Institution: PHYESTA (Physics at Edinburgh and St Andrews)

Unit of Assessment: UoA 9 - Physics

Title of case study: Millimetre wave Instrumentation for High Field Electron Paramagnetic Resonance

1. Summary of the impact

Impact: Economic and societal
The Millimetre Wave and Electron Paramagnetic Resonance (EPR) group has developed internationally award-winning instrumentation, and associated components that have been produced commercially by Thomas Keating Ltd. They have also led a pioneering public understanding programme (PUP).

Significance: Thomas Keating have developed a range of new product lines serving > 20 international customers including [text removed for publication] of recent orders. The PUP has reached ~82 000 attendees.

Reach: Systems have been sold internationally and PUP has developed into specific exhibitions at a range of science centres.

Attribution: The work has been led by PHYESTA Researcher Dr Graham Smith

2. Underpinning research

Electron Magnetic Resonance (EMR) or Electron Paramagnetic Resonance (EPR) is a characterisation technique used in materials science, physics, chemistry, biomolecular science, biomedical science and geoscience. Paramagnetic centres and defects can define a materials electronic, optical, mechanical, chemical, catalytic and enzymatic properties. EPR is a technique that identifies these centres and gives detailed information about the local atomic environment and is often able to link structure to function. One of the fastest growing applications is based on site-directed spin labelling in biochemistry, where pump-probe pulse EPR-based techniques (PELDOR measurements) are rapidly becoming the method of choice for accurate long range distance measurements in biomolecules in the 2-12nm range, strongly complementing X-ray crystallography and NMR techniques.

In 1993 Graham Smith, Jim Lesurf and Peter Riedi designed a new type of multi-frequency cw mm-wave electron paramagnetic resonance spectrometer that employed novel quasi-optical techniques. This design [R1] became the blueprint [R2] for the first generation of successful high field (mm-wave) EPR spectrometers that was adopted by many major mm-wave EPR labs across the world. It went on to become an EPSRC National Chemistry Facility run by Smith. (GR/S72306/01)

The crucial breakthroughs achieved in realising high performance in a (scalable) mm-wave EPR spectrometer were due to the adoption of low loss, high performance quasi-optical techniques, combined with the development of new mm-wave components and new measurement protocols. The success of this project led to a more ambitious funded proposal, led by Smith in 2003, to the Basic Technology programme of RCUK (GR/S85719/01). The project, entitled 'Bringing the NMR Paradigm to EPR', was the top ranked proposal among 140 initial submissions across all scientific disciplines. In this four year grant, the first two years were spent developing the underlying basic technologies, the next year constructing the instrument and the final year developing the control software required to produce complex and arbitrary pulse sequences on sub-ns timescales at kW power levels. Further development work was funded through a subsequent EPSRC translation

grant (EP/F039034/1). As part of the development work and within the on-going associated mm-wave research, the team also developed a range of pioneering components including isolators [R3] and corrugated feedhorns [R4] that had clear commercial value.

The new EPR instrument now provides around two orders of magnitude improvement in concentration sensitivity compared to Brukers flagship X-band (or W-band) commercial system [R5]. (This corresponds to nearly four orders of magnitude reduction in averaging time for common pulse measurements). To put that into context, the previous 60 years of EPR perhaps only saw one order of magnitude improvement in continuous wave concentration sensitivity.

The large range of mm-wave applications and projects within the group, together with broader mm-wave applications (car radar, mm-wave astronomy, earth resource studies, fusion diagnostics) also led to successful outreach bids (e.g. EPSRC grant EP/H047964/1) designed to highlight this area of science to the general public and attract school children to technology and science.

In 2011 Graham Smith was awarded the Silver Medal for Instrumentation by the International EPR Society in recognition of his contribution to EPR spectrometer design. The medal is only awarded once every three years worldwide. In recognition of the EPR work, Graham Smith, has also been invited to assume a number of leadership roles in the UK and international communities including: President, European Federation of EPR Groups (2009 - Present); Chair of Royal Society of Chemistry EPR Group (2012), Deputy Chair, European COST network on “Advanced Paramagnetic Resonance Methods in Molecular Biophysics” (2003-08).

