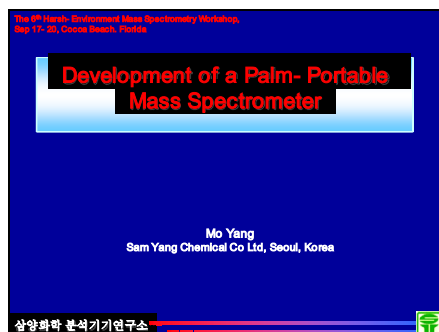


## Development of a Palm Portable Mass Spectrometer\*

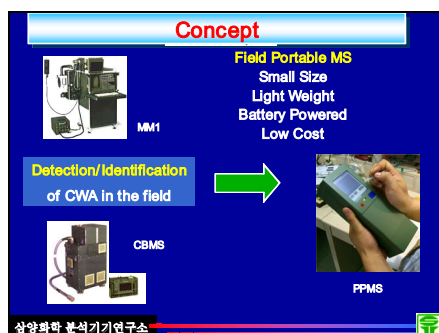
Mo Yang, Tae-Young Kim, Han-Gyu Kim, Hyun-Cheol Hwang, Seok-Kyung Yi, Do-Hoon Kim  
Presented at the 6<sup>th</sup> Harsh Environment Mass Spectrometry Workshop, September 17-20, Cocoa Beach, Florida

슬라이드 1



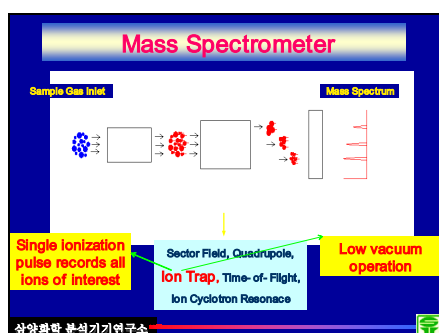
Thank you everybody for remaining to the last talk. I would like to introduce the development of a Palm Portable Mass Spectrometer. In the first half I will show you the technical details and then I would discuss some practical issues in the PPMS applications.

슬라이드 2



You know well that mass spectrometer is one of the most powerful tools for chemical analysis. But its use in the field for detection and identification of chemical warfare agents was very limited because of its heavy weight and large size. MM1 and CBMS are ones of the mobile mass spectrometers developed for military use. They are about dish washer size, weighing up to 100 kg, and draw about 2 kW power. So the concept of the PPMS project was reducing their size and weight, operating with a battery, but without losing the advantages of a mass spectrometer.

슬라이드 3



There are various mass spectrometers. The reason why we prefer Ion Trap MS is that it can record whole ions of interest with just one pulse of ionization. And it works under relatively low vacuum. That is another advantage for battery operated mass spectrometer.

## Development of a Palm Portable Mass Spectrometer\*

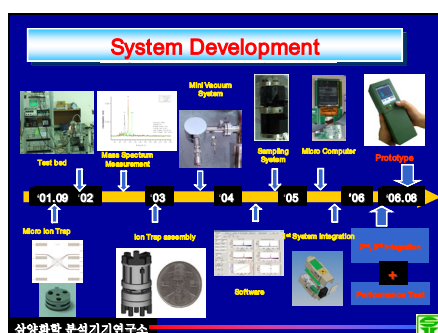
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슬라이드 4



If you want to make a mass spectrometer in small size, then not only the ion trap, but all the other necessary parts also must be miniaturized simultaneously, such as ionizer, ion detector, vacuum system, sampling system, control electronics, including power supply. All parts must be integrated together in a small comfortable case and software must be able to control them.

슬라이드 5



This slide shows the chronicle history of the PPMS development.

Theoretical simulation of the ion trap geometry was confirmed by measuring the mass spectrum on a laboratory test bed, and then the ion trap assembly is engineered.

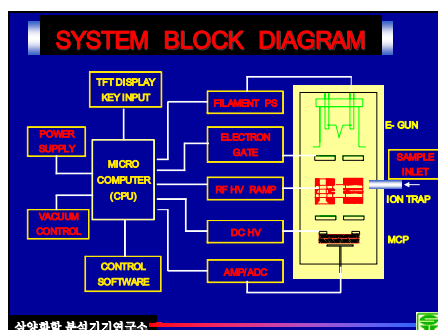
The biggest challenge was the miniaturizing the high vacuum system. We have studied various mini high vacuum pumps and decided to go with ion getter pump.

