part, including power supplies and vacuum pressure in the chamber, and then turns on the ion getter pump. And if the vacuum pressure is high enough then the software checks on the electron gun, RF generator, ion detector, signal amplifier, etc.

Should everything be all right, then it displays "ready to measure" and waits for a command. It takes a couple of minutes, depending on the vacuum.

For every measurement, you should first measure a blank sample. And make sure that there is no signal. Then approach the sample targets. In this case, we are demonstrating benzene, toluene, and xylene.

After the measurement you have to check up the blank sample again. Here you see some memory effect, but it disappears with time.

Right here is the measured data saved in the memory. Display the results in a computer screen, then it looks like this.



These are the specifications of the PPMS

The mass resolution is not very high but the resolution is generally not that serious in the military use for CWA detection.

In fact if you compare this resolution with that of a IMS, this should be excellent.

The detection limit of 6 ppm is not very good. It should go down to at least 10 ppb.

The size is 1.5 liter and 3 pounds – this is the smallest MS so far – but still too big to carry in the battle field for a combat soldier.

So what should we do?

Next Challenge in
Shrinking Mass Spectrometer

1. MS in Mobile Phone Size
2. High Sensitivity
3. GC/MS in Pocket Size
4. Custom-Made MS
5. Harsh Environment

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The next challenge should be, first of all, shrinking the mass spectrometer small as possible.

Well, pocket portable in a mobile-phone size would be acceptable.

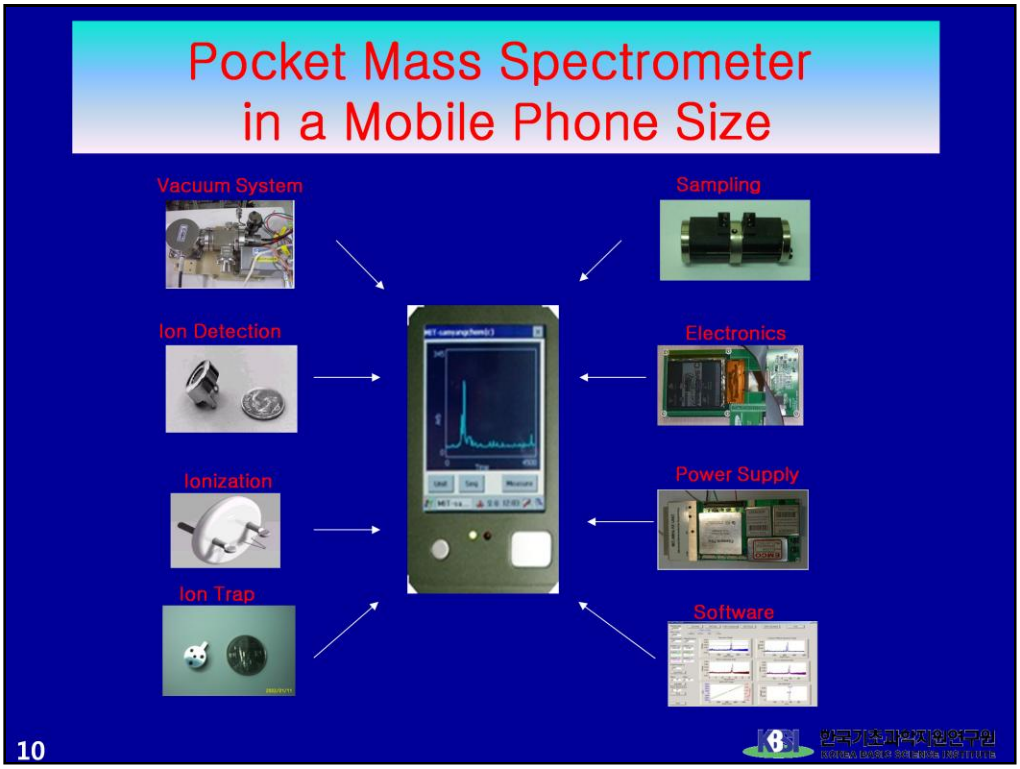
The detection limit should be much enhanced. At least up to human nose sensitivity.

Addition of chemical separation GC in a pocket size MS would be great.

Custom-made MS means that its detection capabilities and features should vary for every application.

Sometimes it might need to operate in a harsh environments such as in a glow discharge plasma.

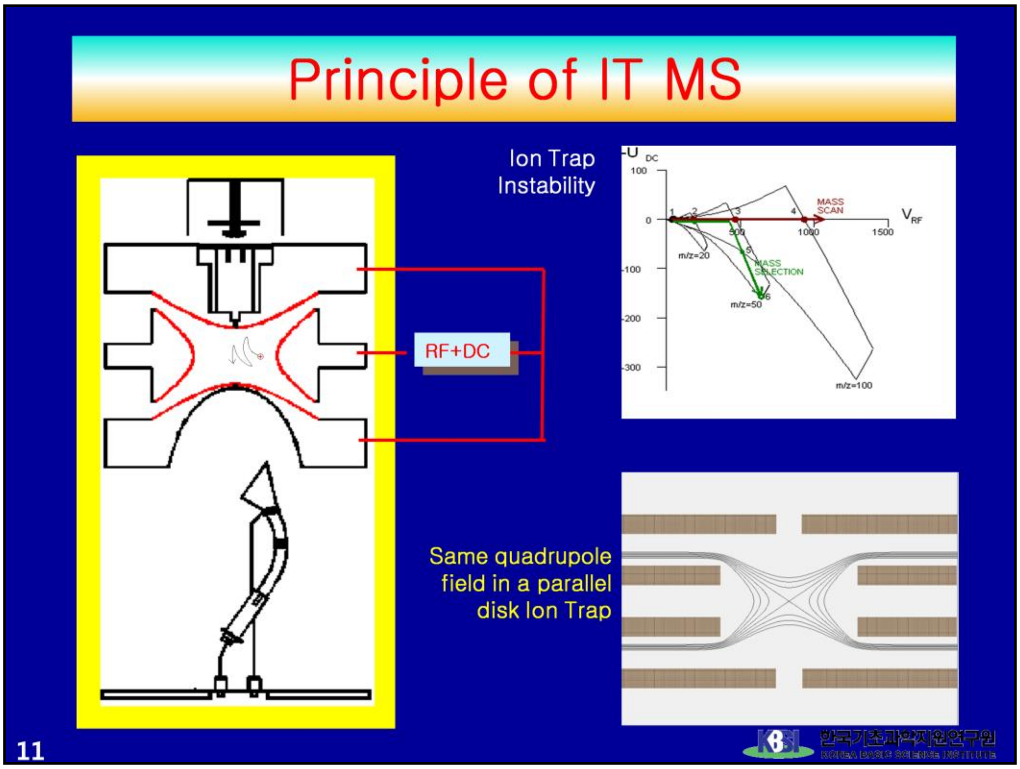
For the time being, our effort in this project is being concentrated in number one and two.



An ion trap is a very smart ion separator that does not lose the MS capabilities even in a very small size.

