

epr news letter

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50

YEARS



The Publication of the International
EPR (ESR) Society



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Bruker has been a leading provider of high-performance magnetic resonance instruments and solutions for molecular and chemical research for the past 50 years. The “50” year on the cover embodies the famous Bruker logo.

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ETH

Eidgenössische Technische Hochschule Zürich
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Editorial

Dear colleagues,

As for me, it was easy to remember that 2010 marked the 50 years for Bruker. How come? Ten years ago, in 2000, Dieter Schmalbein came to Kazan on the occasion of the Zavoisky Award 2000 awarded to Bruker "for the achievements in the development of instruments leading to novel applications of the EPR technique". As a part of the Zavoisky Award ceremony, he gave a brilliant public lecture devoted to the 40 years of Bruker that was a real success story. It was such an impressive story that in ten years it was not surprising that I remember it. Dieter found it especially fascinating that in 2000 there were two Zavoisky Award laureates and that another Zavoisky Award laureate was Harden McConnell. It made Dieter's eyes glisten when recollecting that in the seventies he visited McConnell's lab and was given just ten minutes to describe Bruker instrumentation. And what progress made in some thirty years!

It is also not surprising that the IES owes special thanks to Bruker, our Patron, and that this special 50-years-of-Bruker issue was prepared as a token of our gratitude and appreciation of the contribution this company has made to the EPR community worldwide.

It was possible to have a color hard cover of the EPR newsletter. This terrific decoration was also due to an additional generous gesture of Bruker. In the end of 2002, when I became editor of the EPR newsletter, Arthur Schweiger commented that it would be good to have a hard cover of the newsletter in color. Well, it was a good idea but as it often happens with good ideas, to implement them, you need money which you do not have. I called Dieter Schmalbein and told him about this idea and asked him if he could kindly consider a possibility that Bruker would cover this additional cost. And yes, this was an instructive example of how fast Dieter could come to a decision! He asked me only one question: "How much does it cost?" And I have to admit that when it came to the money issue, even his voice had changed. It was a voice of a hard-boiled businessman who was

estimating whether the expenses were worth the effect. Within a second he decided that the sum I mentioned was acceptable and he said: "OK, go ahead with it!"

This issue speaks for itself. In addition, you could refresh in your memory some of our previous publications: "Memories of the Hutchison Jr. Group" by Arthur Heiss, Ralph Weber and John Weil (13/3, pp. 16–17), "Playing Flute" by Uwe Eichhoff (14/3, 8–9), "Milestones in the Bruker Commercial ENDOR History" by Peter Höfer and Dieter Schmalbein (16/2-3, pp. 26–27), "Dieter Schmalbein: 65th Birthday, but No Stop in Sight" by Arthur Heiss, Andreas Kamrowski, Diether C. Maier and Peter Höfer (17/2-3, p. 14), "40 Years of Bruker (UK) by Roger Ladbury (17/2-3, pp. 14–16), and "Workshop on Quantitative EPR" by Dave Barr, Sandra Eaton and Gareth Eaton (18, p. 32). Hope I did not miss anything.

With all my heart I thank all people who contributed to this issue! It was really a delight to work on it. In particular, I thank Keith McLauchlan and Hans Wolfgang Spiess twice: Keith for his life story in the "Five Years After" column (p. 5), which also gives us an opportunity to congratulate him on his 75th birthday (see also 16/1, pp. 8–9), and for his article in the EPR newsletter Anecdotes column (p. 12), and Hans Wolfgang for his interview on the occasion of his Zavoisky Award 2010 (p. 3), which also gives us an opportunity to congratulate him, and for his contribution to this issue as President of ISMAR (p. 20).

Finally, I share with you Ulrich Haeberlen's comments on 50 years of Bruker: "A firm, like a human being, a star and the entire universe, goes through a sequence of life cycles: childhood, youth, awkward adolescence, maturity, etc. Since some time, Bruker has reached, as has our sun, the stage of maturity and we all hope, as we all do in the case of our sun, that it will remain in that stage for a long-long time ahead." I could not think of a better resume!

Laila Mosina



Zavoisky Award 2000 ceremony, September 29, 2000, Kazan. From left to right: Dieter Schmalbein, Kev Salikhov and Harden McConnell.

PS A recent email message from Erwin Hahn had me thinking that the caption to Abragam's picture with his cigar which read: "SMOKING – NO HYDROGEN!" (a sign once posted on the office door of Anatole Abragam – a short example of his humor) published in the EPR newsletter 20/1, p. 9 (2010) is hardly discernible (white letters on the light gray background). Sorry!

IES business

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Bruker and the International EPR Society

I am happy to write in recognition of Bruker BioSpin's Fiftieth anniversary.

The membership of the IES, the international EPR community and EPR researchers all over the world greatly benefit from the availability and quality of Bruker EPR spectrometers. In the fifty years since its inception, Bruker BioSpin has become a worldwide market leader in NMR, EPR and Preclinical MRI research tools. The Bruker BioSpin Group develops, manufactures and supplies technology to commercial enterprises, research establishments and international corporations

across countless industries and fields of expertise.

While any business is interested, first of all, in the commercial success of its products, the interests of EPR researchers lie in obtaining new knowledge. Happily, Bruker and EPR researchers have had a long and productive symbiotic relationship. The successes of Bruker have provided us with means to advance in achieving our goals. Our needs have stimulated Bruker's production of new scientific instruments.

The IES, representing researchers from around the globe, wishes to recognize Bruker BioSpin's 50th anniversary, its contributions to the field, and to thank Bruker for being a long-term Patron of the IES. We are most grateful for their continued support. We look forward to many more years of fruitful cooperation.

Jack H. Freed
President of the International EPR Society



Interview of Hans Wolfgang Spiess on the occasion of his Zavoisky Award 2010*

Who introduced you into magnetic resonance?

When having to decide which field of science to study, I reckoned that my intellectual abilities were not good enough to study physics, but I thought I might master chemistry. Then, as a chemistry student at the University of Frankfurt, I was fascinated by Prof. Hermann Hartmann, who introduced quantum mechanics to physical chemistry in Germany. Thus, it became clear to me that I should join his group for thesis work. At that time, Prof. Hartmann himself was already quite remote from his coworkers and had 'Habilitationen' to run the subgroups devoted to different techniques. Thus, it was Hans Sillescu, the

* To be published in the second edition of the book "Electron Paramagnetic Resonance: From Fundamental Research to Pioneering Applications & Zavoisky Award" (ed. Kev M. Salikhov, AXAS Ltd, Wellington, New Zealand 2009) (www.treasuresofeureka.com)



The 2011 Bruker Prize

Thomas Prisner
University of Frankfurt
Germany

Awards

NMR guy, who offered me a project for such work. But when I started, he was just on leave for a postdoctoral stay at UCLA. After my thesis work on quadrupole coupling and anisotropic chemical shifts in cobalt complexes and postdoctoral work with Prof. Raymond K. Sheline in Tallahassee, Florida, it was again Hans Sillescu, who helped me to find a position at the famous Max Planck Institute of Medical Research in Heidelberg in the group of Prof. Karl Hausser. There I met a colleague, who introduced me into NMR theory and NMR hardware, Ulrich Haeberlen, from whom I learned a lot. When Hans Sillescu became a full professor at



the University of Mainz, he asked me to join his group to build up a NMR lab devoted to the study of structure and dynamics of polymers, a field I was - and still feel myself to be incompetent. As Hausser's interest was primarily in EPR, I could also observe important developments going on in this field, but it was only well after I became a director at the newly founded Max Planck Institute of Polymer Research in Mainz that I could build up an EPR group myself.

Is there an aspect that distinguishes your scientific work from that of others in the field?

The magnetic resonance phenomena in condensed matter that I worked on throughout my career are usually described by 'Spin Hamiltonians', products of space- and spin-dependent terms. While most of my colleagues were working on designing ingenious methods of manipulating the spin-dependent part of the Hamiltonian, my aim was always to obtain the information on the space-dependent part directly, i.e., the part that is of interest to a broader community. The best example showing that approach is probably the determination of the angle by which molecules rotate in a solid from a Lissajous figure displayed in a two-dimensional exchange spectrum. Other examples include the use of the rotor phase in Magic Angle Spinning (MAS) NMR to determine the orientation of macromolecules in drawn fibers.