The pulse sampling valve reduces the pumping load and extends the life time.

And then we have developed a micro computer for PPMS.

Actually we have repeated designing, engineering, testing, many times. And finally got this shape.

슬라이드 6

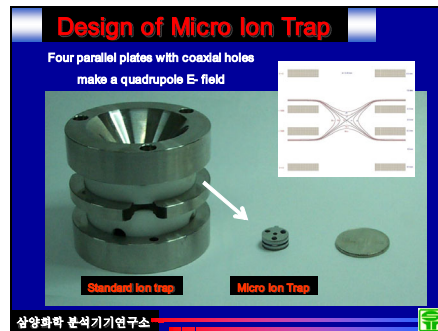


This is the system block diagram. Here is the ion trap assembly. The sample goes from here. The electrons accelerated from here and ionize the molecules here, the mass spectrum is measured here by a MCP ion detector. The micro computer controls the electron emission, electron gate and RF generation. Detected ion signal is amplified and digitized for further data processing.

## Development of a Palm Portable Mass Spectrometer\*

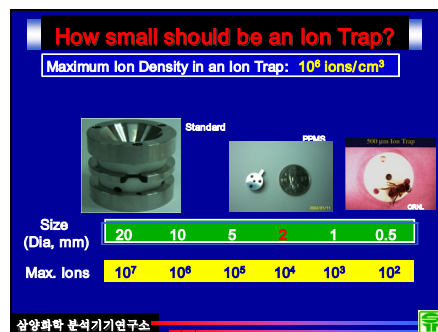
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슬라이드 7



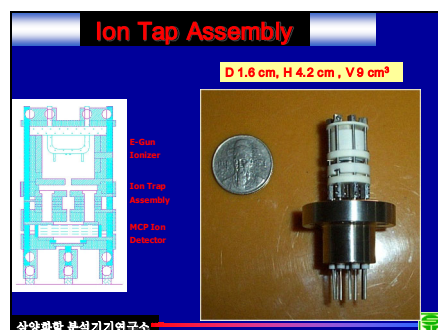
This picture compares the size of the standard ion trap and the micro ion trap used in the PPMS. It consists of four parallel plates with coaxial holes that makes a quadrupole electric field inside virtually the same as that of standard ion trap

슬라이드 8



Now the question is how small the ion trap should be. This is the standard commercial ion trap and this is the half millimeter ion trap that was developed at the Oak Ridge National Laboratory. A small ion trap has many advantages but you have to consider this parameter too. The maximum ion density trapped inside of the ion trap is limited by about  $10^6$ /cm<sup>3</sup>, because of their repulsion force. This means that the total number of ions trapped inside will be less by smaller ion trap. This is an adverse condition especially when you detect trace gases in the air in ppm concentration. PPM means that 1 target ion in million of air molecular ions. So, considering the detection sensitivity, we have decided to make the ion trap in 2 mm size. In practice, the control electronics and high vacuum system still do not follow the reducing the size of an ion trap.

슬라이드 9

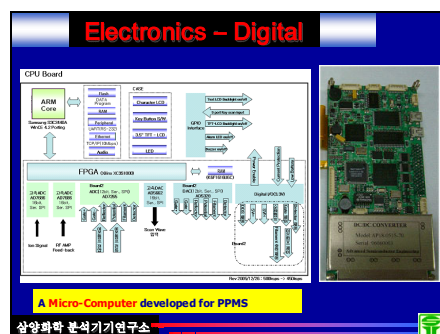


This is the cross section of the ion trap assembly. This coin is the same size of US quarter. You can see the assembly procedure. That consists of 74 pieces, made of either ceramic or stainless steel. The engineering tolerance was less than 10  $\mu$ m.

## Development of a Palm Portable Mass Spectrometer\*

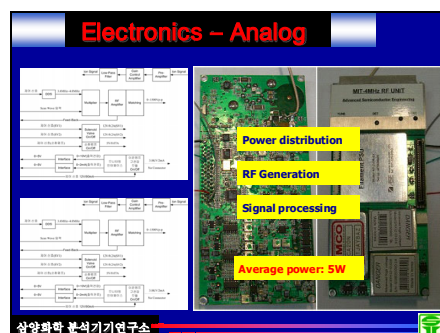
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슬라이드 10



We have developed an imbedded micro computer, using an ARM 9 CPU. The printed circuit board is a 7 layer board with more than 5000 connections.