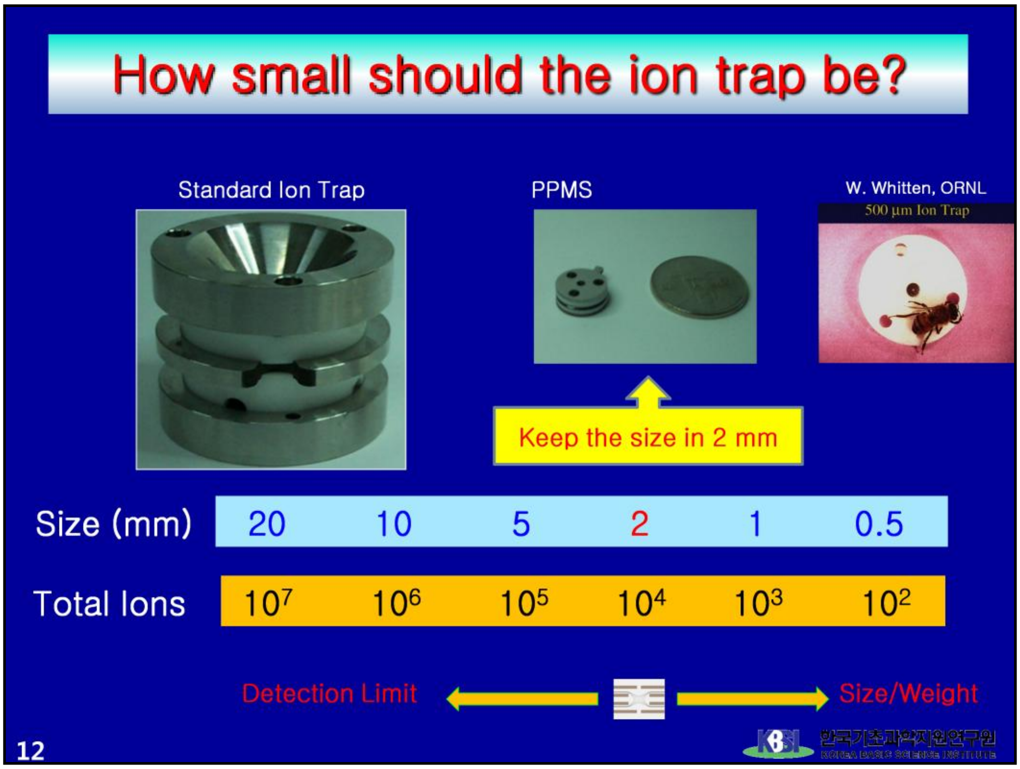
But a small ion trap does not mean a small mass spectrometer.
All other peripheral parts should be small too for a pocket portable MS.

How small can all these parts be reduced?



Do I need to introduce what an ion trap is? Well, skip this.

We have introduced in PPMS a new Ion trap geometry as four parallel disk ion trap with center hole. As you can see here, it can make a quadrupole field very same to the standard hyperbolic ion trap. This means that in this geometry the instability diagram is as good as in the hyperbolic ion trap.



This (left) is an old standard ion trap from Finngian MAT. Inside diameter is 20 mm and out diameter is 60 mm.

This (center) is the ion trap used for PPMS, inside diameter is 2 mm . And this (right) is the 0.5 mm ion trap from ORNL. Bill Whitten made this.

The question is what size of the ion trap should be the best.

Smaller the size then the total number of trapped ions is also smaller because of the ion repulsion force.

So in this direction, smaller size would be an advantage but at a cost to the detection limit.

In the other direction, should the total number of ions be enough, then the size should be larger.

Compromising between the size and the number of total ions, I think that about 2 mm ion trap would be appropriate.

The size of the complete mass spectrometer is anyway determined not by this ion trap size but by many other parts.

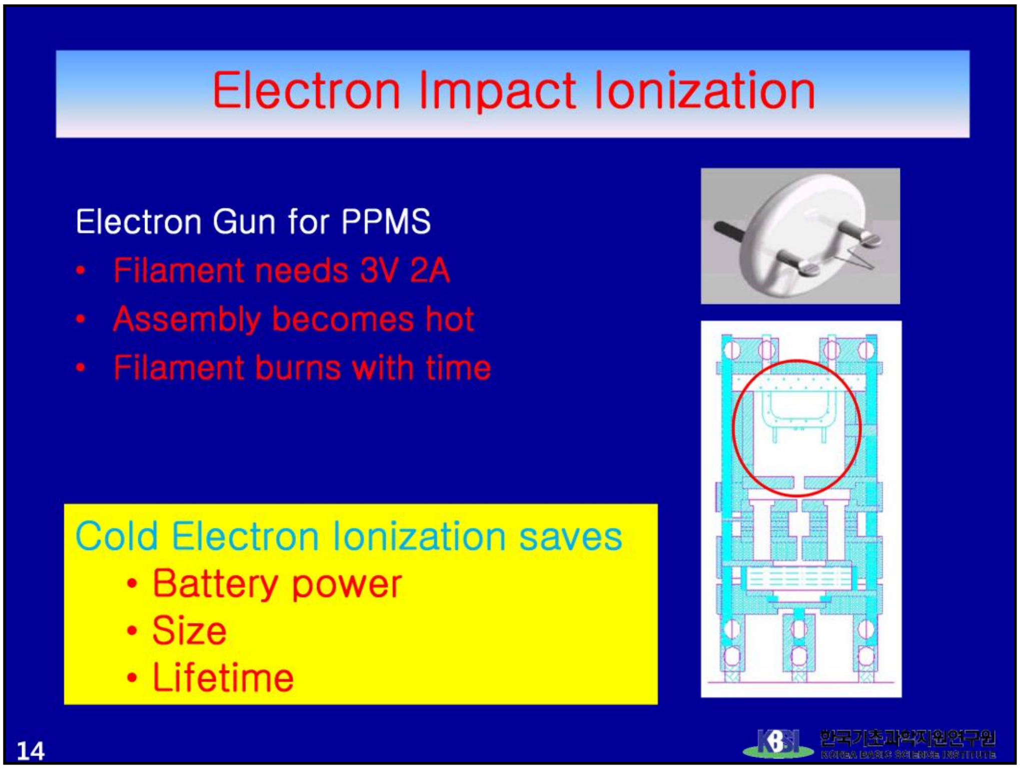
This is the cross section of the ion trap assembly in the PPMS.

(Video)

The size is 16 mm diameter and 42 mm height. But there are 74 SS and ceramic parts assembled together.

Here the active space of ion trap is so small and the other parts are just for mounting and electric connection.

If you precisely design it then the assembly size can be reduced with the same ion trapping volume.