How did your experience in NMR help you in EPR?

In the early days of magnetic resonance, the communities of NMR and EPR were interacting a lot. Later, they separated more than I feel they should have done. That gave me a chance to introduce concepts from NMR to EPR, albeit sometimes a bit too early, as I underestimated the technical difficulties associated with the much higher EPR frequencies. This holds for two-dimensional exchange EPR and in particular for introducing MAS into EPR. Both approaches can now be realized much better than at the time when we did such experiments, due to admirable advances in both sample spinning and microwave technology. On the other hand, four-pulse double electron-electron resonance (DEER) based on the ingenious approach introduced in Novosibirsk by Alexander Milov, Kev Salikhov and Yuri Tsvetkov to measuring dipole-dipole couplings between electron spins is a case where cross-fertilization was highly successful. Using the concept of first generating an echo to overcome the dead time of the receiver, a concept well-established in NMR, boosted the applications of this technique to measure distances in the nanometer range in macromolecular systems, including protein folding and protein complexes. It is a pleasure to watch this technique develop, based in particular on the work of my former coworker Gunnar Jeschke, now at ETH Zürich.

Did you ever benefit from analogies between magnetic resonance and other techniques or introduced concepts of magnetic resonance to other fields?

Analogies play a central role in my scientific work. In terms of statistical physics, the beauty of neutron scattering manifests itself in the possibility of directly determining the correlation functions of molecular motions. This made me think of whether one could do something similar in NMR and led me to the idea of generating deuteron spin alignment through the application of the famous three-pulse sequence and eventually two-dimensional exchange NMR. The opposite direction was pursued by my coworker Manfred Wilhelm, now a Professor at Karlsruhe, in his ingenious idea to develop Fourier rheology. This now provides

us with unique insight in the non-linear flow of polymers, colloids or even cells.

Apologies?

With the enormous development of science worldwide and with increasing interdisciplinary work it becomes ever more difficult to give proper credit to those who have used similar or sometimes even identical ideas prior to us. In fact, I know of specific cases, where I became guilty of not properly citing the previous work of others. Although I could partially rectify such omissions by giving credit to the pioneers in subsequent publications, I would like to take the opportunity to formally apologize here in writing.

What did you find most rewarding in your career?

After all, people are much more important than science. Our position as professors and scientists offers unique possibilities to interact with young people, being able to foster them in their development and observe how they mature. Moreover, as scientists we come in contact with many interesting persons beyond science, e.g., in the humanities, law, arts and even politics at home and throughout the world. At the same time, I always felt it rewarding that in science one has a chance to remain modest, as one is always reminded how difficult it is to even make the slightest advance, which in retrospect looks so simple.

Anniversaries



Five years on

I have been asked why I pursued a career in science. The answer must be that it was because how I was brought up. My father was an aircraft designer and was Project Engineer of many of the famous UK war planes including the Beaufighter, the Blenheim and the Brigand whilst later aircraft which he also Project Engineered included the Bristol Freighter, Concorde and the Lightning fighter. My elder brother graduated in Physics, designed and built satellites and computers and became Chief Executive Officer of National Air Traffic Services, the UK Air Traffic Control organisation. He later became Chief Executive of CANSO, the international Air Traffic Control organization.

I came late to ESR. My first research was on Nucleation and Crystal Growth and then I built a mass spectrometer for the observation of gas phase free radicals produced in a furnace attached to the ion source. As a post-doc I turned to gas phase radiation chemistry at the NRC in Ottawa but following an accidental exposure to ^{60}Co radiation left that area. I returned to the UK to the Na-

tional Physical Laboratory to work on high resolution NMR with J.A. Pople and D.H. Whiffen. I was very lucky in my timing since this was an extraordinary time for innovation in that subject and I was associated with many quite novel techniques. I rapidly joined the international conference circuit and in 5 years did two lecture tours of the U.S. It was a surprise when I joined Oxford to be told that I would not be allowed to continue in this field, although it was my publication record in it that got me the post, since the Head of the Laboratory was himself an NMR man, and he felt that his young staff should do something different.

I had no idea what to do but had the good luck that one of my undergraduate students came to ask me whether free radicals, which he had learned about in a lecture that morning, existed in solution besides in the gas phase, and if so how would I identify them. This happened on the very day that George Porter was awarded the Nobel Prize for his flash photolysis experiments and so I was able to answer that one detected them using UV spectroscopy. But then I realized that Porter detected them, but could not identify them, whereas I knew that one could identify free radicals in solution using ESR. It seemed an obvious thing to try on radicals produced by flash photolysis and the following day I discussed with Peter Atkins whether it would be possible (we worried about the Uncertainty broadening). It seemed so and we decided to give it a go. It was the first experiment I had ever done in ESR.

Ignorance of the difficulties involved saved the day – I had no idea how difficult it was to create a sufficient concentration to observe since UV lasers were not available then, I had no idea that no transient recorder with sufficient speed existed, and I had no idea that we would have to handle data faster than had been previously accomplished, since direct memory access was not then known. So we had to solve these problems ourselves, which was great fun although a commercial nitrogen UV laser giving 1mJ per pulse became available in time to save us. We designed

the system to be able to observe within the first microsecond of radical lifetime, which gave us the bonus of observing electron spin polarization. Barry Smaller, using different electronics, accomplished the same thing at the same time, whilst Dick Fessenden and Bob Schuler were the first to publish spectra showing polarization (from radicals in a steady state concentration).

For those of us working in the early 1960 period choice of research topics was easy. Few of the physical techniques now used on an everyday basis then existed in a state of immediate use to chemists. So it fell to my generation to invent them. Life for young scientists is now more difficult since almost any experiment one can think of can now be done, and the emphasis has changed from technique-development to problem solving. To identify new problems is the hardest part of science – one can keep repeating existing experiments on closely-related systems but this fails to introduce new ideas. Now ESR scientists have to deal with not only chemical applications but also molecular biological ones, and most of us lack training in the two disciplines. It is particularly difficult for non-expert molecular biologists to identify the important problems in biology rather than simply applying existing methods to more and more systems. So I am delighted, and full of admiration, when I see these aims accomplished. There is some wonderfully original research being done. But good scientists always worry about the next experiment rather than on dotting i's and crossing t's on the present one, and continuous innovation is necessary.

Finally, I was asked what I would have done differently, given the chance. The answer is absolutely nothing. My research life has been one big enjoyable adventure and it still surprises me that people have actually paid me for my self-indulgence. And what other life could have given me such a wonderful set of international friends? Seeing them is actually the thing I miss most in my retirement.

Keith McLauchlan

Are you interested to become a member of the International EPR (ESR) Society?

Please find the registration/information form for new/continuing members of the IES and non-credit-card payment instructions for individual members on this Web site: www.epr-newsletter.ethz.ch/contact.html

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www.epr-newsletter.ethz.ch/corporate_sponsors.html



BRUKER celebrated its fiftieth anniversary on September 7, 2010. Bruker Physik AG was founded by Professor Günther Laukien, then a professor of the Institute for electronic Circuits at the University of Bochum, and four others, including Dr. Bruker, in 1960.

First Decade: 1960–1970

Sited initially in Karlsruhe to produce power supplies, high frequency units, electromagnets and eventually NMR/EPR spectrometers, the company moved to newly established buildings in Karlsruhe Forchheim (today Rheinstetten) in 1964. That same year Bruker Spectrospin was started in Wissembourg, France. The next year a cooperation with Spectrospin AG of Switzerland was established.

The EPR Division of Bruker Physik was headed by Walter Riemer, a physicist who joined the company in 1968. He had developed a transistorized EPR spectrometer with a large-screen rapid scan display. Competitors abounded, including Varian, AEG, Radiopan Poland, Hilger & Watts and even a Russian spectrometer.

Bruker's presence in the United States began with the formation of Bruker Scientific Inc. in Elmsford, NY to market high resolution NMR spectrometers. This location was soon joined by an office on the west coast in Mountain View, CA.