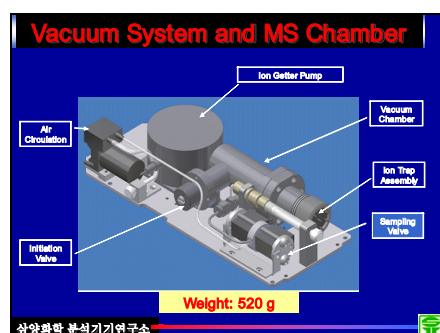
슬라이드 11



This is the analog electronics board that provides various DC voltages from a battery, generates RF HV, and records the ion signal.

The electronics all together draws the power of 5 watts in average.

슬라이드 12

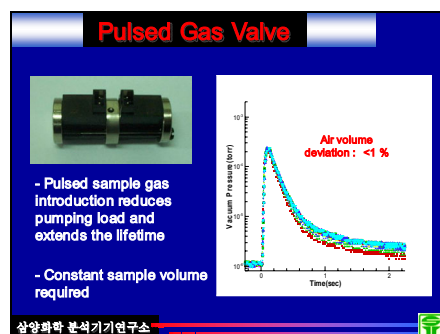


The ion trap assembly is mounted inside of this vacuum chamber. This is the Ion Getter pump and here is a valve for initiation of the high vacuum and this is the sample gas valve with air circulation. This mechanical hardware part weighs only 520 g. If you already have control electronics, then adopting this hardware only would work too.

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슬라이드 13



This is the pulsed gas sampling valve. Pulsed gas introduction reduces the pumping load in the battery operated vacuum system.

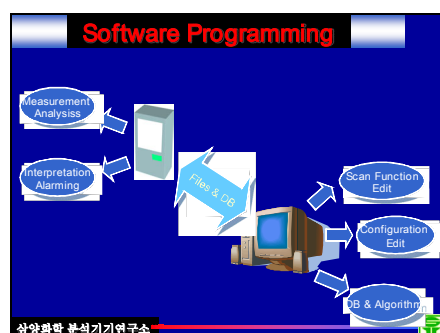
Once you open the valve, it sprays exactly the same amount of air into the vacuum chamber by every opening. The inside pressure goes up to  $10\text{e-}4$  torr maximum and drops to  $10\text{e-}6$  torr in 2 seconds. During this period, mass spectrum is measured 8 times.

슬라이드 14



All integrated final shape looks like this. The size is 8.2 x 24.5 x 7.7 cm and the total weight is 3 pounds. Battery weight is excluded because you can use a various size of batteries. If you use 400 g battery then the operation last about 10 hours, and 200 g battery then 5 hours.

슬라이드 15

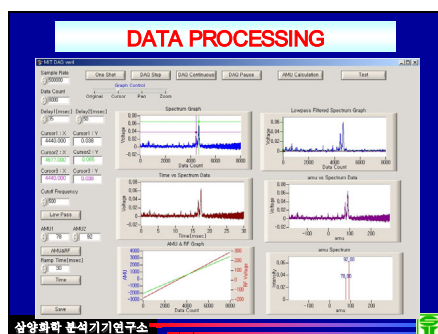


This is the software programming.

## Development of a Palm Portable Mass Spectrometer\*

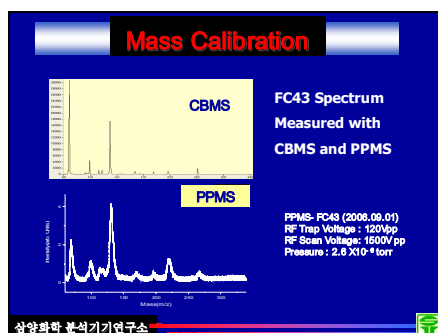
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슬라이드 16



The raw ion signal from the ion detector is recorded like this, but if you filter out the RF background then it becomes cleaner like this. You can plot them either in time scale or in mass scale. And digitize them, it looks like this.