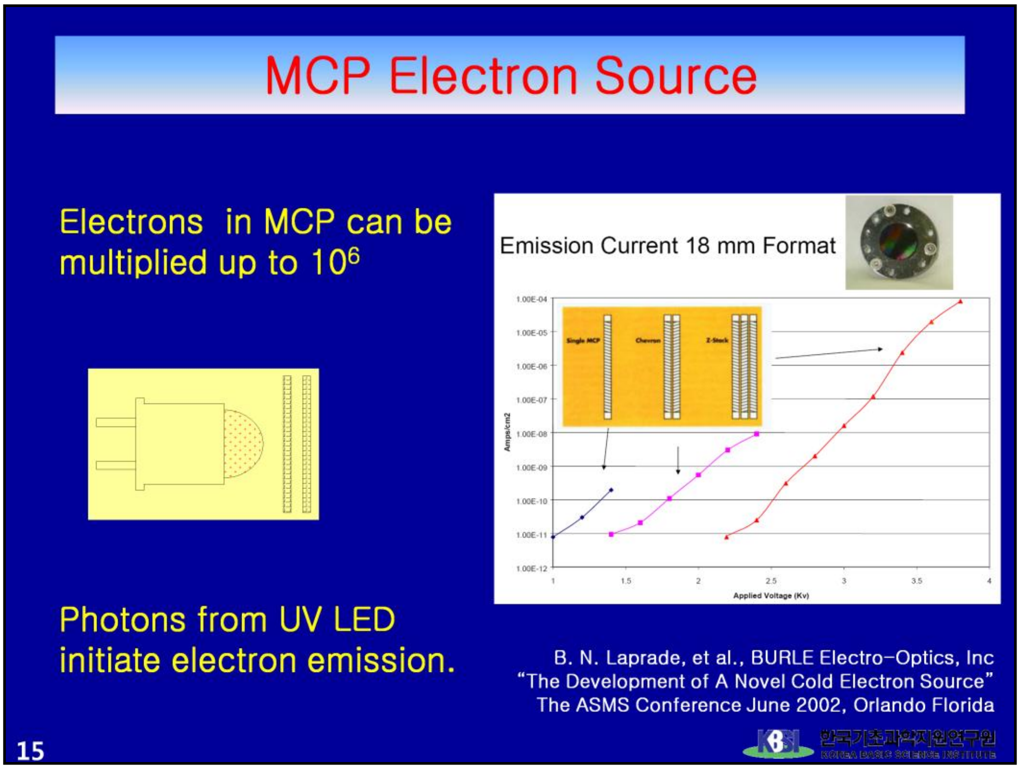
The first attempt to reduce the ion trap assembly is with the electron gun.

E-gun needs 3V 2A and becomes very hot, so this region needs a large space to diffuse the heat.

And the filament burns with time.

So, a cold electron ionization would be nice for saving battery power, reducing the size, and extending the lifetime.

But how?

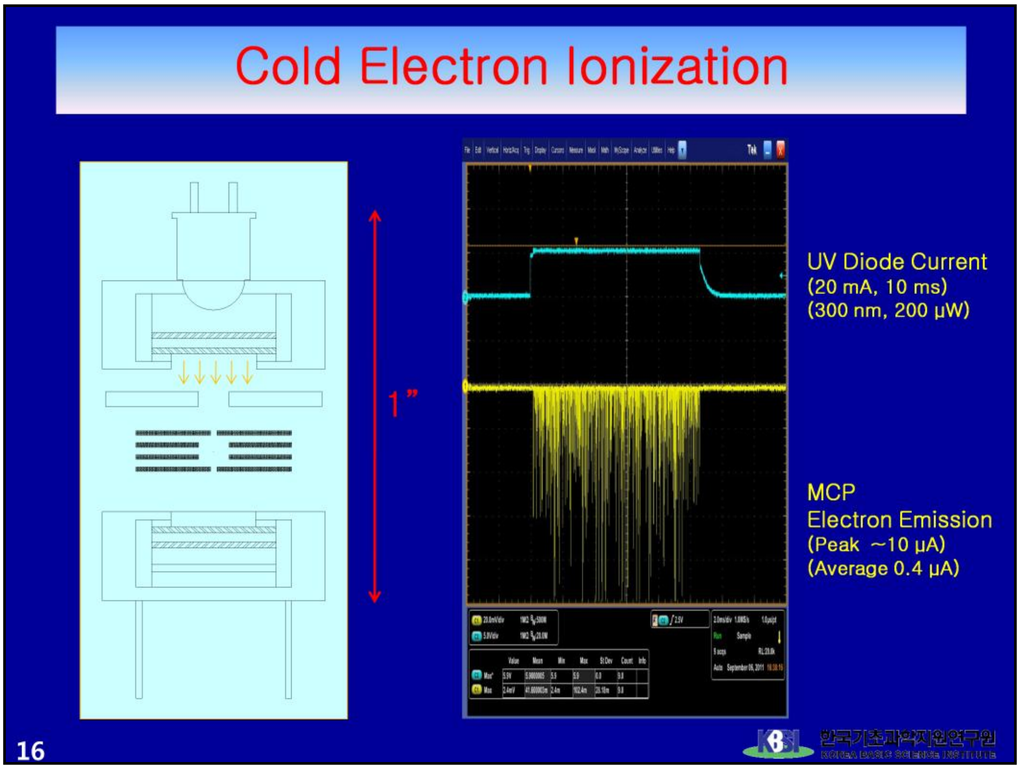


This picture is from ASMS archive, presented by BURLE Electro-Optics Company 10 years ago, introducing a cold electron source.

One muti-channel plate generates electron emission at about 0.1 pico ampere with 18 mm MCP.

Two plates, then 10 nano ampere, and three plates then up to 10 micro ampere.

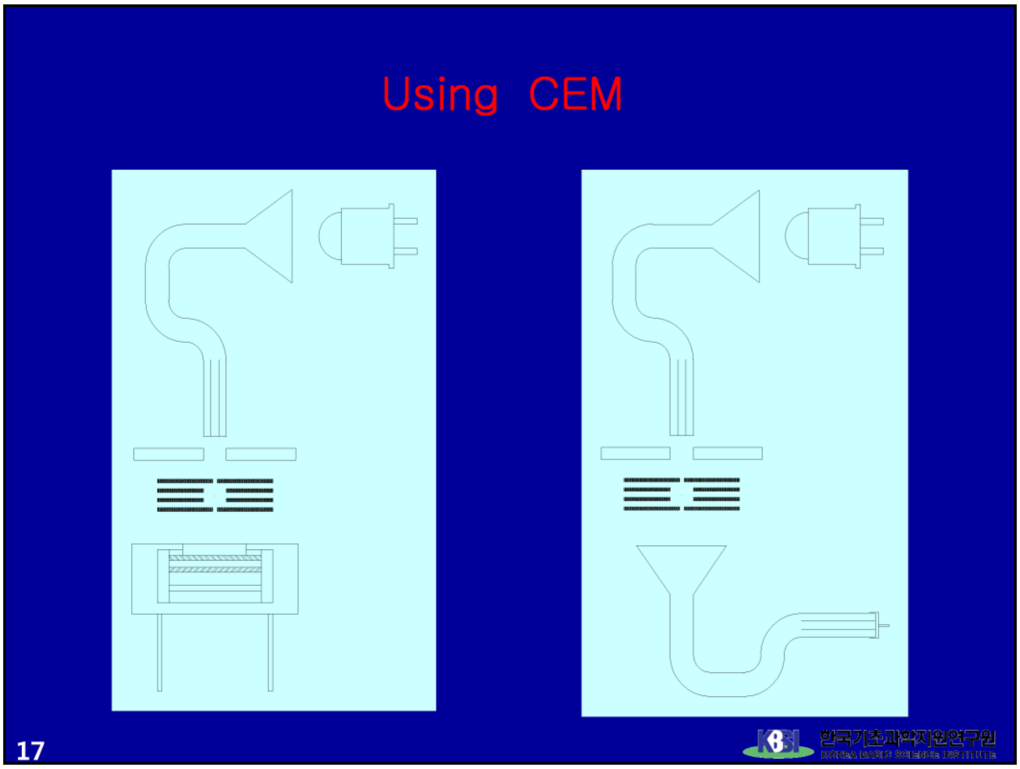
How about using a UV diode for initiating electron emission? A decade ago, there was no UV diode with a wavelength shorter than 400 nm available commercially but now it is different.



