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NEW - SIS TD-56

The New SIS TD-5 is shipping. The main new feature is the Windows-based software for control and monitoring of the system.

NEW - NIST 057

NIST/EPA/NIH Mass Spectral Library

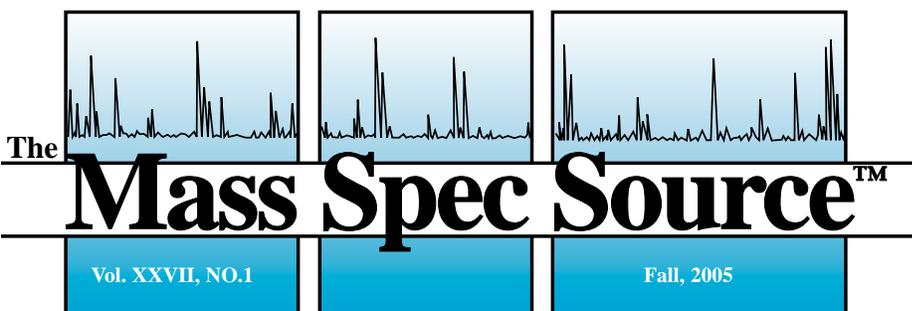
NEW 2006 - 2007 Catalog is in Production



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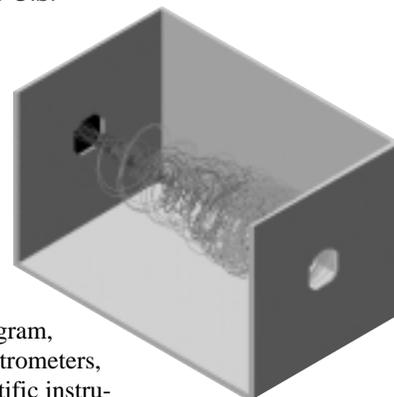


For Mass Spectrometry and Chromatography

NEWS from S.I.S.

SIS Acquires License to Continue SIMION Development.

SIS obtained an exclusive license agreement from the U.S. Department of Energy's Idaho National Laboratory (INL) for the rights to develop and maintain the software code for the SIMION suite of ion optics modeling software. The agreement will allow SIS to enhance, update and maintain the software, to satisfy the needs of the user community, and benefit the industrial partner and the government. Additional details are available on the web at: www.simion.com.



SIMION 3D, originally developed by INL employee David Dahl, is an award-winning Windows PC based program, widely used by manufacturers and designers of mass spectrometers, electron microscopes, electron multipliers and other scientific instruments to study the optics of charged particles through electric and magnetic fields in two and three dimensions. SIMION is designed to provide direct and highly interactive methods, balancing ease-of-use, speed, accuracy, and affordability in order to simulate a variety of real-world ion optics problems. SIMION can model complex problems using a workbench strategy that can hold up to 200 2-D and/or 3-D electrostatic or magnetic field arrays, each of up to 50,000,000 points, which the user can visualize in 3D and cut away to inspect ion trajectories and potential energy surfaces to gain intuition and collect quantitative data.

SIS has distributed SIMION since 1996 and has more recently developed accessory tools (SIMION SL) to expand the capabilities of SIMION to include the importation of CAD files directly into SIMION, a new compiler and other tools requested by customers. Similar features along with an updated user interface are planned for inclusion in the next major release of SIMION scheduled for sometime in 2006. SIS has also established a SIMION web site (www.simion.com) to provide customers with information and support on SIMION.

NEW Product - CPO Ion Optics Modeling Software

If SIMION is not powerful enough for your ion optics modeling applications, SIS now sells and supports CPO - Charged Particle Optics Software. CPO is a software application that calculates electrostatic/magnetic fields and the trajectories of charged particles through those fields, a bit like SIMION. However, CPO differs fundamentally in its more powerful and accurate methods of calculation (Boundary Element Method--BEM), and it offers well-tested space-charge, cathode emission, and other advanced features. Details are available on our web site at: <http://simion.com/cpo/>

Yttria Coated Mass Spectrometer Filaments

by John J. Manura, Scientific Instrument Services, 1027 Old York Road, Ringoes, NJ 08551

Historically most mass spectrometers have used plain uncoated filaments usually constructed of rhenium, tungsten or an alloy of rhenium and tungsten. In the past twenty or so years, several manufactures have tried using thoria (thorium oxide) coated iridium filaments in their mass spectrometers or leak detectors. This thoria and yttria coating technology came out of the vacuum tube industry in the 1940's and early 1950's. The thoria coated iridium filament provides longer filament life because the thoria work function was lower than tungsten, the filament required less power and it operated at lower temperatures. The major disadvantage of thoria is the environmental issues due to the exposure to the alpha particles emitted by thorium. Yttria (Yttrium Oxide) has been used as a replacement by several manufacturers of leak detectors and ion gauge tubes. SIS has been investigating Yttria (Yttrium Oxide) as a replacement for use in mass spectrometer filaments. The work function of Yttrium and Thorium are very similar (3.1 eV versus 3.41 eV respectively) and Yttria does not present the environmental issues associated with Thoria.