Highlights Bruker

- 1960 Bruker Founded
- 1963 First NMR Pulse Spectrometer
- 1964 Buildings in Rheinstetten
- 1967 Cooperation with Trüb Täuber
- 1967 Bruker Elmsford USA
- 1969 First FT-NMR

Highlights EPR

- 1967 ER 400 Vacuum Tube EPR Spectrometer
- ER 414/418 Transistorized EPR Spectrometers

Second Decade: 1970–1980

Early in 1973 Dieter Schmalbein, a doctoral student of Professor Laukien, joined the EPR and took over the lead of the small EPR group in Karlsruhe. The group at that time was working on upgrading the product line to meet the requirements of Dr. John Weil, who had demanded performance and capabilities not offered by other vendors. Dr. Weil was willing to work with Bruker and share his ideas if he could get the research system he wanted; consequently the Karlsruhe team was fully occupied. Dr. Schmalbein, however, wanted to develop a smaller, easy-to-use, less expensive instrument. This led to the startup of a second EPR division at the plant in Wissembourg, France with Victor Ringeisen, the engineer in charge of the workshops.

The result of that collaboration, the ER 200tt, became the first truly competitive instrument available from Bruker. It

offered good performance, automatic tuning and matching of the sample at a competitive price and sales began to grow.

During this time Bruker introduced the first dedicated pulsed NMR, the WH90, (=work horse) which set the stage for all modern NMR spectrometers. Bruker Magnetics was opened in Burlington, MA to market Solid State NMR spectrometers and manufacture superconducting magnets for the WH270 270MHz High Resolution NMR.

Then in 1974 construction was started on a new building in Billerica, MA and the formation of Bruker Instruments Inc. which combined both the Bruker Scientific and Bruker Magnetics operations. Dr. Arthur Heiss returned from Karlsruhe in 1975 to manage the EPR marketing effort in the United States.

Highlights Bruker

- 1971 Bruker Canada
- 1972 First Supercon NMR WH270
- 1973 NMR minispec
- 1974 First Bruker Infrared System
- 1975 Bruker Medizintechnik
- 1975 Bruker Japan
- 1978 Bruker Meerestechnik
- 1978 Bruker Rheinhafen Plant

Highlights EPR

- ER 420 EPR Spectrometer with B-NC 12 Computer
- ER 4114HT High Temperature Cavity
- ER 200 Compact Spectrometer
- ER 4103TM Resonator
- ER 200tt plus EN200 ENDOR/Triple
- ER 10 EPR minispec

Third Decade: 1980–1990

The 1980's saw many changes at Bruker, notably the cooperation with IBM Corporation, which wanted to enter the scientific instrumentation field to recover prestige in the scientific laboratory lost in the previous decade to Data General and Digital Equipment Corp. IBM would re-label and market scientific instruments manufactured by others having negotiated suitable distribution agreements. This provided Bruker with a large capital infusion and allowed IBM Instruments to distribute Bruker's iron-magnet NMR, EPR, FR-IR, Mass Spec and Polarography instruments under the IBM name; Dr. Heiss moved to Connecticut to continue marketing the EPR product line. Bruker retained distribution of supercon NMR's so the facilities in Billerica, MA were retained. IBM leased several buildings in Danbury, CT and prepared for an influx of orders. Despite an aggressive advertising campaign, the scientific community did not immediately switch allegiance to IBM, and sales were hard fought and won on performance and competitive pricing.

During this period Dr. Dieter Schmalbein together with Dr. Reinhard Biehl, enhanced the research level system with the introduction of a microprocessor based digital Hall Effect Field Controller, new gaussmeter, and new signal channels. The new powerful Aspect data acquisition system was also available as an accessory. This instrument, the ER 200D, ►

EPR in the 50 Years of Bruker

Highlights Bruker

1980 Cooperation with IBM
 1980 Bruker Mass Spectrometry
 1980 MM1 Mobile Mass Spectrometer
 1981 Bruker Japan New Bldg.
 1982 Bruker FT-ICR Mass Spec
 1987 IBM Instruments Closed
 1990 Bruker FT-Raman
 1990 Bruker Saxonia-Leipzig

Highlights EPR

ER 200D
 ER 031M Digital Field Controller
 X-Band Transient Bridge
 First Royal Society Bruker Prize
 ESP 300 Fully Computer Controlled System
 ESP 380 First Commercial Pulse EPR
 FlexLine Series of Resonators
 ECS 106 Compact EPR Programmable Goniometer

firmly established Bruker as the leader in EPR instrumentation. The collaboration with IBM had helped Bruker increase its technical standard, evidenced by Varian dropping EPR from its product line in 1982.

Bruker was rapidly expanding around the globe. Bruker Japan, founded in 1975, moved into a new building in Tsukubain, near Tokyo, 1981. In the former Soviet Union, Bruker representatives Dr. Uwe Eichhoff and his wife, Barbara, covered the instrumentation market from their room in the Hotel Ukraina, and established a Bruker office in the Institute of Chemical Physics at the Russian Academy of Science in Moscow. Many fruitful collaborations with scientists from Kazan, Moscow and Novosibirsk followed.

The Chinese market was especially daunting, yet in 1982 while attending an exhibition in Tianjing, a tender for several EPR spectrometers was announced in the Beijing newspaper. The tender was awarded to Bruker and the resulting contract for 8 large systems to 8 different cities established Bruker EPR in Asia.

In Karlsruhe, manufacturing facilities also expanded, having previously acquired the large mechanical facility in the Rheinshafen, with the addition of a company next to Bruker in Rheinstetten. This became the Bruker Elektronik GmbH in 1975, when Bruker Analytische Messtechnik GmbH was formed to encompass the NMR, EPR and FT-IR Divisions. Bruker Elektronik remains the electronic circuit board production facility for all of the various Bruker Divisions until 2010 when it was merged with BioSpin GmbH in Karlsruhe.

In 1986 Dr. Dieter Schmalbein decided to develop an FT-EPR spectrometer although all experts were of the opinion that this is technically not feasible and if, the market would be so small that the project must fail. Following initial failures to build such an EPR system, Bruker intrigued Dr. Károly Holczer with the task of constructing an EPR spectrometer capable of performing all the common and scientifically reasonable pulse experiments known to NMR. The bridge proposal comprised ca. 20 times the microwave components of a standard CW bridge and the development thoroughly stressed everyone in the Division. The ESP 380 was exhib-

Royal Society of Chemistry / Bruker Prize

1986 Martyn C. R. Symons	1999 Jan Schmidt
1987 Klaus Möbius	2000 Dante Gatteschi
1988 Hanns Fischer	2001 Jürgen Hüttermann
1989 James S. Hyde	2002 G. R. & S. S. Eaton
1990 Jack H. Freed	2003 Wolfgang Lubitz
1991 E. de Boer	2004 Wayne L. Hubbell
1992 George Feher	2005 Klaus-Peter Dinse
1993 Neil M. Atherton	2006 Yuri D. Tsvetkov
1994 Arthur Schweiger	2007 Daniella Goldfarb
1995 H. M. McConnell	2008 Edgar Groenen
1996 Brian Hoffman	2009 Gunnar Jeschke
1997 Keith A. McLauchlan	2010 Ronald P. Mason
1998 John R. Pilbrow	

ited at the 1987 Rocky Mountain Conference and was the first fully functioning commercial pulse EPR system. Dr. Holczer took a professorship at UCLA in 1989, but the door for routine pulse EPR was open. The task now was to convince the scientific community – Dr. Peter Höfer, from Prof. Mehring's group in Stuttgart, joined Bruker in 1988 and rapidly demonstrated the capabilities of the new instrument. In 1989 the enhanced version ESP380E was introduced along with a new low-cost CW system, the ECS-106. This was the first fully computer controlled EPR, a system without any manual controls.

Fourth Decade: 1990–2000

The IBM PC began to acquire more capabilities in the 1990s, but it was still not up to coping with the needs of a computer controlled EPR spectrometer. For this task, a Motorola chipset in a VME structure and the OS9 real-time operating system was chosen. In this way, the asynchronous interrupt demands of acquisition could be satisfied, but the user interface was primitive and awkward. The ESP 300E provided an enhanced user interface and the ability to export data via ftp, but was still keyboard based. To overcome the PC's limitations, Diether Maier, leader of the EPR development since 1991, designed the EMX series, introduced in 1994. This system utilized the Windows™ user interface with the acquisition tasks offloaded to an onboard networked processor, the Transputer™, located in the field controller, signal channel, and separate microwave bridge controller.

