Insight

A regular update to the semiconductor industry

October 2008

SAFC Hitech™ Opens Its Doors

To further highlight the new SAFC Hitech™ operational capabilities a series of events have been staged for trade journal editors to see behind the scenes at various production sites.

In early summer the Sheboygan, Wisconsin, US site opened access to its new cleanroom facilities installed as a significant investment to improve packaging capabilities. This $9 million facility provides a state-of-the-art environment for filling ultra-high quality product into a wide variety of vessels without contamination.

In late summer the Bromborough, UK site was visited by the trade press and the improved services available at this location were demonstrated.

In both cases the message was clear, the SAFC Hitech entity is bigger and better than ever with an enhanced capability to meet customer needs and deliver the products required now and in the future. Be it compound semiconductors, silicon devices, photovoltaics or a host of other fields SAFC Hitech has the chemicals and expertise to suit all comers.

"One of SAFC's primary business objectives is to continue to build SAFC Hitech into a global leader in the supply of ultra-pure, high quality materials and technical solutions to the electronics industries we serve," commented SAFC President, Frank Wicks.

"As the demand for new and increasingly efficient materials continues to grow, so does the need to attain higher and higher levels of quality and dependability from our products."

To further communicate developments at SAFC Hitech the website (www.safchitech.com) has latest news and product offerings with the return of the familiar periodic table gateway to the precursors. This interface allows rapid location of chemicals by element with detailed information just a click away. The container returns policy is also available along with other practical information for our customers.

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SAFC Hitech™ Enabling Technology

The Role of Modelling in Novel Precursor Development

The requirement to develop new chemicals for an expanding set of material systems for next generation devices depends highly on the expertise of the synthetic chemists at SAFC. In their studies to understand the fundamental nature of a specific molecule and its potential as a precursor for CVD/ALD they must use all the tools available to them to ensure the focus of laboratory work is not allowed to deviate from the most promising target compounds. Any time spent studying the wrong chemical delays the introduction of the next product range to meet the strict timetable set out by customers to ensure their own roadmaps are adhered to.

With this concept in mind SAFC has a comprehensive set of protocols to assess progress in each research area and to ensure the best molecules are identified as quickly as possible, so that they can be rapidly moved from characterisation samples of a few grams, through the upscale and purification strategy establishment, to final sample despatch for deposition trials. The development cycle is summarised in Figure 1 below:-

The key factor when beginning any new project is establishing which chemicals to start looking at and, whilst literature can be trawled and in-house expertise employed, the array of potential precursors for any particular circumstance is extensive. Each time the above cycle is performed valuable resource and time is employed; hence the minimum number of iterations is critical for an efficient research effort. The procedure to narrow down the number of options in the "Molecular Design" box, prior to starting even preliminary synthetic trials, is now falling increasingly into the realms of theory (as well as chemical experience with similar metal compounds and ligands) and so modelling of ideal precursor systems is becoming highly relevant and important to SAFC as the precursor developer.

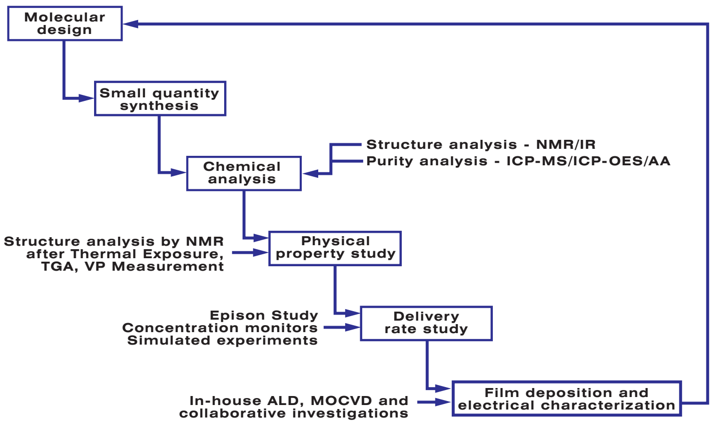


Figure 1: Development cycle

The main problem with previous modelling solutions for CVD/ALD has been the complexities involved with the large heteroleptic molecules, for example MethylcyclopentadienylZirconiumMethoxyMethyl (ZrD-04). A recent collaboration with Simon Elliott and Aleksandra Zydor at Tyndall National Institute as part of the EU-supported REALISE project has begun to shed light on how molecules behave in the ALD process based on their chemical properties. In this way, simulation is gradually moving from merely explaining experimental data to predicting future chemical synthesis trials.