MECHANISM OF EMISSION

It has been reported by several authors in the early literature that free Yttrium (Y) is released within the Yttrium Oxide coating during the heating of the filament during the activation phase and this free Yttrium (Y) migrates to the surface of the oxide coating. It is this free metal film of Yttrium (Y) on the surface of the oxide coating that results in the emission characteristics of the Yttria coated filaments.

PREPARATION OF FILAMENTS

The filament wires were spot welded to metal body filament presses. (Fig. 1) The filaments were thoroughly cleaned and Yttria (Yttrium Oxide) was coated onto the filaments using an electrophoretic process. After coating the Yttria onto the filaments, they were inspected for integrity of coating and the film thickness was measured.

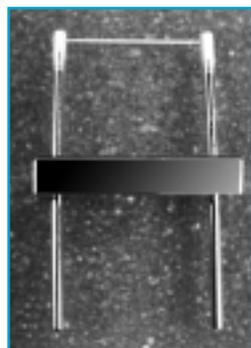


Figure 1 - Yttria Coated Filament

Yttria was coated onto various filaments wires and the emission characteristics were studied. Filaments were tested on the SIS filament testing station shown in Figure 2. This station has been used in filament studies

we have published previously and is routinely used to study filament behavior. This filament testing station permits the simultaneous study of up to 12 filaments. The DC voltage and current through each filament can be varied and the emission current between the filament and a collector is measured. The emission voltage between the filament and the collector was set to 70 volts DC, which is the standard emission voltage used in most EI mass spectrometers. For each of the studies as the filament current was increased in 0.1 amp increments, the filament current, the filament voltage and the emission current were measured using 3 digit digital voltage and current meters. Filament temperatures were calculated using the Stefan Boltzman equation using the measured filament current and voltage as well as the physical dimensions of the filament wire.

COMPARISON OF THORIA AND YTTRIA COATINGS

The chart (Fig.3) compares two Iridium filaments, one coated with Thoria (Thorium Oxide) and the other with Yttria (Yttrium Oxide). The filaments consisted of a filament press with a 10.0 mm length of 0.007" diameter Iridium wire. Yttria