The UV diode is mounted in front of a 5 mm MCP and we measured the electron emission.

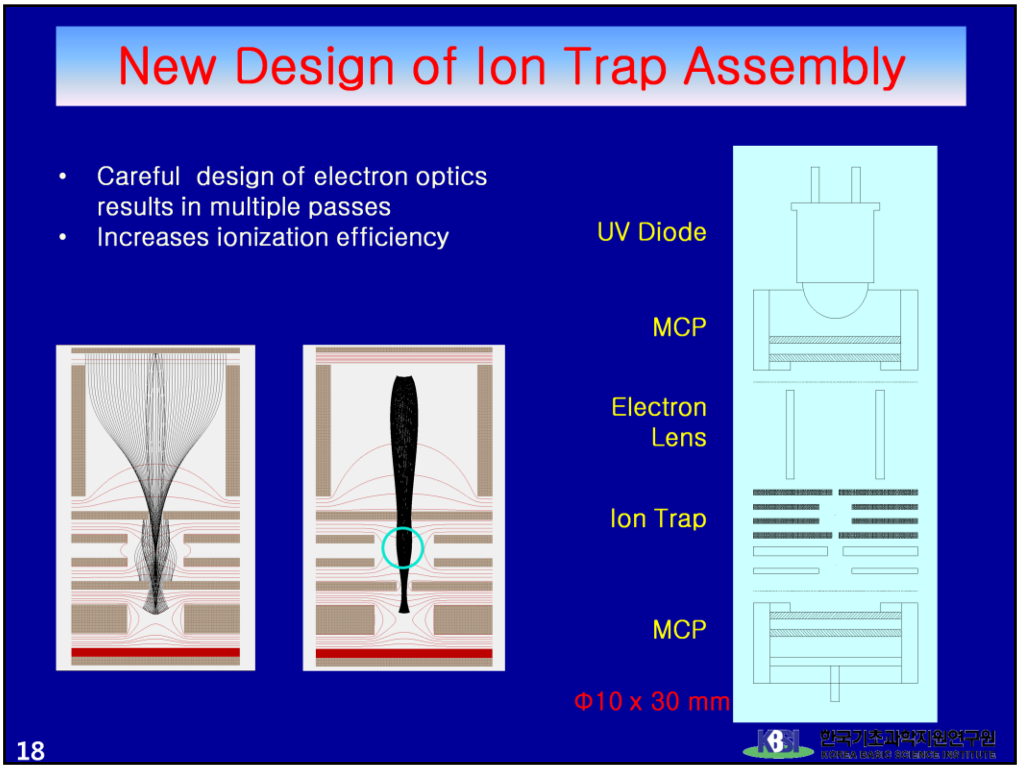
Take a look at the electron current. We estimated the number of electrons up to 10 to the order of 10.

That should be enough for ionization in a mass spectrometer.



This is another possibility, using CEM.

The electron focusing would be better but the size becomes about 10 mm bigger.



If you carefully design the electron optics, then an electron can fly back and forth hundred times.

This geometry will enhance the ionization efficiency.

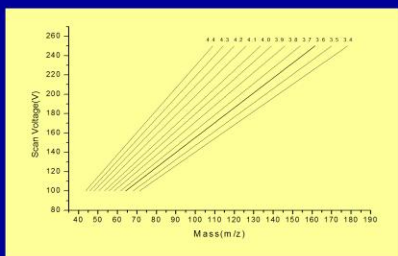
So final design of the ion trap assembly looks like this.

The size would be 10 mm diameter with 30 mm height. Then the volume is about 3 cm^3.

RF High Voltage for PPMS

- Ion trap instability: $q_z = -8eV / m r_o^2 \Omega^2$
- RF at 3.900 MHz with 1500 Vpp max.
- Mass range: 300 amu.

Mass vs. Voltage by Different RF Frequency



RF Module developed for PPMS

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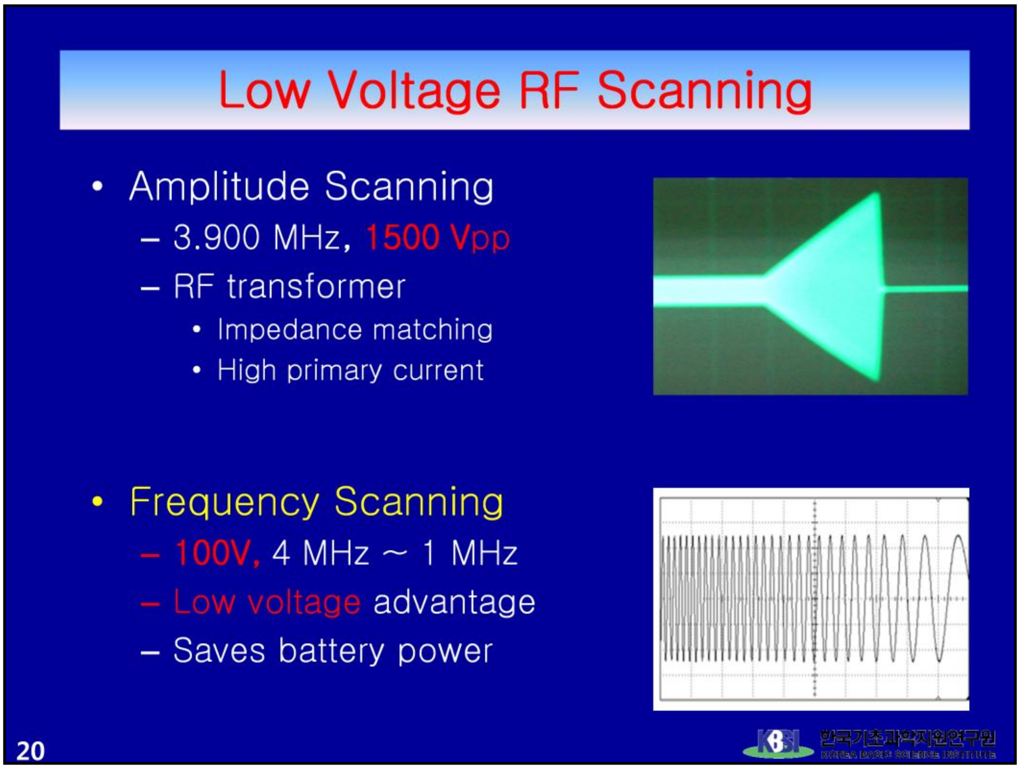
For the 2 mm ion trap, 1500 Vpp with 3.9 MHz was good for mass scanning up to 300 amu.