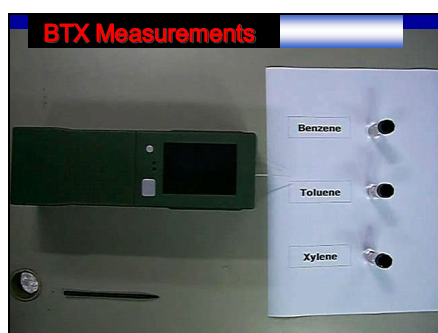
슬라이드 17



We calibrated the mass position with the standard mass spectrum of FC 43. The upper spectrum is measured with CBMS, lower one is measured with PPMS.

The exact mass calibration is pretty good. The mass resolution is not that good as in CBMS. But considering the size and weight, we think that it is good enough for identifying CW agents in the air in real-time.

슬라이드 18



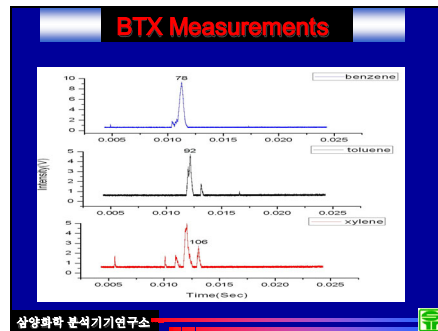
This is a demonstration of detecting toxic industrial chemicals in the air, such as benzene, toluene, xylene.

When you turns the power switch on, then it examines all the parts by itself. Everything all right, then it gets ready and waits for your command. Then first you should check up the blank test. And then approach to the vial and measure the vapor coming out from it. After the measurements, you check up again blank test.

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슬라이드 19



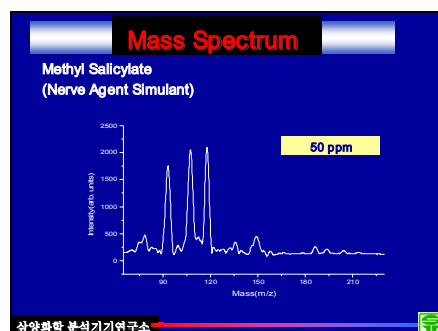
Apparently they look similar but if you plot the three spectra together then they look like this.

슬라이드 20



The PPMS was officially tested by Korea Research Institute for Standards and Science. The officially confirmed detection limit is 6.4 ppm for toluene in the air and 53 ppm for TCE.

슬라이드 21

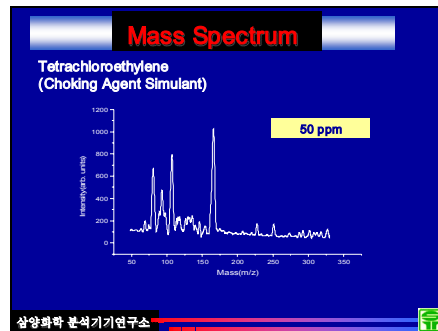


This is the mass spectrum of a nerve agent simulant, Methyl Salicylate. We are not allowed to test with real CW agents so we have tested with such a simulant only.

## Development of a Palm Portable Mass Spectrometer\*

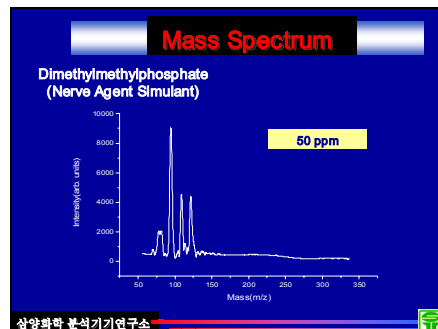
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슬라이드 22



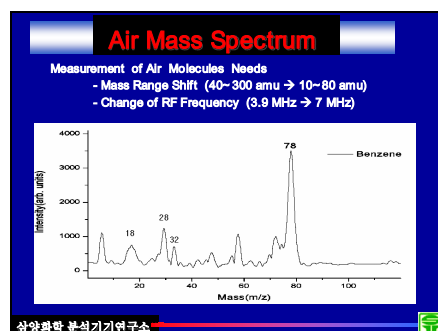
Tetrachloroethylene is used as choking agent simulant.

슬라이드 23



DMMP is a nerve agent simulant. Its chemical structure is very similar to sarin gas, the notorious nerve agent.

슬라이드 24



The PPMS is designed for measuring the trace gases in the air so the air ions are eliminated and the mass scans from 45 to 300.

However, ones of you in space sciences might be interested in measuring rather simple gases for studying the planet atmosphere or frozen gases. In this case you have to shift the mass range, changing the RF frequency from 3.9 MHz to 7 MHz.