A major problem for any instrument manufacturer is the acquisition of semiconductors in a rapidly evolving electronic world. The obsolescence and discontinuance of supply of major components, such as the Transputer™, led to yet another redesign and the implementation of Ethernet connectivity between the individual spectrometer modules. It also became necessary to bring the manufacture of a solid-state X-Band microwave source in house, leading to the implementation of a microwave development group in Wissembourg. At the same time, a major software project to address the continuing problems with Windows™ was undertaken. The result was Xepr™. This Linux-based program with inherently multi-dimensional data structures was conceived to provide

EPR in the 50 Years of Bruker

the software basis for the new eleXsys Series of CW and pulse spectrometers.

It was decided in 1993 to expand the existing multi-frequency capabilities to W-Band and the microwave group faced the challenge of developing oscillators, mixers, up- and down-converters matched to the unique demands of spectroscopy, as most commercially available components were designed for radar applications. This led to the heterodyne bridge design concept which allowed many different frequencies to be based upon the sensitivity and switching capabilities of the X-Band IF bridge.

Highlights Bruker

- 1991 Raman Microscope
- 1992 First 750 MHz NMR
- 1994 New building in Ettlingen
- 1995 First 800 MHz NMR
- 1997 Prof. Laukien died
- 1997 Bruker Daltonics
- 1997 Bruker acquires AXS from Siemens
- 1998 Bruker Optics

Highlights EPR

- WinEPR
- EMS 104 Alanine Dosimetry
- ESP 300E enhanced 32 bit version
- EMX Series
- ESP 360 DICE ENDOR
- Xepr EPR System Software
- eleXsys E500 E580 E600 E680
- AquaX – Flow System
- SuperX Bridge with 3000:1 S/N

Fifth Decade: 2000–2010

Bruker was honored with the prestigious Zavoisky Award in 2000 “...presented in recognition of a work dedicated to electron paramagnetic resonance and, in particular, the awardee’s achievements in the development of instruments leading to novel applications of the electron paramagnetic resonance technique.”

The Fifth Decade at Bruker was one of corporate consolidation and expansion through acquisition of new technologies. Bruker BioSpin was formed in 2001 to bring together all of the Bruker companies specializing in magnetic resonance. Bruker had achieved dominance in the fields of NMR and pre-clinical MRI as well as EPR. Bruker acquired Vacuum-schmelze Hanau in 2002 to ensure the supply of wire for superconducting magnets. The Bruker Daltonics group was the first of the Bruker companies to be listed on the NASDAQ stock exchange, soon followed by Bruker AXS. In 2003 Bruker Daltonics and AXS merged to form a single listed company joined by Bruker Optics in 2006. All of the Bruker companies were merged in 2008 adding Bruker BioSpin to Bruker Corporation (NASDAQ: BRKR). Bruker expanded again in 2010 with the acquisition of Veeco’s atomic force microscopy and optical industrial metrology units.

Bruker EPR also continued to expand and upgrade the product line with the introduction of the new EMXplus

and EMXmicro spectrometers incorporating newly designed field controllers and signal channels as well as upgrading the microwave bridge electronics to direct Ethernet control. The eleXsys Series were similarly upgraded with the introduction of the eleXsys-II product line and enhancements to the E540 EPR Imaging spectrometer to include high field gradient capability for X-Band materials imaging. The development of a new cryogen-free 12T superconducting magnet and a quasi-optical bridge has extended Bruker EPR to 263GHz with both large-sample non-resonant probes and high sensitivity single-mode resonators.

The Xenon™ software package has been introduced to allow the EMXmicro/plus spectrometers access to the Linux platform and many of the capabilities of Xepr™ with a very user-friendly interface. Xenon™ incorporates both the SpinFit and SpinCount modules for accurately titrating mixtures of spin adducts and reference-free measurements of spin concentration.

Bruker Corporation, today led by Dr. Frank Laukien, has revenues that exceed the US\$1 billion mark which are directly attributable to the company’s commitment to customer service, innovation, continuity and product quality. Continued progress is assured through the confidence and reliance on more than 4000 highly motivated employees and through continuing excellent customer relations. As one of the leading analytical instrumentation companies, Bruker is committed to developing innovative solutions to tomorrow’s analytical questions and thereby securing an ever-successful future.

Highlights Bruker

- 2000 Bruker Daltonics listed on NASDAQ
- 2001 Bruker BioSpin formed
- 2001 Bruker AXS listed on NASDAQ
- 2002 Bruker acquires Vacuum-schmelze Hanau
- 2003 Bruker Daltonics and AXS merge
- 2006 Bruker Optics joins Bruker Corp.
- AVANCE III NMR Family
- AVANCE 1000 1 GHz NMR
- DNP at 400 MHz / 263 GHz
- Bruker Energy & Supercon Technologies
- 2008 Bruker BioSpin joins Bruker Corp.
- 2009 Bruker acquires ACCEL Instruments GmbH
- 2010 Bruker Acquires Veeco AFM and Optical Industrial Metrology Instruments

Highlights EPR

- Zavoisky Award
- EMXplus
- EMXmicro
- E540 EPR Imaging
- eleXsys-II
- E700 E780 263 GHz
- Xenon Software
- Quantitative EPR published by Springer
- Spin counting

Dieter Schmalbein
Arthur Heiss



1



2



3



4



5

Photo 1: Class in Denver at the Rocky Mountain Conference 2004.

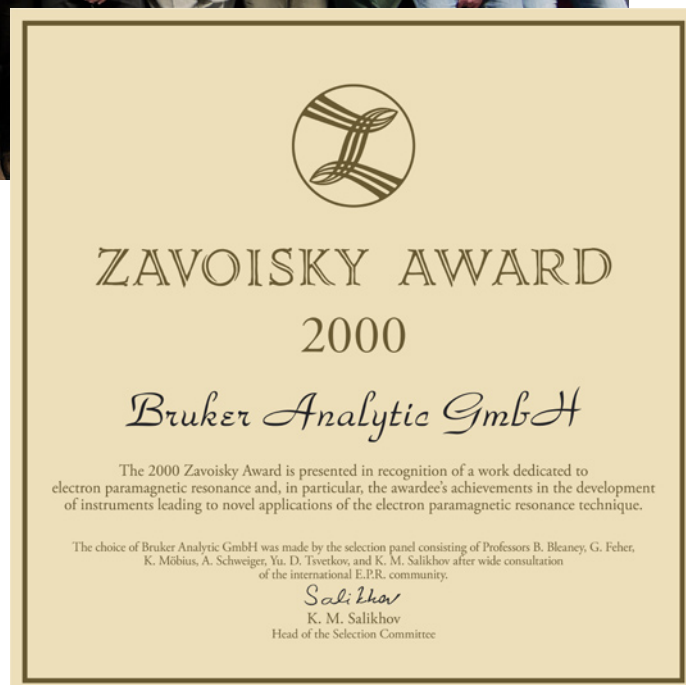
Photo 2: Demo lab (Bruker BioSpin, Billerica MA USA).

Photo 3: Meeting of the German / US team at the Rocky Mountain Conference 2010 to discuss strategies. From left to right: Arthur Heiss, Ralph Weber, Peter Höfer, Dave Barr, Dieter Schmalbein and Patrick Carl.

Photo 4: Dieter Schmalbein (center) in discussion with the NMR Manager Dr. Tony Keller (left) and Dr. Gerhard Roth (right), the manager of the Bruker superconducting high-field magnets.

Photo 5: ESR 2010: this is part of the EPR team today. There are always some people missing who are on installations somewhere in the world.

Photo 6: Zavoisky Award 2000 Diploma.



Lifetime of 28 Years of a Bruker EPR Spectrometer

During my scientific career of more than half a century I used a commercial spectrometer for a bit more than the second half of it. In the period 1955/1958 I constructed my first EPR spectrometer as part of my Thesis at the ETH in Zürich. It had a superheterodyne receiver with a local oscillator klystron and an intermediary receiver working at 30 MHz, “organized” from an old TV set. This first, and the second one, also a superheterodyne, used 9 GHz microwave radiation and was operational at the Battelle Memorial Laboratory in Geneva where I met my long-time collaborator Walter Berlinger.

Together we then came to the IBM. Laboratory in Rueschlikon near Zürich in 1963 where a successful long-time enterprise started with many EPR results, yielding on the order of 30 Letters to the Physical Review, and a series of larger publications with many collaborators. This spectrometer was again of the heterodyne type and allowed a modular setting with the possibility to apply hydrostatic and uniaxial stress, frequency-dependent illumination, a



temperature stability of better than 10 mK, and temperatures from the pumped helium range to 1300 K. It worked at 19 GHz.