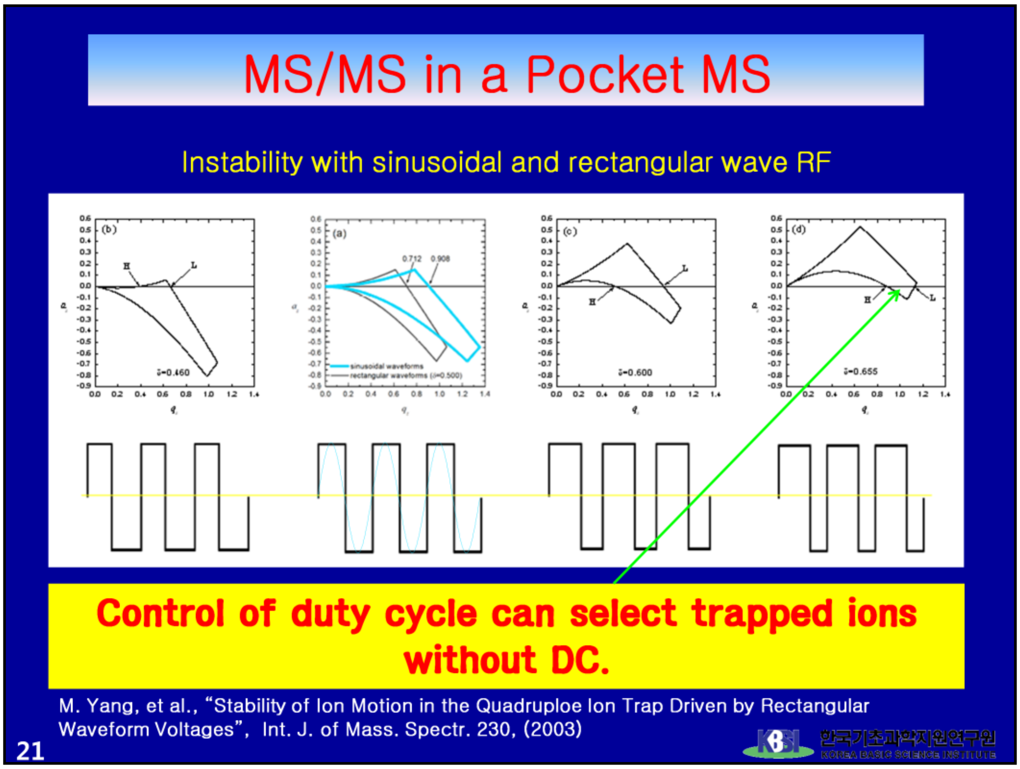


Generally RF voltage scanning is used in an ion trap mass spectrometer.

But in a circumstance when high voltage is not allowed, then frequency modulation is another alternative.

For ion mass up to 300 amu with 100 V, frequency modulation should be from 4 MHz to 1 MHz.

Another advantage of frequency modulation is that it saves high current for RF transformer. So much of battery power will be saved.



Some people ask me whether MS/MS could be possible in such a small mass spectrometer. I would say yes.

Here the blue figure is the ion trap instability diagram with sine wave RF.

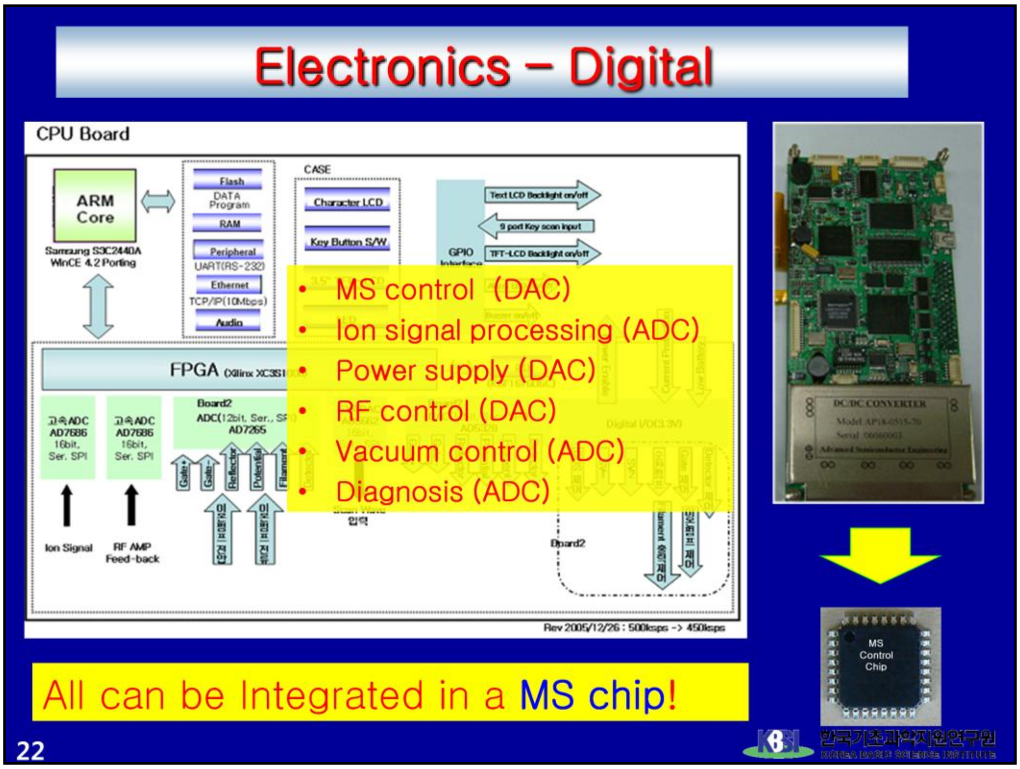
But with a rectangular waveform of RF, the instability diagram changes like the black area here.

One interesting result is that when the duty cycle changes, for example positive phase is shorter than negative, then the instability changes like this(left).

In the other direction, the positive phase is longer than the negative, then the instability region bends up a little bit. Change the duty cycle more, then like this(right).

This means that with control of the duty cycle in the rectangular waveform, you can select trapped ions without using extra DC voltage.

Then it is possible to measure the fragmentation mass spectrum following a collision induced dissociation.