This is a result of one time experiment and we did not try much for the optimization.



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슬라이드 25

**Summary**

- A palm-portable mass spectrometer has been developed for field use.
- Mass Range: 40- 300 amu
- Mass Resolution: 2 amu at  $m/z=106$
- Detection Time: 0.1 sec.
- Clean-up Time: 5 sec.
- Size: 8.2 x 24.5 x 7.7 cm, (1,547 cm<sup>3</sup>)
- Weight: 1.44 kg (without battery)
- Average Power Consumption: 5 W
- Life Time: 8000 hr expected with normal operation (every minute detection)

삼양화학 분석기기연구소

This is the summary of the PPMS. The size is 8.2 x 24.5 x 7.7 cm<sup>3</sup> and weighs 1.44 kg.

The detection time is 0.1 sec and clean-up time is 5 sec so that in every 5 second, you can analyze new sample gases.

Its life time is mainly determined by the ion getter pump. Pre test shows that its life time is expected about 8000 hours assuming every minute measurement.

슬라이드 26

**What should be improved further?**

- The ultimate operational requirements are different depending on the applications.
- End user's response will accelerate the further R&D.

삼양화학 분석기기연구소

Certainly there are many things we should improve further, but the question is how far we should develop. How high the sensitivity? Resolution? Detection time? Size? Weights?

So the further development should be oriented by the response of the end users. So let me brief the practical issues in the applications.

슬라이드 27

**Applications**

- Military
  - CWA Detection/Identification
- Environmental
  - Real-Time Air Pollution Monitoring
- Homeland Security
  - Explosive/Drug Detection
- Space Exploration
  - Gases on planet's surface
  - Trapped Gases in Rocks
  - Frozen Gases on Comets
  - Gas Leak Detection

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The PPMS could find applications in many areas such as military, environmental sciences, homeland security, and space explorations.

If you could verify any organic gases on the Mars, it would be a great milestone.

One more application you can think about is a disposable mass spectrometer for gas leak detection. This small and cheap MS is attached on the leak suspected area on the rocket and pops off just before the launch, then the challenger disaster could have been avoided.

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슬라이드 28

**Military**

1. Size small as possible
  - MS chip
  - Mobile phone size MS
2. Detection sensitivity
  - Detection limit 0.1 ppm
  - Sample gas concentrator
3. Real-time detection
  - 0.1 sec for 10 ppm
  - 100 sec for 0.01 ppm
4. Military Requirements
  - MIL-STD-810/461

삼양화학 분석기기연구소

Military application is on which we are now concentrating most of our efforts.

The size can be still reduced but PPMS is already good enough.

Required detection limit of CW agents in the air is usually 0.1 mg/m<sup>3</sup>. And the PPMS is a little bit short to this requirement. So we are considering to attach a sample gas preconcentrator. This will certainly increase the sensitivity up to 1000 times but it will lose the detection time.

The fast measurement in real-time is also very important in a chemical war operation, especially for the situation that the gas concentration changes rapidly or you are monitoring the poison gases in the air from a fast moving vehicle or aircraft.

슬라이드 29

**Environmental**

1. Organic vapor in the air
  - Toxic industrial chemicals
2. PPB concentration
  - Sample gas concentrator
3. Detection time
  - Few minutes allowed
4. Hand portable size

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In the environmental application the most of the target gases are organic vapors in the air. This requirement is not far from the military application. However, the mini size is not that critical here so I will skip this.

슬라이드 30

**Homeland Security**

1. Organic vapor in the air
  - Explosive vapors
  - Drug vapors
2. PPB concentration
  - Sample gas concentrator
3. Detection time
  - Few seconds allowed
4. Palm portable size for drug inspection

삼양화학 분석기기연구소

Now a day, no liquids or gels allowed to carry on the airplane.

You might be getting used to, but scientists should change this kind of weird regulations.

Well, for checking up the bottles, just open the bottle cap and measure with the PPMS. Identifying the vapor from inside is very easy, as you see in the demonstration video.

However, detecting explosives without opening the bottle would be still an open challenge because some explosives have very low vapor pressure.

Detection time of a few seconds should be all right, since passenger moves about that speed.

The size of the detector does not have to be so small in the airport, I think.

Maybe if you want to inspect illegal drugs in the car

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trunk or in a pockets, then the inspector would prefer a small detector on his palm.