Many substantial results in the fields of ferroelectricity, photochromics, structural phase transitions and critical phenomena were obtained. The first observation of the EPR of ions with high valence such as Fe^{5+} or Co^{4+} or negative effective U-centers led to my promotion as an IBM fellow in 1982. There were six of us with this status at a time when the IBM

Alex Müller and his wife Ingeborg at the gathering celebrating 100 years of Alfa Romeo, 11 September 2010, Champex Lac Valais, Switzerland.

company had about 420 000 employees. With this status one could choose projects of one's own taste, and this helped in the discovery of high-temperature superconductivity. On becoming a fellow one was allowed a “gift”, and I asked for a Bruker 9 GHz spectrometer, which was accepted.

Congratulations to Bruker Corporation on the Occasion of Its Golden Jubilee*

Last year, Bruker Corporation could celebrate its Golden Jubilee, a perfect instance to look back and ask about the reasons for the remarkable success of the most relevant company active in the field of magnetic resonance. Indeed the continuous growth of Bruker Corporation during the past 50 years can fill initiative and innovative entrepreneurs with confidence. After all, courage and creativity are decisive for success, irrespective of the size of the company. Money-mindedness of investors alone is insufficient for a positive development. History demonstrates, also in the realm of magnetic resonance, that initial success might lead to haughtiness and to un-



derestimation of the motivated competition. Another lesson that can be learned concerns the leadership of high-tech companies. Never invest in companies that are led by lawyers and MBAs who lack sound technological experience. Technical and scientific knowledge, as well as skin-contact with the market are essential for avoiding adverse developments. No global financial crisis is necessary for demonstrating the devastating effects of poor decision mak-

ing. A comparison of the recent history of Bruker and Varian reveals several principles of wise governance. Bruker escaped many lurking dangers by wise personal politics and long-term vision. The sound technical knowledge of the CEO is still the best warranty against bold management errors.

As long as Europe possesses companies with initiative of the quality of Bruker Corporation, the long predicted commercial decline of Europe is not in sight. Despite the fact that Bruker Corporation is today legally a US company, the spirit of the company is still solidly “European” and promises rewarding investments for investors, superb high quality products for the spectroscopist and analytical scientist, and an inspiring working place for potential employees.

Let us hope that this jewel among the spectroscopy-oriented companies will prosper for many more decades to come.

Richard R. Ernst,
Nobel Laureate Chemistry 1991

* Read also an article by Richard Ernst “Zürich's Contribution to 50 Years Development of Bruker” published in *Angew. Chem. Int. Ed.* 2010, 49, 8310–8315. (<http://onlinelibrary.wiley.com/doi/10.1002/anie.201005067/pdf>)

Keith Blazey, now since long in retirement, and working in my group, was mainly using it in the Rueschlikon Laboratory. Then, when I reached 70, I moved to the Physics Institute of the University in Rueschlikon and was allowed to take the Bruker spectrometer with me, as it belonged to me as a Fellow of the IBM company. Since then it has been in use continually - that is a total 28 years.

Of course on the electronic side parts have been replaced by more up-to-date ones. This can be regarded for the Bruker company as a sign of reliability and continuing service. Also, the microwave cavity has been modified in such a way that most of the EPR applications possible with the early superheterodyne spectrometers could be carried out with the high-frequency modulation in operation with the Bruker spectrometer. This has even permitted photochromic research by detecting EPR simultaneously under illumination and variable electric current conditions.

K. Alex Müller
Nobel Laureate Physics 1987



45 Years Devoted to EPR: Another Anniversary of Bruker BioSpin

Memory is at the Beginning of the New

In the history of science there are many examples that significant steps in the advancement of knowledge are initiated by the invention of new experimental tools that allow for scaling the dimensions of our abilities to look at the world around us. Prominent examples are the inventions of the microscope, the telescope, and the spectroscope, whose extension from the visible light via the microwave and X-ray spectral regions enabled us to observe new details of the atomistic world and to change

paradigms from classical to quantum physics. But, for gaining new understandings it is generally required to involve a large number of researchers in the field, in addition to the original inventors of the new tools. Such tools were indeed made available to more and more researchers by skillful people, be it expert lens grinders in the Galilean times or dedicated physicists and engineers in modern times.

This line of thinking seems to apply also to EPR spectroscopy in general and to Bruker BioSpin in particular. For the real breakthroughs in the molecular-level understanding of complex paramagnetic systems, Zavoisky's invention of EPR in 1944 had first to be taken up by numerous laboratories from academia, research institutions and industry. This enabled highly motivated scientists to use the new EPR technique, to improve and expand it, and to learn to analyze the rather complex EPR spectra in order to contribute to the advancement of knowledge.

Thus, after the first creative steps by rather few dedicated laboratories in the development of EPR and its extension to the multi-resonance, multi-frequency, multiple-pulse and high-field domains, a really broad range of exciting EPR applications had to wait for commercial analytical instrument makers, such as Varian in the US and Bruker in Germany (and also, although on a smaller scale, AEG in Germany and JEOL in Japan). Varian, although the first commercial EPR and ENDOR manufacturer, and always profitable in this division, dropped out of the EPR business in 1982. This was decided just at the dawn of a remarkable renaissance in EPR spectroscopy. It was due to the successful efforts of a few laboratories to introduce fast microwave pulsing and high-field/high-frequency capabilities – very much by way of analogy to what had happened in NMR spectroscopy a decade earlier. Apparently, Varian did not arrive at a very wise decision but, strangely enough, it was also adopted by the AEG management.

Dr. Günther Laukien at Bruker, however, was wiser and, rightfully, the EPR community praises him for his decision to continue to invest in sustaining improvements of their EPR spectrometers. Moreover, Bruker BioSpin has continued up to now to introduce commercial state-of-the-art variants of new EPR methodologies originally invented in dedicated EPR laboratories around the world. Bruker's decision to stay in the EPR business did not only secure a world-wide leading role in commercial EPR fabrication, but also led to a multitude of exciting EPR applications in chemistry, physics

and biology. This is mirrored by an impressive growth of the EPR literature during the last 20 years. A few of Bruker's more recent milestones in commercial EPR instrumentation development are:

Their first FT-EPR spectrometer (1987), their first pulsed ENDOR spectrometer (1993), their first high frequency (95 GHz) cw and pulsed EPR spectrometers (1995), and their first very high frequency (263 GHz) EPR spectrometer (2009). The full list of their "firsts" is impressively long, and the technical and scientific excellence of the people at Bruker BioSpin responsible for those achievements is highly appreciated by the international EPR community. As a logical consequence, Bruker BioSpin was honored by the prestigious Zavoisky Award (2000), a well-deserved recognition, indeed!

There is also the human aspect to be mentioned on such an anniversary occasion: The Bruker scientists maintain direct contact with the EPR community by showing up at EPR workshops wherever they are taking place in the world! There one can meet them more as a colleague than as a customer. On such occasions it was always my pleasure to discuss with Dieter Schmalbein, Reinhard Biehl, Karoly Holczner, Peter Höfer, Andreas Kamlowski, Ralph Weber, and Arthur Heiss.

Reinhard Biehl was very close to me as a former highly gifted student and creative collaborator, but also as a most impressive human being. After his PhD student and postdoctoral time in my group he moved to Bruker in the early 1980's. There he got heavily involved in the development of cavity resonators and pulse EPR instrumentation. His wide-ranging knowledge of the physical sciences, and his innovative ability for tracing the right way out of a difficult problem placed him among the key players in research and development of modern EPR spectroscopy. He was a demanding discussion partner and always asked for complete dedication to the given task. His personal and scientific life reminded of a candle burning from both sides. He died much too early in 1987 at the age of only 43 years.

Memory is at the beginning of the new: The EPR community wishes Bruker BioSpin ongoing success of the EPR division allowing the Bruker scientists and engineers to stand in their tradition of always striving for the "new" in EPR spectroscopy - also in the years to come after this 50th anniversary.