Personnel

Key PHYESTA researchers involved in this work were Dr Graham Smith (Present throughout period of assessment), Dr Jim Lesurf (Reader to 2004, Honorary Reader 2004 - 2013) and Professor Peter Riedi (Professor to 2003, Professor Emeritus 2003 - Present), Dr Duncan Robertson (PDRA 1994-1999, 2000 - Present), Dr David MacFarlane (PDRA 2002 - Present), Dr Paul Cruickshank (PDRA 2004-2010), Dr David Bolton (PDRA 2005-Present) and Dr Robert Hunter (PDRA 2006 - Present).

3. References to the research

The quality of the underpinning research is best illustrated by [R1], [R3], [R5]. *[Number of citations]*

[R1]	G. M. Smith, J. C. G. Lesurf, R. H. Mitchell, and P. C. Riedi, "*Quasi-optical cw mm-wave electron spin resonance spectrometer*", *Review Of Scientific Instruments*, **69**, p. 3924, (1998), DOI: 10.1063/1.1149200,URL: tinyurl.com/pupxktn *[70]*
[R2]	B.M. Gilbert, M.J. Davies, K.A. McLauchlan, G. M. Smith, P. C. Riedi, "*Progress in High Field EPR*", RSC Specialist Periodical Reports on Electron Paramagnetic Resonance, **17**, (2000), DOI: 10.1039/9781847553546-00164, URL: tinyurl.com/prrv8x2 *[unknown]*
[R3]	R.I.Hunter, D.A.Robertson, P.Goy, G.M.Smith, “*Design of High Performance Millimeter Wave and Sub-Millimeter Wave Quasi-Optical Isolators*”, IEEE Transactions on Microwave Theory And Techniques, **55**, p. 890, (2007), DOI: 10.1109/TMTT.2007.895152, URL: tinyurl.com/pcax8dk *[16]*
[R4]	J.McKay, D.A.Robertson, P.A.S.Cruickshank, R.I.Hunter, D.R.Bolton, R.J.Wylde and G.M.Smith, "*Compact Wideband Corrugated Feedhorns with Ultra-Low Sidelobes for Very High Performance Antennas and Quasi-Optical Systems*", IEEE Transactions on Antennas and Propagation, **61**, p.1714, (2013), DOI: 10.1109/TAP.2013.2243097, URL: tinyurl.com/ojukn4w *[0]*
[R5]	P. A. S. Cruickshank, D. R. Bolton, D. A. Robertson, R. I. Hunter, R. J. Wylde and G. M. Smith, “*A kilowatt pulsed 94 GHz electron paramagnetic resonance spectrometer spectrometer with high concentration sensitivity, high instantaneous bandwidth and low deadtime*”, *Review of Scientific Instruments*, **80**, p. 103102, (2009), DOI: 10.1063/1.3239402, URL: tinyurl.com/prrv8x2 *[27]*

4. Details of the impact

The breadth of impact of the mm-wave activity is mainly evidenced by the commercial success associated with the EPR program, but we would also point to the success and societal impact of the more general mm-wave outreach program that arose from the EPSRC Public Understanding funding.

Economic Impact.

Commercialisation of EPR instrumentation is performed under licence by our partner Thomas Keating Ltd. Examples of these systems can be seen on the front page of the Thomas Keating we site [S1]. These high Field EPR and DNP systems (or components) have been sold around the world, and cost between £50K – to over £1M depending on the specification. They can be found at the United States National High Magnetic Field Laboratory (NHMFL) in Tallahasee; European High Magnetic Field Lab, Grenoble; Max-Plank Institute, Mulheim; Santa Barbara; Cornell; MIT; North Eastern University; Budapest; Lausanne; Warwick & Nottingham amongst other groups. The most recent orders [text removed for publication] for the pulse spectrometer include both the US Pacific Northwest National Laboratory (PNNL) and the US National High Magnetic Field Laboratory in Tallahassee. Both these systems have now been delivered to specification.