슬라이드 31

**MS on the Planet Surface**

1. Gas Pressure
2. Temperature
3. Frost, humidity
4. Dust Storm
5. Static Charge
6. Electromagnetic Interference
7. Landing Shock
8. All Automatic



**small and light !**

삼양화학 분석기기연구소


Saying about mass spectrometry on a planet surfaces, you should consider the harsh environment before the MS functions. Gas pressure, temperature, frost and humidity, dust storm, static charges, electromagnetic interferences, etc. The instrument must survive from the landing shock and all functions must be automatic including fixing the trouble by itself.

So fulfilling those requirements, the mass spectrometer must be small and light, because the transportation to a planet is very expensive.

슬라이드 32

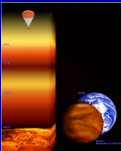
**Mars**

1. Glow-discharge gas pressure
  - 0.7 ~ 0.9 kPa of CO<sub>2</sub>
  - All voltages lower than 100V
2. Temperature fluctuation
  - 133 ~ 293 K
3. Landing shock



**Venus**

1. Hot temperature
  - 228 ~ 773 K
2. High gas pressure
  - 9.3 MPa of CO<sub>2</sub>
  - Pulsed gas sampling
3. PPMS under parachute ?



삼양화학 분석기기연구소

On the Mars surface, the most critical problem would be the gas pressure of 7 Torr. This is a very active glow discharge region so that any voltage higher than 120V may not be exposed to the Mar's atmosphere. Otherwise, just one pulse of glow discharge break down may destroy all electronics. You have to shield all the HV components, cables, and connectors very carefully, or you have to make the mass spectrometer with any voltages below 100V, including ionization, mass separation, and ion detection, and vacuum pump. Well, this would be a quiet new concept of mass spectrometer that would be possible with PPMS.

On the Venus, the most critical problem is not the pressure but the hot temperature. It goes up to 480 degrees C. The vacuum chamber and ion trap assembly may survive in that temperature but electronics would not be able to. If you slowly descend the mass spectrometer into

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the Venus atmosphere under a parachute, then very fast measurement in real-time would be required, as of PPMS.

슬라이드 33

**Moon**

1. Trapped gases in the rock
  - Isotope Ratio
2. High vacuum surrounding
3. Cold/Hot temperature  
100 ~ 400 K

**Comets**

1. Frozen gases
  - Microparticle MS
  - Real-time
2. High vacuum surrounding
3. Cold temperature

상암화학 분석기기연구소

On the moon and comets, surrounding is high vacuum.

In this environment, the most interest is how to vaporize the solid particle sample into the mass spectrometer.

We know that a couple of aerosol particle mass spectrometer has been developed for real-time measurement.

This system could be applied to this mission but small size would be again another scope of development.

슬라이드 34

**Further Developments**

1. Enhance the Sensitivity
2. Enhance the Mass Resolution
3. Smaller, Lighter, Less Power
4. Harsh Environment

Who needs what?

**For collaborations,**

please, email to Mo Yang,  
<dryangmo@yahoo.com>

상암화학 분석기기연구소

Conclusions.

We should develop the PPMS further, enhancing the sensitivity, resolution, smaller size, and that capable to work in the harsh environments. But how far should we go? Who need what resolution? Who need what sensitivity?

We could make a mass spectrometer in mobile phone size, but who needs it?

In fact I once planned to develop a MS chip that integrates all control electronics in a finger nail size but the company has stopped it because they could not find any prospective end user in large quantity.

Well, should any of you consider the PPMS application seriously, we would be happy to collaborate either in research or business development.

However, if you ask me to provide a couple of sample set just for evaluation, then it would be somewhat awkward to follow since one unit

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developed for military application would not meet the space requirements.

Instead, I would like to suggest that you describe your operational requirements and we discuss how long it should take, and how much it would cost, and how to secure the ultimate specifications.

These are my associates for PPMS project.

From the left, Dohoon Kim is a chemist, Hyuncheol Hwang is a mechanical engineer, Taeyoung Kim is a chemist and PPMS project manager, Seokkyung Yi is a physicist and software programmer, and two electronic engineers in analog and digital, Junghoon Chung and Hangyu Kim. And the rightmost is Mo Yang who has directed.

Thank you very much for your attention.

- This project has been fully supported by the Korea Dual Use Technology Center.

슬라이드 35