Klaus Möbius



Serving the EPR Market across 50 Years

I wonder if the readers of the EPR Newsletter have ever thought about what really bad customers of EPR equipment they are. Each of us wants something special. The EPR market is not one market, but a large number of small markets across biology, chemistry and physics;

The Influence of Bruker

ESR had a much more difficult gestation than NMR. Firstly because its applications were limited to samples containing unpaired electrons and secondly because microwave techniques were not well developed. The wide application of NMR caused highly sophisticated techniques, in magnet manufacture, computing power etc to be developed whilst the basic radiofrequency electronic methods were well established. In contrast, ESR was limited for the most part by technology, although as a result of war-time radar equipment was available at X-band (X-band radiation is transmitted through clouds). Some extraordinary fundamental work of microwaves was done at Bell Telephone during the War, and served as our Bible. In 1960 there existed a number of homebuilt instruments, and early commercial ones from Varian, culminating in the E4, a workhorse machine for standard problems. But Varian then ceased to develop and make ESR spectrometers, and the void was, to the great benefit of ESR spectroscopists, filled by Bruker.

Dieter Schmalbein was already with the company and he interacted with Klaus Möbius in Berlin. At the time Klaus, with Reinhard Biehl, was transforming ENDOR spectroscopy in solution with some brilliant innovations. Dieter

across solids liquids and gases; across practical applications and basic science; and more – each of these minimarkets needs unique EPR accessories. The typical customer who lives by government grants needs a quotation for his/her proposal, and then expects it to be still valid when the money becomes available a year later. Moreover, the funding agency may have cut the expected award by 10%, and still there is an expectation that the equipment can be purchased. Bruker has served this simply terrible market with grace and energy and high competence for fifty years. It is amazing and we all should be grateful.

Across these fifty years, I myself have been a Bruker competitor, a Bruker consultant, and a very good Bruker customer, so I have seen the firm from many perspectives. The collective personality of the company includes, based on my observations, the following characteristics: extreme loyalty and dedication in serving their customers and the field of EPR in general, steadfastness across a half century of technological and market change, and a high level of professionalism in manag-

ing their business. Few scientific communities have been so fortunate.

The technology of EPR has been changing continuously over the half century, driven by new applications, computers, innovations in microwave systems, and novel digital devices. There have always been academic innovators in the EPR world who strive continuously to advance the field. The stress on Bruker management not only to deploy financial and engineering resources wisely in the commercialization of selected academic advances, but also to pursue their own substantial and innovative contributions to the field must have been considerable. In addition there has been a continuous call on engineering resources just to keep the product line up-to-date. My compliments to the Bruker EPR management team for its wise leadership in keeping these demands in balance.

Also, the Bruker guys have become everyone's personal friends.

Best wishes to them and their firm for the next half century.

James S. Hyde



persuaded Reinhard to join the company and they set about introducing these techniques on a new generation of spectrometers. I believe that it was the impact of these that persuaded Bruker to maintain production of ESR ones, although concomitant developments in computing on the NMR side of Bruker allowed them also to provide a (rather idiosyncratic) computer on the spectrometers. This initially led to computer-control of experiments, but probably more importantly at the time when by no means all of those who used ESR knew how to solve the spin Hamiltonian, enabled users to analyse their spectra with immediate effect using the software provided

I owe a particular debt to Dieter and Reinhard (who died tragically young) in that they undertook the broadbanding of my spectrometer to allow transient radicals to be observed, and without charge. Their familiarity with the Maxwell equations and their implications to cavity design always impressed me.

For a commercial company with that rare thing a successful ESR machine on their hands it must have been tempting to sit back and generate some profit. But to their great credit they continued to develop the most sophisticated spectrometers ever produced commercially. Early on they introduced Q-band, and then high-field and W-band spectrometers, both of which introduced new dispersion into spectra and greatly widened the range of applications. They developed extraordinarily sophisticated pulse generators, which in turn allowed the common use of pulse, and multiple pulse techniques, in particular in conjunction with vastly improved computing power. The techniques were originally introduced elsewhere, in particular by Jacob Lebedev at high field (and he developed the microwave techniques and hardware used at these frequencies too) and Klaus, Arthur Schweiger and Jack Freed. But Bruker introduced them into reliable equipment which allowed essentially any ESR experiment ever done to be performed routinely. This has taken a ma-



50 Years of Bruker

I first became aware of Bruker in the late 1960's when first considering the purchase of a commercial EPR spectrometer. A company near the Monash University Campus had become the Bruker local agent and I recall talking with them only to realize that the cost of a CW instrument was beyond the funding available to me at that time. During 1973 I served on the National NMR Sub-Committee of the Australian Research Grants Committee, charged with selecting national Pulsed NMR Spectrometer. After much deliberation, we chose Bruker, one of the earliest pulsed NMR instruments they made. From memory I recall the terminology of pulse-free-precession. This was a time when it was thought, wrongly as it turned out, that one instrument would be sufficient for the whole of Australia!!

At the 1987 EPR Symposium in Denver, Bruker exhibited its prototype ESP380E spectrometer. Many of us looked upon it with awe, thinking it would be a dream to own such an

instrument. An opportunity presented itself in 1991 through a large equipment fund administered by the Australian Research Council. The bid was successful and our spectrometer, installed early in 1993, still runs today!

I have been privileged to witness the high quality production facility at Rheinstetten firstly in 1990 and again in 1992.

I wish to add my congratulations to Bruker for their contribution to developments in magnetic resonance and for the quality of their instruments during the past 50 years.

John Pilbrow

All is Well What Ends Well

My first encounter with EPR occurred in Florence in the early 1970s and, although it may be embarrassing to admit the spectrometer was a VARIAN E9 which, by the way, is still working. I was interested in transition metal complexes in low-symmetry environments to check the possibility of using ligand field models to calculate the electronic levels in the non-cubic symmetry. The Florence Institute of Inorganic Chemistry specialized in five coordination and much effort was made to understand the electronic structure. Initially, I used single-crystal electronic spectroscopy and decided to forget, for a while, five coordination to investigate a copper(II) compound, $\text{Cu(en)}_3\text{SO}_4$, where en stands for ethylene-

tion which splits into ${}^2A_{1g}$ and ${}^2B_{2g}$. On the other hand, the ground state becomes 2E in trigonal symmetry without breaking the degeneracy. From polarized electronic spectra we suggested that the trigonal symmetry was an average due to the dynamic "tetragonal" distortions. In order to find the "smoking gun", we decided to use the brand new VARIAN EPR spectrometer, which was available in the lab, and the temperature dependence of the spectra was a good reward of our efforts. In fact, at room temperature the spectrum was quasi-isotropic, as a result of the fast hopping, on the EPR time scale, of the system between three equivalent distortions along x -, y -, and z -axes. As a confirmation, below 160 K the spectrum became anisotropic suggesting that hopping was blocked. The g -values did not quite comply with the rules, and since $g_z < g_x, g_y$, we assumed that they corresponded to the rare tetragonal compression. I presented these conclusions at a conference and the very polite Dirk Reinen, chairman of the session, suggested to me the right interpretation. At low temperatures the individual copper coordination is tetragonally elongated, the elongation axis of one ion corresponding to the compression of the neighboring one. The two signals are averaged by the intermolecular exchange.

A very good start indeed! Luckily errando discitur* and provando e riprovando** I improved so much to convince Bruker to give me the award of year 2000, and here is the last

major, and continuing, technical investment for which we are all grateful.

Throughout the period Bruker has not only produced fine spectrometers but has actively encouraged their application to new fields of research. Our Community has much to be grateful for. But our personal thanks should go to Dieter who has driven the whole thing including during those times when the Company itself was a little reluctant to invest in ESR.

I apologise to those who have not been mentioned in this account but who deserve to have been. But this is an account of one company's contribution, and not a history.