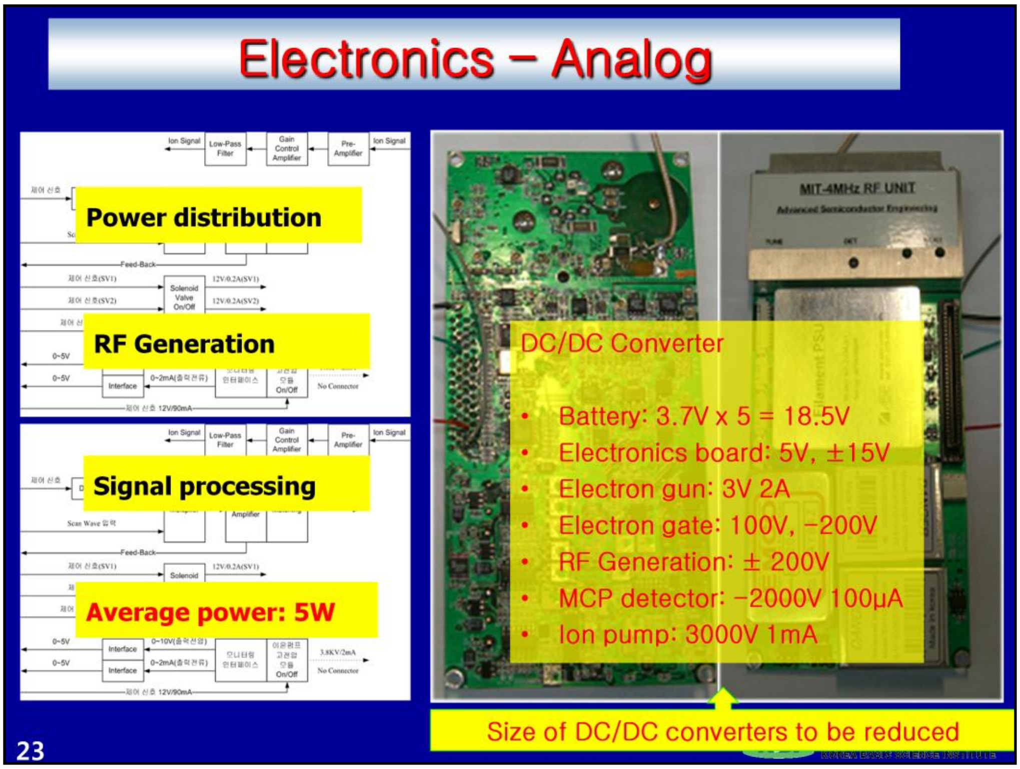


Control electronics are two different categories. One is digital electronics, and the other one is analog electronics.

In this board, ARM9 central processing unit and FPGA (field programmable gate array) accommodate the ion trap control programs and manage various DAC and ADC for ion trap operation.

They all can be integrated into one IC chip. We once asked the people in Samsung electronics if it would be possible to get a chip like this. They asked me back "How many do you need?"

For the time being I have no right answer but if many of you are interested in this and the quantity goes up, then this kind of MS control chip will be soon realized.

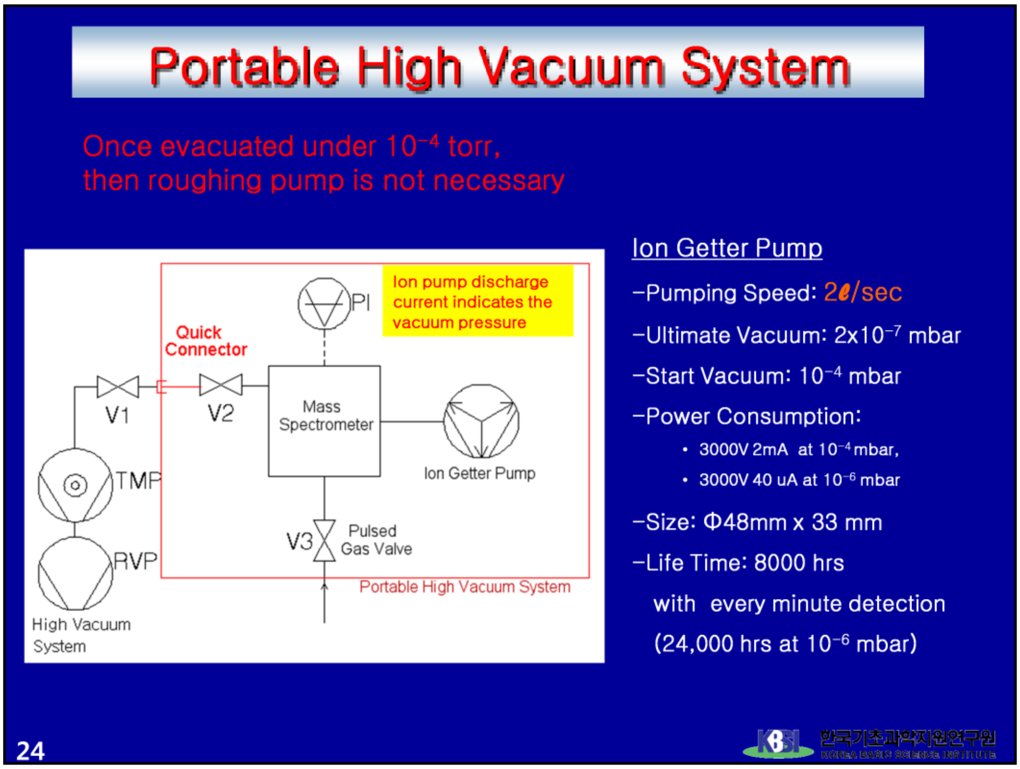


The main functions of the analog board are providing various voltages and generating HV RF.

There are 8 different voltages required but all of them must be supplied by a single battery.

A stack of individual DC/DC converters takes up a large space.

Reduction of size is technically not difficult but it also has to be custom-made. It is also a matter of quantity or money



The biggest technical challenge in shrinking a mass spectrometer is the vacuum system.

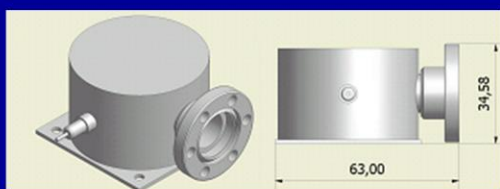
One thing I want to point out here is that the PPMS has no roughing pump. It works with an ion getter pump only.

Of course the ion pump works under 10^{-4} torr. But once this system is evacuated, then the PPMS is detached and the ion pump does not need the roughing pump, even after several days of shut down.

So the vacuum is checked in the morning once, just like you check the battery everyday, and then you do not need to carry the roughing pump all day long without use.
This is the same as you not needing to carry the i-phone battery-charger all day long in your pocket.

Miniaturized High Vacuum Pump

	PPMS	Pocket MS
Chamber Size	9 cm^3	3 cm^3
Ultimate Vacuum	$2x10^{-7}$ mbar	$2x10^{-7}$ mbar
Pumping Speed	2 ℓ/sec	0.7ℓ/sec
Power Consumption	3000V 2mA Max	3000V 0.7mA Max