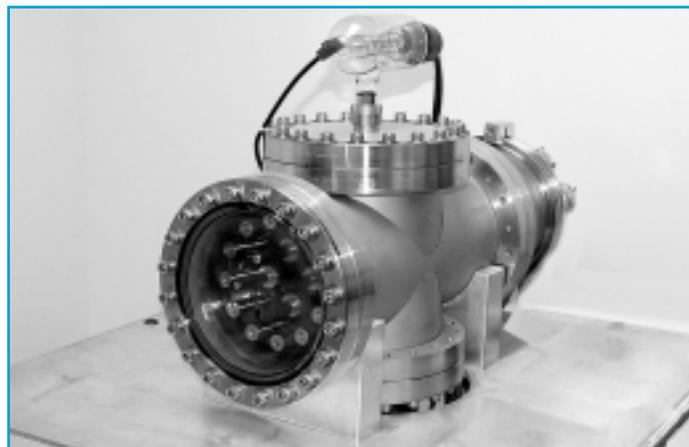


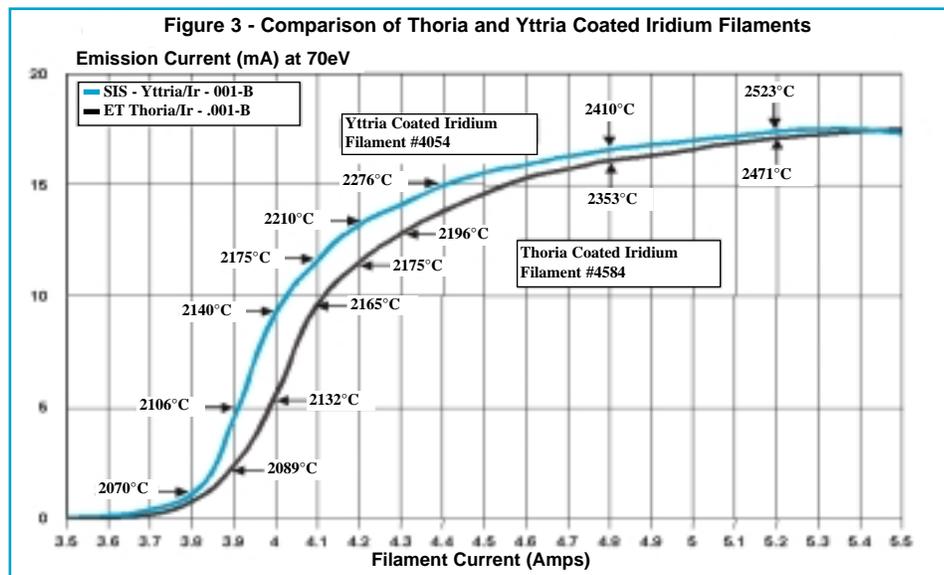
Figure 2 - SIS Filament Testing Station

and Thoria were electrophoretically deposited on the filament wires to a thickness of 0.0005".

As can be seen from the chart (Fig.3) the emission currents of the Yttria and Thoria filaments are very similar. For both the thoria and yttria coated filaments, the filament operates at about 2200°C to achieve 10 mA of emission current. This study and the following studies confirm the feasibility of using Yttria as a replacement for Thoria on filaments for mass spectrometers.

STUDY OF YTTRIA COATED RHENIUM FILAMENTS

Rhenium filaments were coated with Yttria to determine its application for mass spectrometer filament manufacture. Emission plots of both Rhenium and Yttria coated Rhenium are shown



below. Rhenium by itself has often been used as a mass spectrometer filament and therefore emits over a broad current range as shown in **Figure 4**.

As shown in the chart (**Fig. 4**), when the Rhenium filament is coated with Yttria it emits at a significantly lower filament current than the plain uncoated rhenium filament. The Yttria coated filament required about 70% of the current and power to obtain the same emission as the uncoated filament wire. Emission occurred at temperatures between 1850°C and 1950°C for the Yttria coated rhenium filament. The Yttria coated filament provides emission at about 500° lower in temperature than the uncoated filament to achieve the same emission current. This will result in good filament emission at a lower filament temperature and would be expected to produce longer filament life with the Yttria coated filaments.

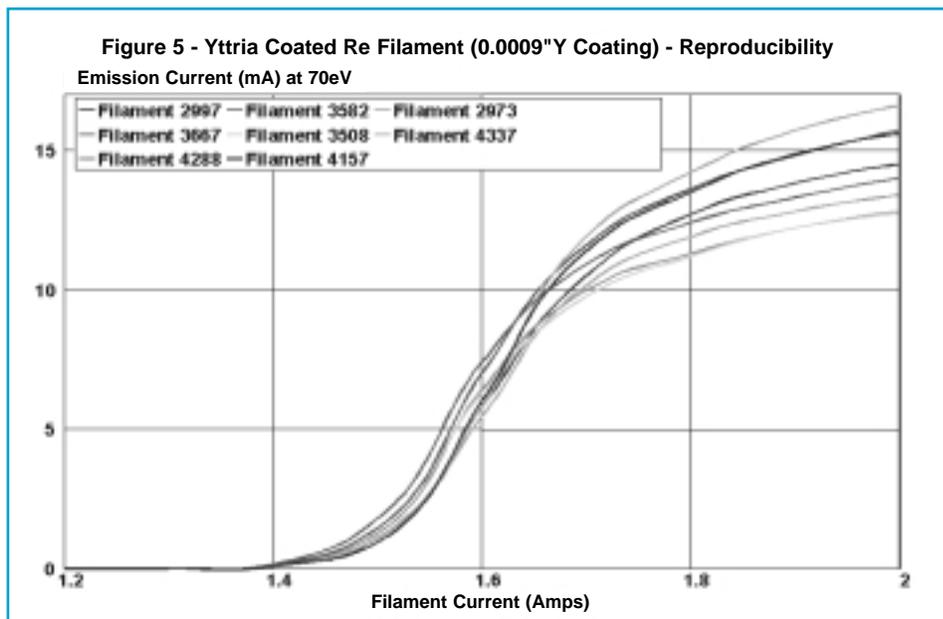
REPRODUCIBILITY OF YTTRIA COATED RHENIUM FILAMENTS

A set of 9 rhenium (.0055" diameter) filaments were coated with Yttria to a thickness of 0.0007" to 0.0010" to determine the reproducibility of manufacturing these filaments. The results are shown in **Figure 5**. The filaments were very reproducible in the emission range of 0 to 10 milliamps of emission, but this variation was probably due to the variation in thickness of the Yttria coatings or variation in the distance between the filament and the collector since different mounting positions were used for each of the filaments in the testing station.