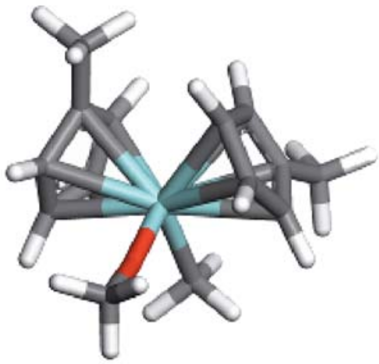


Figure 2: Representation of MethylcyclopentadienylZirconiumMethoxy Methyl (ZrD-04).

The Tyndall approach has looked at the current well-performing precursors and their ALD reaction products as isolated molecules using the TURBOMOLE suite of quantum chemical programs [www.turbomole.com]. In particular the ease of ligand elimination has been tested to predict an order of their release during the different stages of the ALD process [1]. Experimental collaborators have tested this prediction against reactions occurring in an actual ALD chamber using quadrupole mass spectrometry, with outstanding agreement (see Figure 3 below) [2]. How to tune the reactivity of the precursors and alter this mechanism has also been calculated.

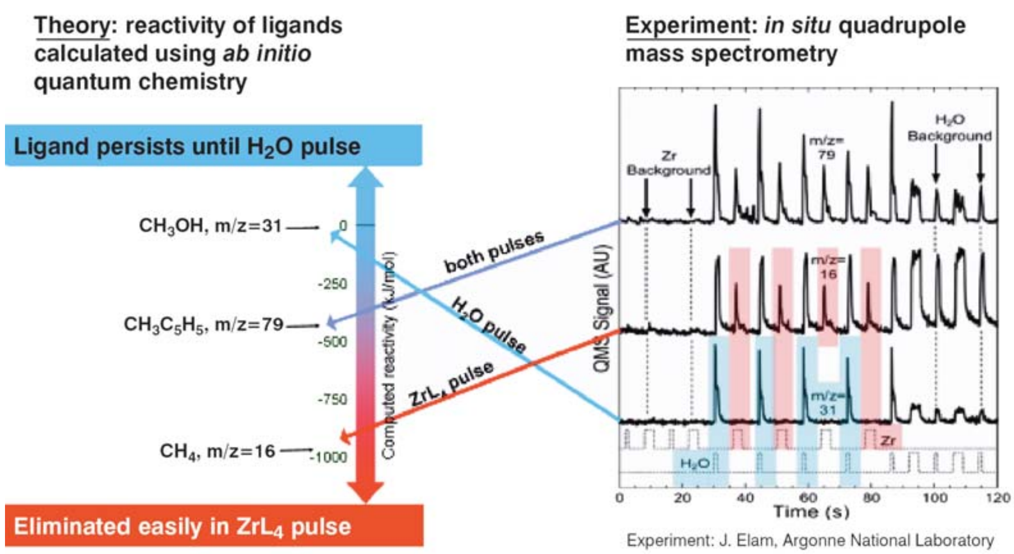


Figure 3: Calculations at Tyndall (left-hand side) indicate that methyl (CH_3-) is the most reactive ligand and that it will be eliminated first during the Zr-pulse. The methoxy ligand (CH_3O-) is computed to be least reactive and so will persist on the surface until the H_2O pulse. The cyclopentadienyl ligand is of intermediate reactivity. QMS data from Argonne (right-hand side) confirm this mechanism.

The next stage will be to predict further improvements to the molecular design of the current best performing precursors. This opens up the possibility of high-throughput precursor screening *in silico*. The challenge will then be for SAFC to ensure that what can be predicted can actually be made and isolated to high purity for use in deposition. However advances on the development cycle will have been made to streamline work schedules and bring new chemicals to the market place on reduced timelines.

SAFC is committed to the supply of next generation chemicals suited to all customer requirements in advance of each technology node and the product development cycle illustrated ensures compliance.

For full details of the modelling progress at Tyndall in relationship to the REALISE project please visit the project website or contact one of the SAFC technical team. The HfD-04 and ZrD-04 results were presented at the Bruges ALD2008 conference and the details are available on request.

References

[1] Surf. Coat. Techn. 201, 9076, (2007)
[2] Appl. Phys. Lett. 91, 253123, (2007)

REALISE
Funded by the European Commission under the FP6 project REALISE (http://www.tyndall.ie/realise)

SAFC Expands TMI Production in Far East

To address the growing demand for III-V precursors on a global basis SAFC Hitech have implemented a multiple production facility approach to provide local support for the three main market areas, namely US, Europe and Far East. With comprehensive production capabilities in Bromborough, UK and Haverhill, US it was decided to install further plants in the Taiwan operation at Kaohsiung to more evenly spread supply capacity.