Ion Getter Pump
for PPMS

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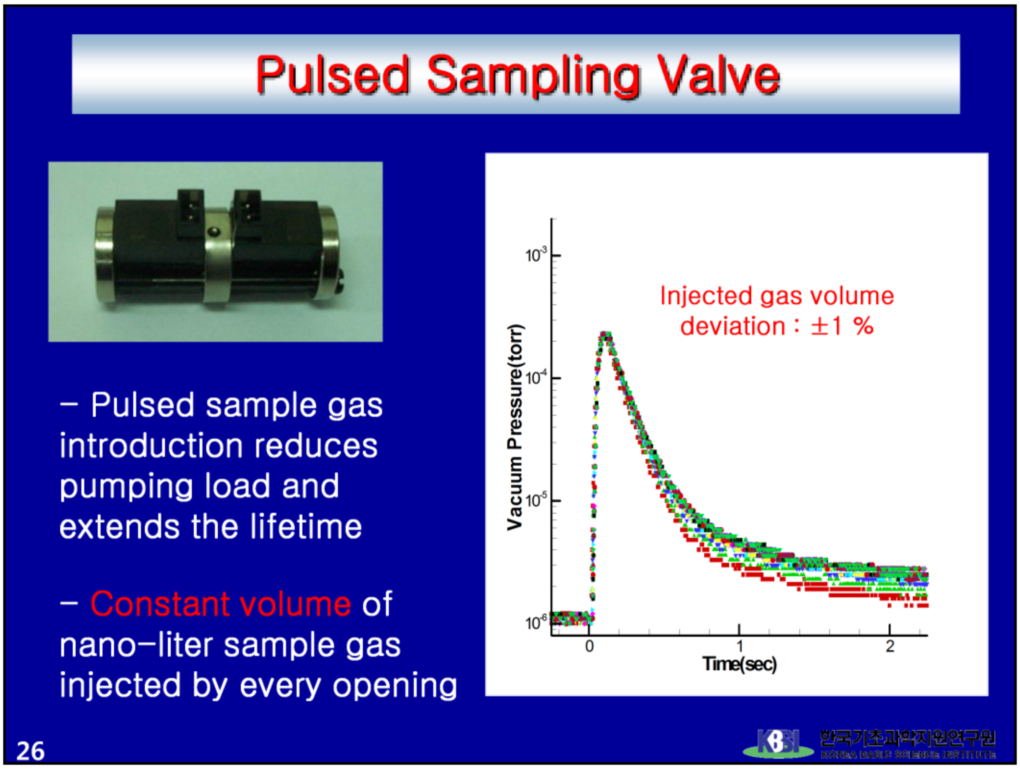
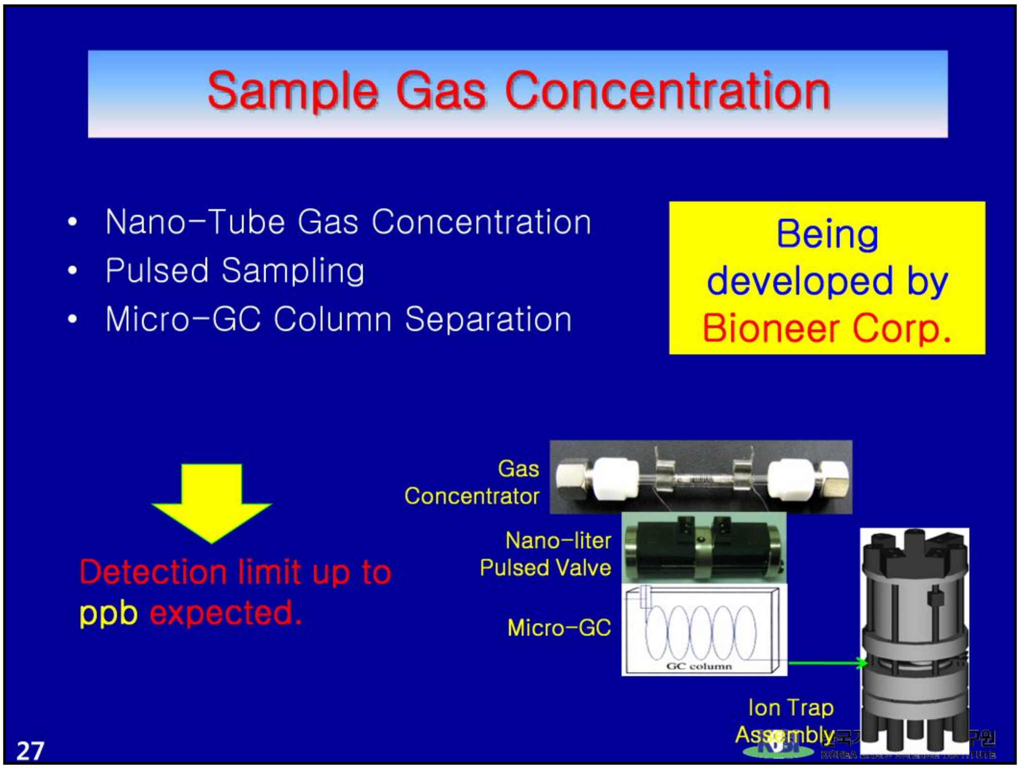
The size of the ion pump can be reduced by half when the chamber volume is reduced.



This pulsed sampling valve is very important because it injects just a nano liter of air sample only when you measure.

You do not need to introduce air gas continuously and pump out which wastes battery energy in a portable MS.

Very nice here is that it always injects a constant volume of air sample so it makes a consistent mass spectrum every time.

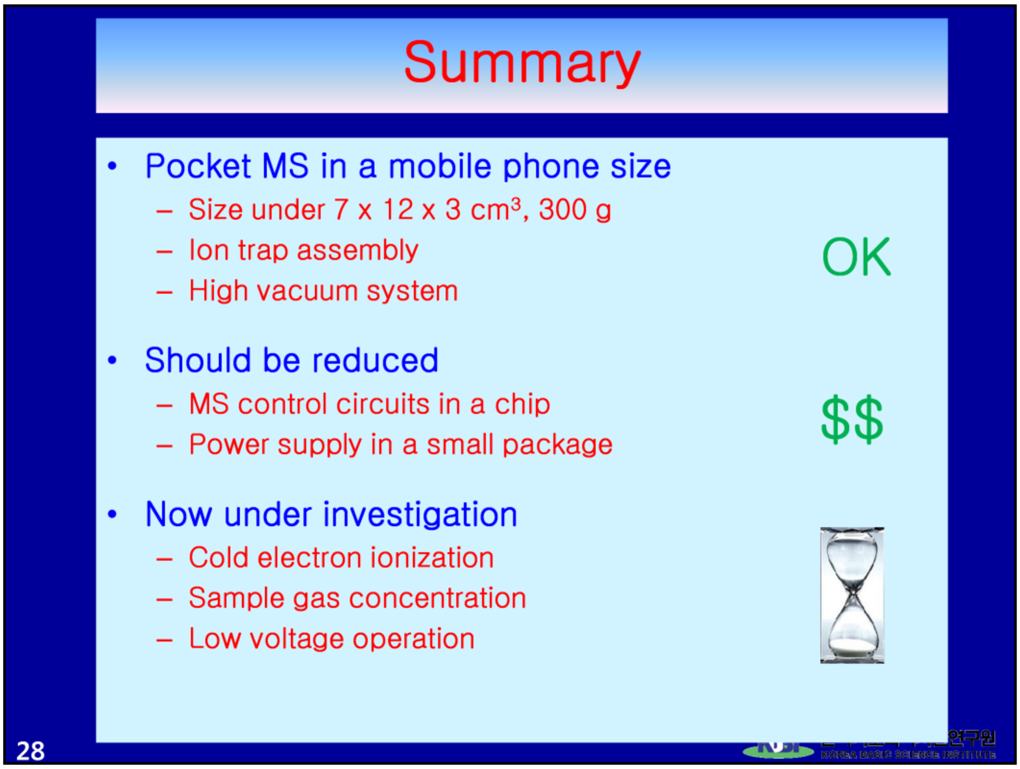


Sample gas concentration would be a another big challenge.

We are expecting detection limit up to ppb, using a pulsed sampling valve after a nanotube gas concentration.

Addition of micro GC will enhance the detection limit too.

This sampling system is now being developed by Bioneer Corporation.



For summary, I would say that the shrinking MS in a pocket portable size would be technically no problem.