In general we have demonstrated that we can reproducibly produce filaments with our processes and that film thicknesses between 0.0005" and 0.0010" thick provide for optimum performance and uniform coatings of the filament surface.

FILAMENT TESTING ON AN AGILENT™ MSD

The next study was done to compare the actual operation of the Yttria coated filaments in a mass spectrometer. Two filaments were installed in an Agilent 6890 MSD. The first filament (**Filament**



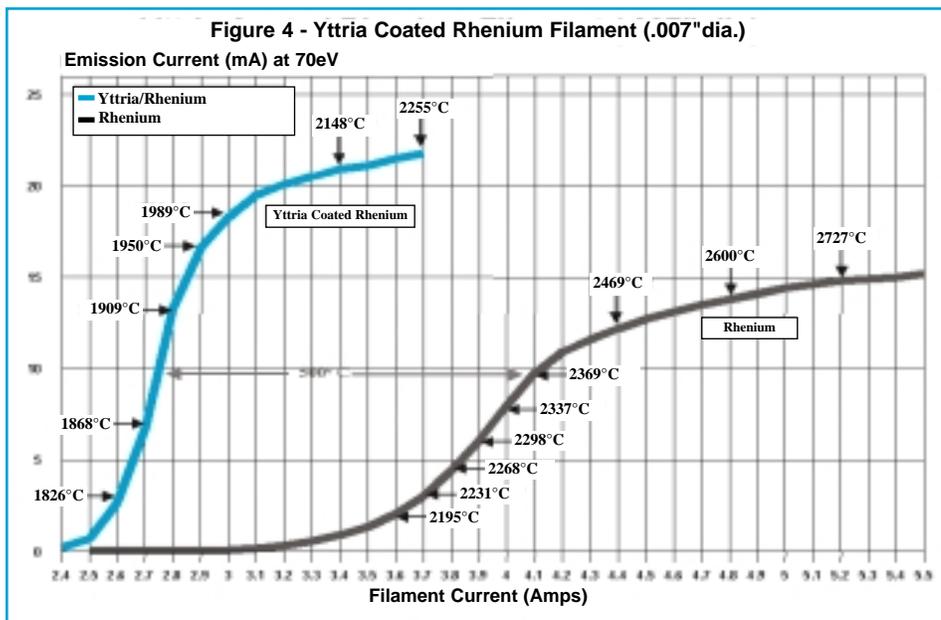
#1) was a plain 0.0055" rhenium filament which is the standard filament normally used in the MSD. The second filament was the same style filament, 0.0055" rhenium, coated with Yttria to a thickness of 0.0005". The mass spectrometer was operated in the normal EI mode and was tuned with each filament using the standard Agilent ChemStation Autotune. In both cases the filament emission current was set to 34.96 in the ChemStation tune setup.

The standard uncoated rhenium filament (**Filament #1**) operated at a measured filament voltage of 2.059 Volts AC. The Yttria coated filament (**Filament #2**) operated at measured filament voltage of 1.455 volts, which is about 70% of the voltage requirements for the non Yttria coated filament. This data agrees with the previous study above in which filament current and power for the Yttria coated rhenium filament were reduced to 70% of that required for an uncoated filament. This reduction in filament voltage and conversely filament current results in lower filament temperature and it is expected that the fila-

ment life will be increased. However, actual lifetimes of Yttria coated filaments in a real world mass spectrometer requires additional testing. It has been reported that these filaments are subject to poisoning by inorganics such as Chlorine and Flourine. The Yttria coated filament has been used in our MSD for about 3 months now and is still working fine.

CONCLUSION

The above studies demonstrate the feasibility of using Yttria coated iridium and rhenium filaments in a mass spectrometer. Yttria is a good replacement for Thoria and eliminates the environmental problems associated with Thoria. Yttria coated filaments require less power than uncoated filaments and the filament operates at lower temperature to achieve the same emission as the uncoated filaments. Historically iridium has been used as a base metal for Thoria and Yttria coated filaments, however we have demonstrated that Rhenium is also a viable alternative to Iridium and may be superior. We have demonstrated the SIS can reproducibly manufacture Yttria coated filaments to meet the end users requirements.