In particular a new Trimethylindium plant has been commissioned that replicates equipment in UK and US. Research Manager Rajesh Odedra (pictured right) oversaw the successful technology transfer with increased volume product purification equipment installed and fully operational during his recent visit to the facility.

Research Manager Rajesh Odedra

To ensure the product from all sites is identical a stringent analytical round robin has been performed along with growth test trials of standard TMI from different locations. All the data indicate the same high purity product is produced and no differences in performance can be observed (see SIMS plot of test structure below)

The successful implementation of extra production capacity will ensure SAFC Hitech can service all its customer requirements going forward together into a bright future.

0.5*μ* UD GaAs cap

0.2*μ* AlAs

0.3*μ* GaInP using test TMI

0.3*μ* AlInP using test TMI

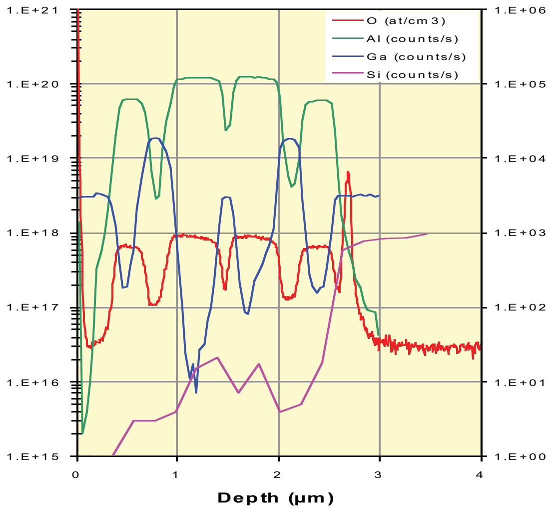
0.1*μ* GaAs marker

0.3*μ* AlInP using established TMI

0.3*μ* GaInP using established TMI

0.2*μ* AlAs

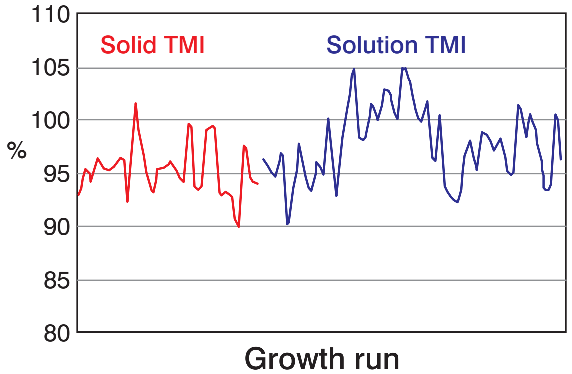
GaAs buffer and n-GaAs substrate

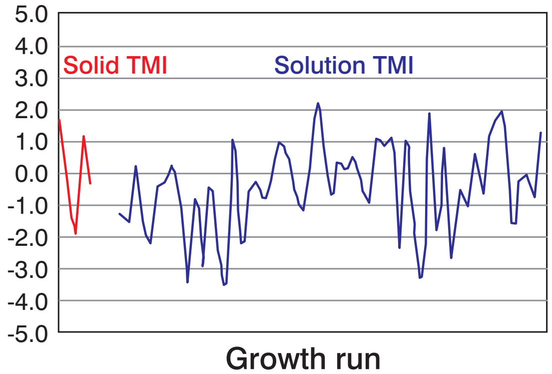


SIMS plot of test structure

Solution TMI™ Performance

In recent years the requirement for high consistency in Indium precursor delivery has been a key issue to address. At SAFC we have developed new bubblers for Solid TrimethylIndium (TMI) whilst still providing the proven technology of Solution TMI. Despite some concerns about the extra solvent component present in a Solution TMI bubbler numerous customers remain firm believers in this concept and obtain excellent process control without any contaminant problems at all. Typical control data is illustrated below from full production scale tools with run to run results showing good reproducibility and target device performance is achieved in all cases. The first figure highlights an increase in average brightness of the final LED device whilst the second illustrates the wavelengths achieved in sequential runs are within ±3.





The Solution TMI is clearly comparable, if not better, in this process than the Solid TMI and so this product continues to offer significant advantages. To discuss further the compatibility of Solution TMI with your process please contact a local SAFC Hitech representative.