Keith McLauchlan



Dante Gatteschi (right) and Giovanni Bizzaro (left).

diamine. The interesting feature was that six nitrogen atoms impose D_3 symmetry on the metal ion that seems to contradict the Jahn-Teller theorem. In fact, the ground state of a d^9 ion in the octahedral coordination is 2E_g which is unstable against a tetragonal distor-

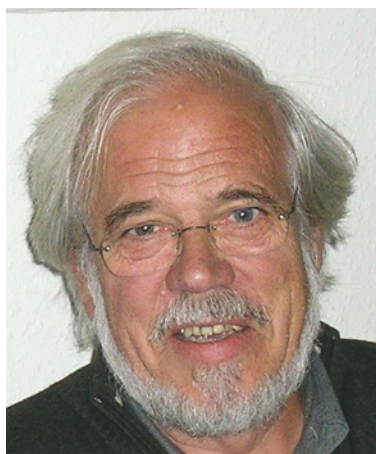
* Mistakes are often the best teachers

**Testing and re-testing

part of the story. I went to Norwich to give the Bruker lecture, which, remembering the hectic start, was entitled “EPR of transition metal ions. A tale of symmetry and of symmetry breaking”. Shortly before the beginning of the ceremony I contacted Giovanni Biz-zaro (Bruker Italy), who was due to give me the prize, and we realized that nothing was prepared. After some panic Giovanni made a big empty envelope which finally was ready for me. It shows up quite well in the official picture of the event! The solid prize came to Florence few days later.

The lab now is equipped with a 95 GHz Bruker E600 spectrometer. The use of high frequency would have avoided the above mistake and, more than that, it opens the doors to the exciting field of high-frequency EPR spectroscopy. But this is another story.

Dante Gatteschi



My Personal Recollections with Bruker in Karlsruhe (Germany)

It is often said that Bruker and its long term “spiritus rector” Günther Laukien are synonymous; if so, then my first contact dates back to 1966. I was a student at Karlsruhe University, had finished my regular Physics courses and was looking for an interesting topic to perform my Diploma thesis in. So, I attended for one semester some specialized lectures and one of them was by Günther Laukien, who at that time was Professor at the Physics Department. The lecture was, of course, on NMR and relaxation. Eventually I did not join with him but worked for my Diploma thesis in another topic. It took nearly ten years before I had contact again, this time with Bruker and its ESR-division as a customer. During my PhD work I had

been initiated to ESR-Spectroscopy and had worked with machines by Hilger and Watts (England) and AEG (Germany), both names long forgotten in the community. I spent a post-doc time in the US where I worked with Varian spectrometers.

When it came time to decide about my first „own“ ESR-apparatus at Regensburg University, I negotiated with Varian but also visited Bruker in Karlsruhe (shortly before Dieter Schmalbein became responsible for the ESR division) and eventually decided for a spectrometer from Bruker. In retrospect, the most important reason for this decision (much against the “main stream“ in those days) was the atmosphere in Karlsruhe which was much alike that one typically finds in a University laboratory. I had the impression I was discussing with scientists rather than talking to company employees. This aspect, for me, has remained a constant parameter and was even strongly enhanced in the era of Dieter Schmalbein with firstly Reinhard Biehl and later Peter Höfer. In more than thirty years of contact I have had with Bruker since then (I was lucky to be able to acquire further instruments over the years for my laboratory thanks to Saarland University and other granting agencies, especially the Deutsche Forschungsgemeinschaft), I have not lost this impression: being among scientists in the Karlsruhe ESR division labs. Despite the enormous growth of the company and its division in that same period, the specific scientific problem and an instrumental perspective in solving it were always the prime target of discussions during my visits. And, there was always enough time for discussions. It is also typical in this context that there has been little fluctuation in the main responsible persons in the ESR division over such a long time so that a strong continuity in contacts has been maintained. The same goes for the technical support for which I will mention Mr. Klausmann as one representative. Of course, many more devoted scientists and technicians have been, and are still involved, in keeping the Bruker ESR division alive and going.

I wish Bruker all the best for its anniversary and for its future; I hope the people in the ESR-division can keep up their quite specific and special style of working with and for the ESR-community even in a globalized world.

Jürgen Hüttermann



50 Years of Bruker

First of all I would like to congratulate Bruker on their 50th anniversary. During ISMAR2010 in Florence there was a presentation about the history of Bruker, and it showed their great contributions to the field of magnetic resonance. We have Bruker’s EMX X-band EPR spectrometer in Kobe. Although we are mainly working on developments and measurements of high-frequency/high-field ESR, the EMX spectrometer is a complementary and nice machine. Its sensitivity is comparable with the conventional SQUID magnetometer and its high sensitivity is very useful when we study the thin magnetic semiconductor films. In many cases we have to cool down to liquid He temperature and the angular dependence measurement at low temperature enable us to identify the paramagnetic centers and ferromagnetic properties. We also study strongly correlated spin systems by ESR and sometimes we want to extend the temperature and the magnetic fields of X-band spectrometer to 0.1 K and beyond 10 T, respectively. However, these might be too much to ask considering the cost.

In 2009 I visited Karlsruhe to attend the International Conference of Magnetism. Taking this opportunity my colleagues and I visited Bruker BioSpin and Dr. Peter Höfer kindly showed us the state-of-art EPR spectrometers, especially the 263 GHz high-frequency EPR spectrometer under development at that time that looked very promising. I was also interested in the X-band EPR spectrometer which enables one to obtain the absolute spin density. EPR has an advantage in separating paramagnetic centers by the difference of resonance fields. This separation is not possible using a conventional SQUID magnetometer which measures the total magnetization of the system. In this case I always felt that it would be

extremely useful if we could obtain the absolute spin density of each paramagnetic center directly from the EPR intensities. Now it is realized and on the market.

Finally I hope that Bruker continues to contribute to our EPR/ESR community and that new developments including high-frequency EPR will come up in future.

Hitoshi Ohta

Bruker Prize Lecture

The ESR Group of the Royal Society of Chemistry is also delighted to celebrate Bruker's 50th Anniversary and to acknowledge the support from Bruker at our conferences and meetings over the past years. In particular, since 1986, Bruker has generously sponsored the Bruker Prize Lecture at the UK ESR Group of the Royal Society of Chemistry's Annual International meeting. This award was initiated following discussions between the Group's Chairman, Prof. Neil Atherton

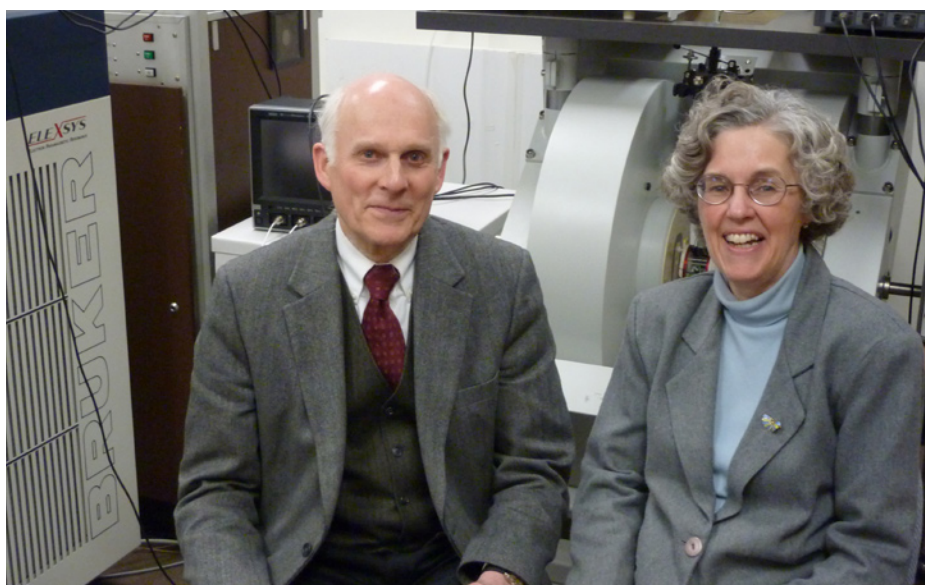
and Bruker's Dieter Schmalbein. It was agreed that Bruker would provide financial support for the lecture but would have no influence or input into the selection process save that the lecture 'be presented by a scientist who has made a major scientific contribution to the field of ESR spectroscopy'. As a past Group chair myself, I can confirm that the selection process is indeed entirely independent.

The first Bruker lecture was presented by Prof. Martyn Symons FRS with his lecture entitled 'Applications of ESR spectroscopy to the study of the effects of ionising radiation on DNA and DNA complexes'. In the intervening 25 years there has been a series of lectures by scientists of the highest calibre from around the world. The 2011 Bruker lecture is no exception and Prof Thomas Prisner (University of Frankfurt, Germany) will be presenting the 26th annual Lecture in April at the Group's 44th Annual Conference in York (www.esr-group.org/conferences/esr2011). After each lecture Bruker has also hosted a reception to celebrate the lecturer. A full list is available at: esr-group.org/Bruker-Lectures.php.