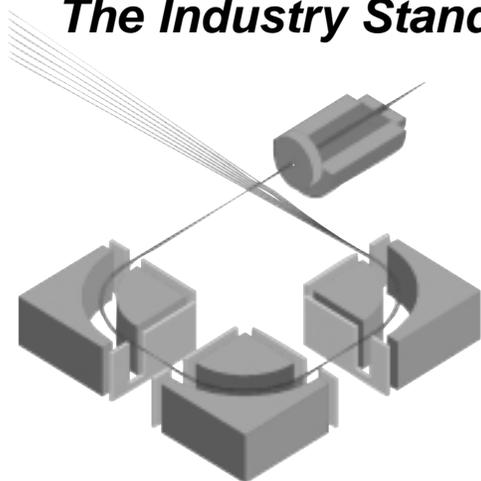


SIS Manufacture of Yttria Coated Filaments

SIS can now manufacture Yttria coated filaments. This can be done in a prototype and production environment. We can coat Iridium, Rhenium or Tungsten filaments with Yttria coating from 0.0025" to 0.0010" thickness. We can manufacture straight filament wires and ribbons as well as coil or pin shaped filaments. We also manufacture filament presses and custom design filament assemblies for our customers. We can work with you to develop and test filaments for your application and consult with you in your filament design. We have capabilities for small to large volume production quantities.

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- Array size increased to 50,000,000 points.
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- Larger Arrays
- Faster Calculations
- Long file name support.
- Data Arrays in User Programming.
- Three new options on the Modify screen.

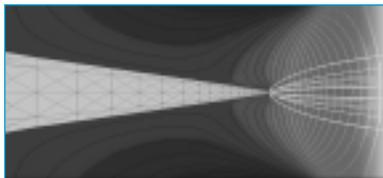


CPO

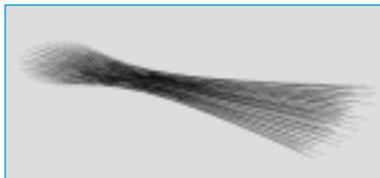
Charged Particle Optics Software

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involving Space-charge, Cathode Emissions and High Accuracy.*

CPO is well suited for



• Fine, open or emitting structures

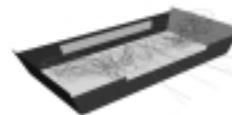


• Space charge

Other Features:

- magnetic elements
- automatic focusing
- aberration coefficients
- scattering
- large number of examples that instruct and confirm accuracy

Applications



Source & emission optics



Analyzers & lenses



Detectors

<http://www.simion.com/cpo>

NEW!

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**The New Scientific Instrument Services 2006 - 2007 Catalog
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1. Would you like:

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 Mass Spec Source Newsletter(MSS) Cryo-Trap(CRY) SIMION

2. What additional services or product lines would you like SIS to provide?

3. What Mass Spectrometer(s) do you have in your lab?

Agilent Technologies

- 5890/5988/5989(A1) GC 5890, 6890(A6)
 5970(A2) 1100 LC/MS(A7)
 5971(A3) Other _____(A8)
 5972(A4) 5975(A9)
 5973(A5)

Finnigan

- 3000/3200/OWA/1020/5100(F1) LC/MS(F8)
 4000/4500(F2) Polaris/ITD(F9)
 Quantum(F3) ICP(F10)
 Incos 50/500/XL(F4) TSQ/SSQ(F11)
 GCQ(F5) MAT90/8200/HiRes(F12)
 Trace/AQA(F6) Other _____(F13)
 LCQ/Duo/Deca(F7)

VG/Fisons/MicroMass

- Platform(VG1) Micromass(VG6)
 LC/MS(VG2) 70/70, ZAB(VG7)
 Autospec(VG3) Other _____(VG8)
 TRIO 1000/2000(VG4) MD800(VG9)
 Quattro(VG5)

Varian

- Saturn I, II, III(V1) Saturn 2000(V2) 1200(V3)

Other Manufacturers

- JEOL(JE1) Shimadzu(SH1)
 Sciex(SC1) Vestec(VE)
 Nermag(NR1) Balzers(BZ1)
 Perkin-Elmer QMass(PE1) Nicolet(NC1)
 Perkin-Elmer MS(PE2) Bruker(BR1)
 Waters Integrity(WA1) Leybold Inficon(LB1)
 LECO(LE1) Ion Spec(INS)
 Extrel(EX1) Other _____(MS)

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