The mm-wave components developed by PHYESTA have also contributed to sales at Thomas Keating in the international metrology, space, earth resource, fusion diagnostics and security industries.

Thomas Keating Ltd is based in Billingshurst in West Sussex, and employs approximately 40 people. The Managing Director has been actively collaborating with the mm-wave group throughout the assessment period. He attributes the early existence of his company to the initial interactions our mm-wave group. Thomas Keating is now widely recognised as "…*perhaps the leading supplier of front end systems for high field Electron Paramagnetic Resonance and Dynamic Nuclear Polarisations ..*" and a leading mm-wave component supplier for whom the collaboration with PHYESTA has "…*played a major role in winning international orders in the space, metrology, fusion diagnostic and earth resource communities.*" [F1]

Prior to this work the UK had no presence and virtually no recognition for EPR instrumentation development. After Bruker and JEOL, Thomas Keating has now probably supplied more systems than any other currently operating company. In 2012, Thomas Keating won the Queens Award for Enterprise: International Trade [S2]. Sales of mm-wave instrumentation based on the original research by Smith made a major contribution to that success, with Pacific Northwest National Laboratory providing supporting evidence. [F1]

The technologies developed have also impacted on many other mm-wave programs within the group. These are largely associated with imaging radars for security applications (funding and contracts from DSTL, Home Office, US Army Research Labs, Millivision, Qinetiq, Alfa Imaging), medical imaging (funding from EPSRC) and for imaging volcanoes in low visibility situations (funding from NERC with a permanent installation at the UK Monserrat Volcano Observatory).

Societal Impact

The mm-wave outreach program during the evaluation period has currently reached approximately 115,000 people across Scotland. This audience figure is made up from ~82,000 as a touring exhibition (Major airshows, BA festival, gala days), ~28,000 in Scottish Science Centres and 4,600 over 133 events in schools (~15% primary : 85% secondary). The touring exhibition displayed at 6 public events before being adapted for stand-alone exhibition and has been on display to the public since November 2012, first at Dundee, then Aberdeen Science Centres.

The programme has also delivered 4 CPD (Continuing Professional Development) events including secondary school physics teachers (~40) [F2], oil industry staff (~20) and St Andrews staff (4). The

associated website [S3] continues to be very popular, receiving nearly 10,000 visits in the past 12 months.

In her supporting statement, the development officer of the Scottish Schools Education Research Centre states *"…By involving subject matter like yourselves in our CPD programme, we are able to offer the highest quality training to teachers. As a result of the CPD courses to which you contributed, the feedback we obtained from the 39 visiting teachers indicated that 75% of the teachers who undertook the CPD training rated the Vision for the Future material as 'very useful…".* [F2]

Our work in outreach is of particular relevance to the Scottish secondary school curriculum directly addressing outcomes SCN 3-11b and SCN 4-11b [F2, S4].

5. Sources to corroborate the impact

[F1]	Factual statement by Project Scientist, Thomas Keating Limited. *Corroborates details of the impact of the collaboration on Thomas Keating ltd*
[F2]	Factual statement by the Development Officer, Scottish Schools Education Research Centre *Corroborates details of the contributions of the Public Understanding exhibit to the Scottish Curriculum for Excellence and the role of the programme in delivering CPD training for teachers.*
[S1]	www.terahertz.co.uk/ *Corroborates examples of the St Andrews instrumentation built by Thomas Keating*
[S2]	www.queensawardsmagazine.com/2012winners \ *Corroborates Queens Award for Enterprise: International Trade won by Thomas Keating.*
[S3]	www.vision4thefuture.org/s1_home/index.htm *Corroborates Vision for the Future, public understanding project.*
[S4]	Curriculum for Excellence Description, p. 269, Available at: tinyurl.com/pyvx3q2. *Corroborates SCN 3-11b and SCN 4-11b in the Scottish School's Curriculum for Excellence.*