New Role for Ann Hughes

Building on the changes to the SAFC Hitech sales teams outlined in the previous Insight newsletter, to provide a focussed group of representatives to service the entire product range of SAFC Hitech entity to the customary levels of excellence expected, a further business development role has been assigned to one of our most experienced Sales Managers, Ann Hughes. Ann will be working with the global sales team to support our proactive work in our core business areas of compound semiconductor materials and gases.

"Our core business areas focus and strategy is important to ensure that we continue the high level of service to our customers and also maintain an innovative and productive approach to product supply. These market areas are seeing growth in certain applications and it is our target to innovate and supply our chemicals and gases critical to the application requirements and the greatest efficiencies."

All those who know Annie will be reassured to have a familiar face driving this effort forward.

Colin Overton Retires

After many years handling the sales accounts for first Metalorganics and then the specialty gases of Epichem/SAFC Hitech Colin has decided to retire to pursue more leisurely interests. The industry has seen significant growth over his time involved with both technical and business aspects and the expertise he gained ensured wide consultation by customers. We all wish him well in his new endeavours and will continue to provide an excellent customer service through the new team of contacts.

SAFC Hitech Launch Green Programme

Introduction

Over the past years, concerns related to the impact of industrial processes on the environment have become increasingly more important to all manufacturing companies. SAFC Hitech follows the lead of its parent Sigma-Aldrich to assess and address "Green" issues across all business areas with a global commitment policy that states:-

Our Global Commitment to Environmental Sustainability, Social Responsibility, and Fiscal Accountability is creating a new level of collaboration with our employees, customers, and the communities where we work and live. SAFC Hitech has continuously worked in applying process improvements to our operations and working environment. This is now being employed to integrate sustainable development programmes into every facility. We support the principles contained within the UN Global Compact, and we strive to support and respect the protection of international human rights within our sphere of influence.

The objectives for each of the three main areas listed are explored further in the summary statements below and provide a comprehensive framework on which to build our individual focussed projects.

Environmental Sustainability

We aim to meet society's needs for products and services with progressively less negative impact on the world we live in. SAFC Hitech is in the process of implementing sustainable development programmes and through these initiatives will promote greater environmental responsibility and support energy conservation, natural resource conservation, material reuse, reduction, and recycling, and the application of green chemistry into more of our processing operations worldwide. We look forward to evaluating opportunities to partner with our customers in these important areas, and we will encourage our suppliers to continually improve their supply operations in support of a healthier and cleaner environment.

Social Responsibility

SAFC Hitech has a long and rich history of social commitment. A part of that heritage is a legacy of giving back and actively seeking to inspire others to be generous as well. Our employees participate in the communities in which they live and work in many different ways from inspiring science in future generations to actively participating and volunteering in a wide range of charitable events. SAFC Hitech supports the efforts of its employees financially, with time and encouragement.

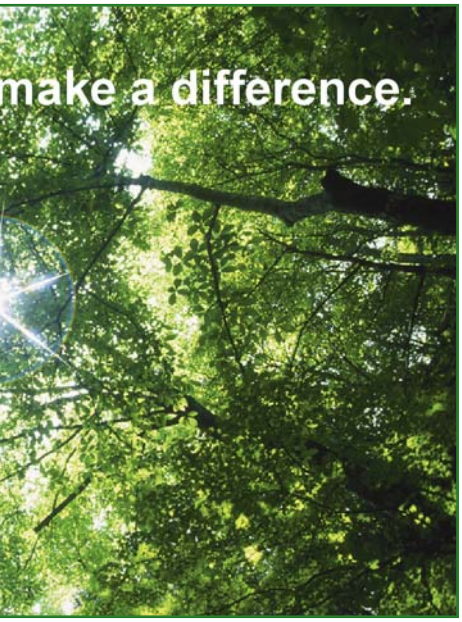
Fiscal Accountability

We strive to provide a high standard of behaviour, along with unquestionable integrity. Continued honest and ethical business conduct is a cornerstone of our 'One Company' values. The Global Business Conduct Policy provides a foundation for good judgment when faced with choices of ethics and conduct. We will work against corruption in all its forms. As part of a public company, it is of critical importance that the Company's filings with the Securities and Exchange Commission be accurate and timely.