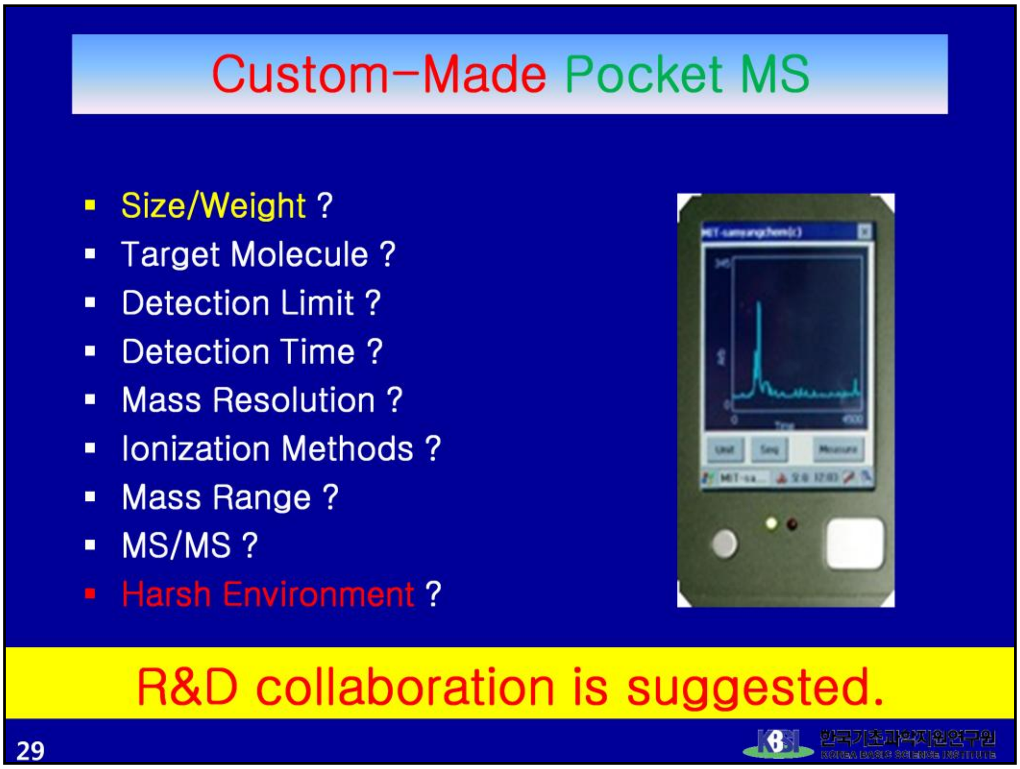
MS control chip and miniaturized power supplies are technically OK but it is just a matter of quantity or money.

Cold electron source has been demonstrated. The focusing and ionization for MS is now under test.

The sample concentration system is also under construction.

These are, I think, just a matter of time.

So I hope that I can show you the results in the next HEMS workshop.



The final shape of the pocket portable mass spectrometer can vary with requirements in every application, depending on the target molecules, detection limit, detection time, etc.

High mass resolution is very important when you measure isotope patterns.

Sometimes chemical ionization is required for thermally labile molecules.

Someone might be interested in heavy mass range, while the others in MS/MS capability.

Operation of MS in a harsh environment such as in the middle of sprite discharge plasma would be of very high interest for space exploration.

However for the scientists who are developing a methods for rapid food screening, for example, or drug inspection on the road, they need a very specified compact portable mass spectrometer but they are not an expert in developing instruments.

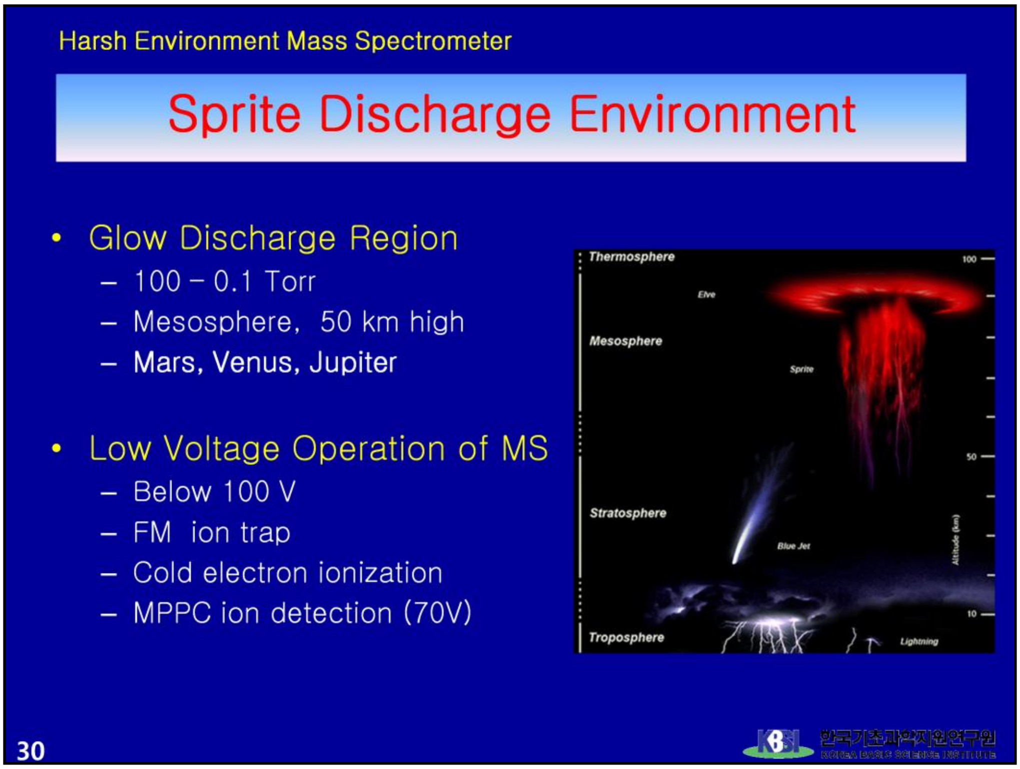
Another problem for an instrument developer is that the quantity of the pocket mass spectrometer for special purpose is not enough to invest time and money.

In this case we can collaborate for developing a custom-made MS for your own purpose.

We can provide the platform of Pocket MS and you modify for your own purpose, saving time and money.

The expenses surely will be much lower than you develop everything by yourself.

One more things, if your research project is funded by the government, then a matching fund is generally provided by Korean government, too.



The sprite discharge is for example one of the harsh environments in space exploration.

On the earth's ground you are familiar with thunderstorm and lightening. But if you go higher above 50 to 100 km, then the gas pressure drops down to several torr.

This gas pressure is in the glow discharge region, where about 150 volts already breaks an electric discharge, just like a fluorescent tube.

This gas pressure is known to be in Mars surface, in the high altitude of Venus and Jupiter.

So a mass spectrometer that survives in this environment and is able to measure the gas composition there should be operated with very low voltages, never higher than about 100V.

I believe that the pocket portable mass spectrometer is very suitable for this purpose.

I would be happy to share all the progress with you.

If any of you are interested in further details of shrinking mass spectrometers, please, do not hesitate asking me or email me.

And should any of you have to develop a special mass spectrometer for your own special purpose, then we cordially invite you to cooperate on a development project together, with your institute and Korea Basic Science Institute. Dr. Kim is available now here and happy to discuss about that.

If you are perhaps interested in commercial products or a business partnership regarding the pocket mass spectrometer, then you can email Dr. Han Oh Park. He is the president of the Bioneer Corporation and he will be happy to discuss about that.

Thank You for Your Attention !

감사합니다 !

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Thank you for your attention.

I would be happy to answer to any questions.

And any of your advice, comments, and suggestions would be appreciated.

Thank you.