SAFC Hitech & the semiconductor industry

With the growth of the semiconductor market, larger and larger volumes of highly hazardous chemicals are being employed. Handling techniques developed for safe and responsible deployment require continuing investigation to ensure ever more rigorous standards are met. To assess and certify a company's progress in this area, the international standard ISO14001 was introduced. This certification operates in a similar manner to ISO9001, which addresses quality issues, but the focus is on the environmental assessment of production processes and strategies to minimise impacts.

Inside the SAFC Hitech operation we are certified to ISO14001 and the protocols required to maintain this standard require active participation in programmes to control and reduce emissions in an ongoing manner. This means that existing processes must be continually assessed and methods developed to increase efficiencies, minimise waste and energy consumption and improve the general sustainability of all production technologies. In particular recycling projects coupled with reduced use of finite resources and substitution of more environmentally friendly materials have led to significant improvements in a number of areas over recent years and these advances will be the foundation for future work across all fields of operation.



Furthermore the whole product lifecycle will be addressed and so the impacts of the new Green programme will be a greater focus on the assessment of Suppliers and the Supply Chain for key products to ensure sustainability and minimum environmental impact. Collaboration with raw material providers to establish robust supply methodologies is critical to service a growing market without negative results in the world around us.

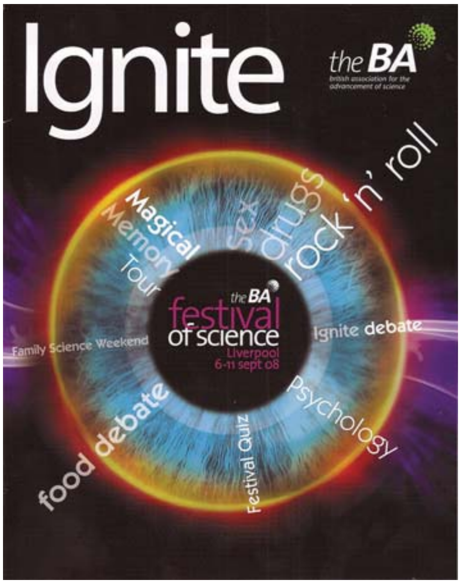
Moving forward along the supply chain SAFC Hitech have already implemented a full service for container return and recycle, however, increasingly the potential to recover exhausted product from customer processes for reintroduction into precursor production processes is raised to reduce waste and improve efficiencies. This task is not simple due to the quality requirements of the precursors and the very high potential for contaminant introduction from material collected from deposition processes. Collaboration with the kit manufacturers and customers will be necessary to establish separation techniques to minimise impurity transfer prior to return for potential reprocessing but just these sort of projects will be progressed as part of the Green effort.

In conclusion, the efforts to ensure that semiconductor precursor fabrication and use processes remain environmentally safe requires continuous improvement in production methods and a wider network of by-product collection and re-use to generate industry standards for the future. SAFC Hitech is committed to establishing frameworks necessary to achieve this goal.

SAFC Hitech & the general public

A further objective to the Green program is to provide social inputs to local communities and to raise awareness of chemistry in general. To achieve this goal SAFC Hitech personnel have been involved in a wide range of activities particularly focussing on interactions with schools. Demonstrations of exciting chemical reactions and effects along with more detailed talks on semiconductor devices have been received well by all and we hope to continue the mentoring of the next generation of would be scientists to increase popularity and provide chemists for the future.

Within the SAFC Hitech facilities initiatives are in place to reduce energy consumption and increase recycling for all the administration functions and these protocols can equally well be applied to home life. Paper, printing, packaging, heating, lighting, local sourcing can all be controlled and limited to impact less on the environmental demands and thus reduce the overall carbon footprint of the company to complement the process reductions also targeted above.



Raising Public Awareness Through Science Promotion

This year saw the largest science festival in the world visit Liverpool, UK next door to the SAFC Hitech HQ in Bromborough. In line with the company's Green Programme, support for this event was seen as a great way to raise the profile of science in the region and so SAFC Hitech were proud to sponsor the festival in general along with a specific series of talks focussing on "New materials for the 21st Century".

The full program is detailed on the British Association for the Advancement of Science website (http://www1.the-ba.net/bafos/events/showevent.asp?EventID=84).

The objective of the week long programme of events was to engage all levels of the public from specialist professionals to school children and all interested amateurs in-between. An array of top scientists and commentators was featured to transform the capital of culture into the city of science.

New SAFC Hitech Research Project

The high profile and expertise of the research team has led to numerous approaches from potential partners to develop new chemistries for a wide range of applications. To support both core and non core product area investigations collaborative research is a key strategic factor and a recent project submission has been accepted for funding by the UK TSB. (http://www.innovateuk.org/aboutus.ashx) The focus of this project will be the improvement of processes to fabricate optoelectronic devices capable of running at elevated temperatures to increase performance and application range. This work involves the same partners from a previous successful collaboration involving novel dopant sources for improved device performance.

Extended Temperature Optoelectronics (ETOE II)

Project Abstract

Development of higher functionality devices employing new materials (AlInGaAs/InP) and their fabrication to high yield and reliability. The project aim is to define viable processes to access a wide range of integrated devices, including tunable lasers with modulators, optical amplifiers and electro-adsorption modulators.

Lead Organisation CIP Ltd
Consortium Members Bookham Technology plc, LSA Ltd, Universities of Sheffield and Surrey, SAFC Hitech Ltd.

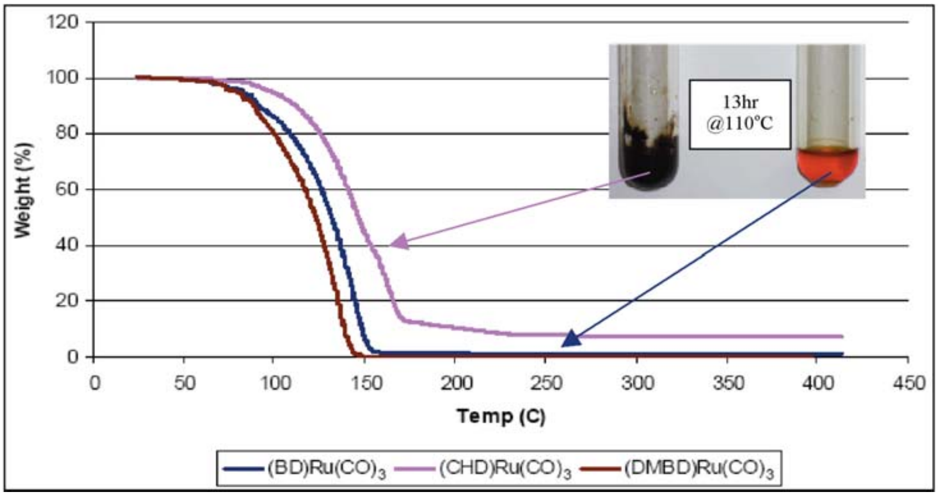
SAFC Hitech is also proud to be involved in the recently renewed PV21 Supergen project (PV Materials for the 21st Century) aimed at building on previous work in the area of solar cell development to consolidate a world leading position in light harvesting and management technologies.

PV21 SUPERGEN

Team members
Universities of Glyndŵr, Durham, Bath, Southampton, Northumbria, Edinburgh, South Bank, Cranfield along with numerous industry partners.

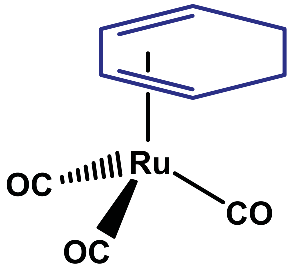
O Free Deposition of Ru Metal Films

Interest in the Silicon semiconductor industry for Ruthenium deposition continues to grow, however, conventional precursors offer an interesting potential limitation for high purity films namely that they require an oxidant to achieve Ru metal layers. The potential is therefore present to also incorporate Ruthenium oxide which whilst metallic in nature may lead to unwanted effects. Ideally an anaerobic solution is needed and to solve this phenomenon SAFC have investigated Ru(0) compounds. The findings have been successful in that a family of diene tricarbonyl molecules have been shown to be capable of use to deposit very high quality Ru metal films without an oxidising atmosphere or coreagent. Initial work focussed on the cyclic derivative cyclohexadieneRuthenium tricarbonyl [(CHD)Ru$(CO)_3$] but later studies have shown that the open dienes offer better chemical properties. It is interesting to note that this is in contrast to the $(RCp)_2$Ru vs $(Diene)_2$Ru case where the close ring derivatives appear best suited to the processes needed to obtain high quality results.

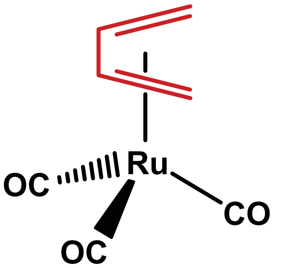


Thermogravimetric analysis of the (CHD)Ru$(CO)_3$ and two open dienes is shown above with a thermal stability test inset. It is clear that the open dienes transport more cleanly at slightly lower temperatures and are more thermally stable over prolonged heating exposure. Indeed in growth trials the precursor temperature for the (CHD)Ru$(CO)_3$ was 10°C higher than the other two sources. Furthermore both the butadieneRuthenium tricarbonyl [(BD)Ru$(CO)_3$] and the dimethylbutadieneRuthenium tricarbonyl [(DMBD)Ru$(CO)_3$] compounds are liquids compared to the solid (CHD)Ru$(CO)_3$.

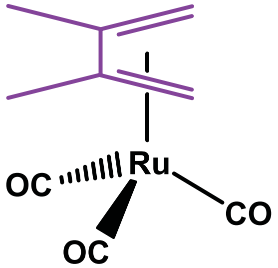
Characterisation of films grown in-house on the SAFC ALD tool also highlight the benefits of the open diene derivatives with faster growth rates and similar or higher resistivities obtained in all cases as shown in the table below. Further work is ongoing to make these exciting new precursors more widely available to interested parties on a research basis to establish the optimum processes going forward.



(CHD)Ru$(CO)_3$
Dep.Rate ≈ 240Å/min @350°C
Resistivity 37$\mu\Omega$/sq



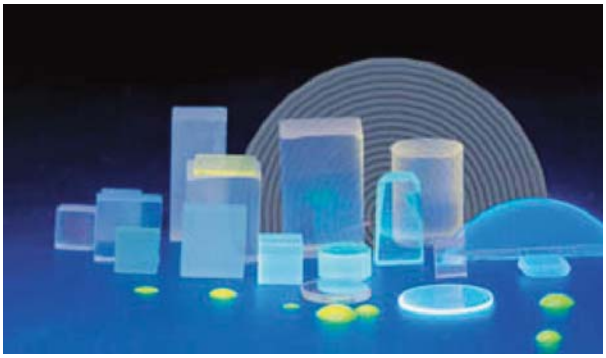
(BD)Ru$(CO)_3$
Dep.Rate ≈ 300Å/min @350°C
Resistivity 36$\mu\Omega$/sq



(DMBD)Ru$(CO)_3$
Dep.Rate ≈ 300Å/min @350°C
Resistivity 49$\mu\Omega$/sq

Scintillation Materials

A scintillator is a substance that absorbs ionizing electromagnetic or charged particle radiation then releases this energy by fluorescing photons at a characteristic Stokes-shifted wavelength, i.e. it glows when hit by high energy particles or photons. Scintillators are therefore similar to phosphors but their short fluorescence decay times and optical transparency at wavelengths of their own specific emission energy set them apart from these materials.



These scintillating compounds find a wide range of uses but are primarily employed in many physics research applications to detect electromagnetic waves or particles. The scintillator converts the energy to light of a wavelength which can be detected by inexpensive or easy to handle detectors such as photomultiplier tubes (PMTs). However, increasing numbers of mainstream imaging equipment for medical imaging and environmental monitoring and mining applications are increasingly employing these highly sensitive detectors.

The most widely used scintillation material is thallium doped sodium iodide [NaI(Tl)] due to its very high light output and ability to produce large size crystals at economic cost. However, it suffers from the disadvantage of being hygroscopic which leads to the requirement for hermetically sealed assemblies to avoid degradation effects. Sodium and thallium doped cesium iodide [CsI(Na) and CsI(Tl)] are also excellent inorganic scintillator compounds. Their different emission spectra maxima and decreased hygroscopicity make them attractive alternatives to NaI(Tl).

Six main characteristics are used to describe the performance of a scintillator as listed below:-

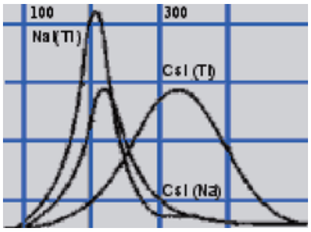
Light output (LO) is the coefficient of conversion of ionizing radiation into light energy. Having the highest LO, the value for the NaI(Tl) crystal is taken to be 100%. Light output of other scintillators is determined relative to that of NaI(Tl) (%). LO (Photon/MeV) is the number of visible photons produced in the bulk of scintillator under gamma radiation.

Scintillation decay time is the time required for scintillation emission to decrease to e-1 of its maximum. The lower the decay time of a scintillator, that is, the shorter the duration of its flashes of fluorescence are, the less so-called "dead time" the detector will have and the more ionizing events per unit of time it will be able to detect.

Afterglow is the ratio of the intensity measured at a specific time (usually, after 6 ms) after the Decay time to the intensity of the main component measured at the Decay time

Energy resolution is the full width of distribution, measured at half of its maximum (FWHM), divided by the number of peak channel, and multiplied by 100. Usually Energy resolution is determined by using a 137Cs source. Energy resolution shows the ability of a detector to distinguish gamma-sources with slightly different energies, which is of great importance for gamma-spectroscopy.

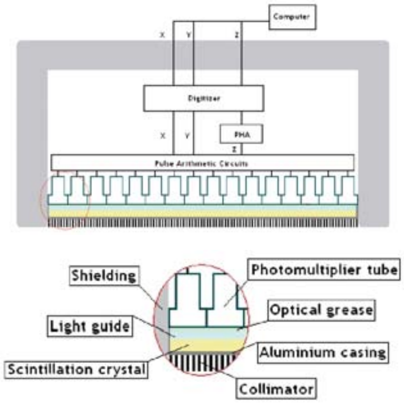
Emission spectrum is the relative number of photons emitted by scintillator as a function of wavelength. The data for the most common crystals is shown in the figure. For coefficient detection of emitted photons, the maximum of PMT quantum efficiency should coincide with I_{max}.



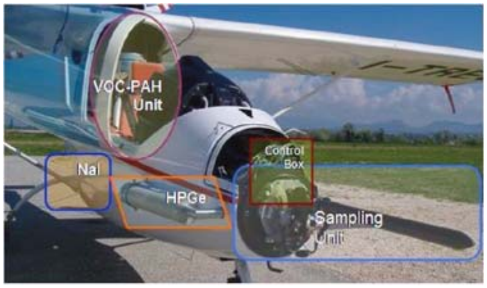
Background is a quantity determined as a number of luminescent pulses emitted by radioactive substance within 1 second in the bulk of the scintillator with the weight of 1 kg.

Selected Scintillator Detector Applications

Gamma camera



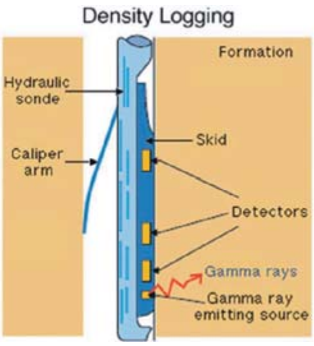
A Gamma camera utilising scintillating materials is used in nuclear medical imaging to view and analyse images of a human body which has had gamma ray emitting radionuclides introduced. A diagram of the detector arrangement is shown and this system accumulates events or counts of gamma photons that are absorbed by the crystal in the camera. Usually a large flat crystal of sodium iodide with thallium doping in a light-sealed housing is used. The highly efficient capture method of this combination for detecting gamma rays was discovered by noted physicist Robert Hofstadter in 1948.



Environmental monitoring

Detection of high energy radiation/particles in the atmosphere at varying heights and their correlation to background readings to assess the spread of contaminants requires exceptionally sensitive equipment. Large NaI crystals can provide this capability to acquire environmental gamma spectra and thus have been deployed in combination with other sensitive tools to provide a complete picture of radiation levels.

Mining/Drilling



To find out whether a well contains oil and/or gas, different types of probes containing various measuring instruments are lowered into the well including a gamma radiation source and scintillation detector. After the gamma radiation enters the porous layer, part of it returns and can be measured by the detector. The energy loss level provides information on the layer.

Data sources

http://www.delftoutlook.tudelft.nl/info/index2506.html?hoofdstuk=Article&ArtID=2452

http://en.wikipedia.org/wiki/Gamma_camera

http://www.iss.infn.it/webg3/g3iss/aereo/systemoverview.html

The SAFC Hitech portfolio encompasses a wide range of Scintillator materials which can be purchased to high specifications to meet the stringent requirements of this market. The rich supply history of these Performance Materials is being highlighted at a Crystal Grade Hildes product launch in October 2008 and to be included in the distribution list please contact Sean Dingman (sean.dingman@sial.com) or your local SAFC contact or visit our booth at any of the forthcoming conferences and tradeshows where our representatives will be present for discussions.

In particular see Sean and Mike Willis at IEEE NSS-MIC 08, Dresden for their presentation entitled "High Purity Halides for Detector Crystal Growth from SAFC Hitech" Wednesday Oct 22nd (www.nss-mic.org/2008).

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