Clearly, EPR is still a rapidly developing field of science, with many potential Bruker lecturers still to be identified. I know that I am not alone in looking forward to many more the Bruker Lectures in the decades to come.

Shirley Fairhurst



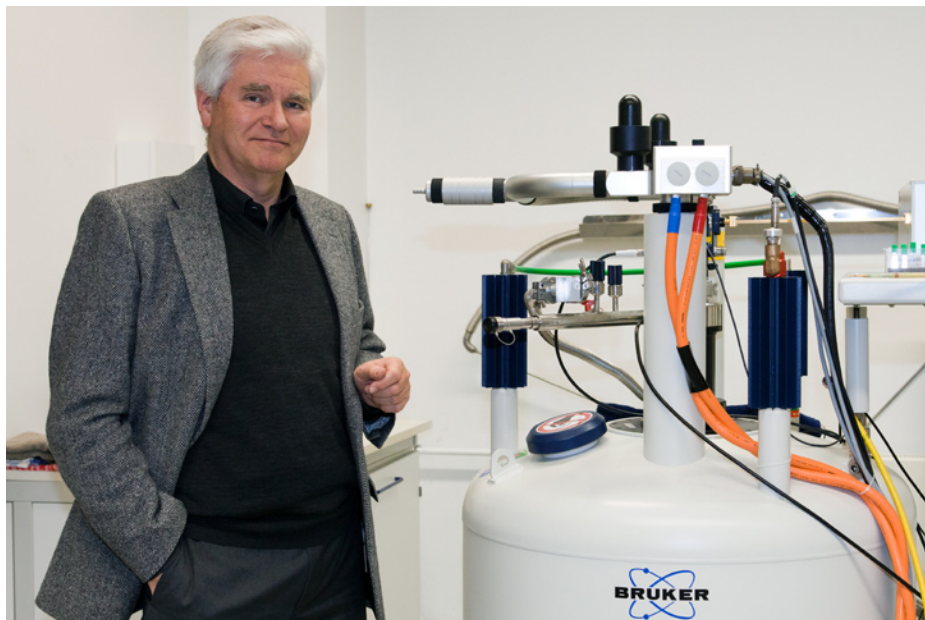
Bruker as Seen from Denver

The first three decades of the history of EPR at Bruker was described by Dr. Dieter Schmalbein in "Foundations of Modern EPR," edited by Kev Salikhov and us (World Scientific, 1998). We first started working closely with Bruker when they helped sponsor the 3rd Annual International EPR Symposium in 1980. Our first Bruker EPR spectrometer was acquired in

1984, via IBM Instruments, who fortunately had hired Dr. Arthur H. Heiss. We now have eight EPR spectrometers, including an E580, two EMX, and locally-built pulsed and rapid scan spectrometers with important Bruker components. Over time, Bruker became the primary sponsor of the EPR Symposium, and enthusiastic participants in our 1987 and 1992 Workshops on the Future of EPR. Art Heiss, Ralph Weber, and Dave Barr are strongly focused on helping students (and faculty) learn

about EPR so that they can advance the science (and buy instruments!). They worked with us to teach nine workshops on various aspects of EPR, from the fundamentals of pulse to how to select a resonator. One of these, the 2008 Workshop on Quantitative EPR, became a textbook on Quantitative EPR (Springer 2010) with Ralph and Dave joining us as authors. We have also published three papers coauthored with Ralph. This background may give us a different perspective on Bruker than others may have – that is, that this is a group of scientists with the "academic" passion for innovation and teaching that dominates their activities in what could otherwise have been a quiet and cautious near-monopoly of a small market. Several times Bruker has pushed a technology to its limit to give researchers a capability that many did not even know that they needed. Disappearances of technologies, such as the transputer just after Bruker converted almost all modules to transputers, have been major setbacks to allocating effort to building new capabilities. Our perspective in working closely with Bruker is that the future of EPR will be exciting, in part because Bruker will continue to produce new capabilities that help us use unpaired electrons in areas from in vivo physiology to quantum computing.

Gareth R. Eaton and Sandra S. Eaton



Bruker BioSpin and the Scientific EPR Community – A Personal Account

If somebody would ask me if there is a company that had a major impact on my scientific work, the answer would be “Yes, certainly: Bruker BioSpin”. It is not only the excellent instruments and the service provided by Bruker, it is the people in this company that make the difference - and there is a story behind it closely related to some important events in my personal scientific life.

Early in 1974 I started to work on my dissertation at the Freie Universität Berlin with Harry Kurreck (Chemistry Department) and Klaus Möbius (Physics Department). The topic chosen was to expand electron-nuclear-double resonance (ENDOR) to non-protein nuclei, which required – next to good samples – also a significant improvement on the instrumental side for handling the required high cw microwave and radiofrequency power levels. Just at this time Reinhard Biehl in the Möbius’ group developed an ingenious novel type of resonator that (together with a new spectrometer design) opened new vistas in the applications of high power cw-ENDOR to paramagnetic systems. Together with many other scientists in the Berlin EPR groups I profited a lot from this development – that we owed to a large extent to Reinhard’s broad knowledge and deep insight in mw and rf technology as well as cavity and spectrometer design. In the early eighties Reinhard joined the EPR group of Bruker, headed by Dieter Schmalbein. And it was around this time that Varian, the main competitor of Bruker, decided to drop its EPR

activities – leaving the market almost entirely to Bruker BioSpin. Reinhard’s work not only contributed to the company’s success to design and build novel state-of-the-art cw-EPR/ENDOR equipment, but also led to the first commercial pulse/FT EPR spectrometer. Unfortunately Reinhard Biehl died, much too early, in 1987 in his early forties.

When I accepted my first permanent position as Associate Professor in Stuttgart in the physics institute headed by Michael Mehring, I had the pleasure to meet Peter Höfer, who had just finished his doctoral degree with Michael in 1988. Peter developed and applied variants of pulse ENDOR, and described the first 4-pulse electron spin echo envelope modulation 2D experiment (HYSCORE). He also joined Bruker BioSpin in 1988, and with his truly outstanding knowledge and technical skills acquired in Stuttgart has been for many years one of the key players in the development of pulse EPR instrumentation in the company.

When I accepted a Chair for Physical Chemistry at the Technische Universität Berlin in the early nineties we had the grants to buy several Bruker spectrometers for our new laboratory. Owing to the novel excellent pulse X-band EPR/ENDOR machine we were soon able to expand our applications, from radicals to transition metal centers, e.g. in photosynthetic proteins. Friedhelm Lenzian and those coworkers who joined me from Stuttgart, in particular Hanno Käss, established excellent contacts with Bruker BioSpin, which helped enormously in running and maintaining the highly complicated spectrometers.

In the mid-nineties the first commercial high field pulse/cw EPR machine at 94 GHz (W-band) was introduced by Bruker. The EPR community in Germany was greatly interested, and with assistance from the Large Equipment Program of the Deutsche Forschungsgemeinschaft, three of these machines were bought and installed at German universities. We received one of the W-band spectrometers and made it available to other EPR groups in the framework of the DFG Priority Program “High Field EPR” (1998–2004). Shortly thereafter I left and the W-band instrument stayed in Berlin with my former collaborator Robert Bittl, who became the successor of Klaus Möbius at the FU Berlin.

In the year 2000 I accepted a Director’s position with the Max Planck Society at Mülheim/Ruhr, more than 500 km West of Berlin. At the new place, assisted by Ed Reijerse as group leader, we set up a new large EPR laboratory with currently 10 stand-alone instruments covering the frequency range from 2 to 244 GHz. Again Bruker BioSpin was instrumental in this endeavor: we have purchased seven machines over the last decade. For example, we received the first Bruker pulse Q-band EPR/ENDOR/ELDOR spectrometer, which soon became the “working horse” in our laboratory – and it still is the most demanded and best-suited machine for studying metalloenzymes and related model complexes. The excellent performance of this spectrometer with respect of sensitivity, long-term-stability and resolution – together with our home-built Q-band resonator – was the basis for much of our successful EPR work, e.g. in the field of oxygenic photosynthesis and biocatalysis in general. This would not have been possible without the excellent work of the physicists, designers and engineers at Bruker BioSpin – and the very good personal relationship between them and the members of my group over almost three decades of scientific work. I also want to thank the responsible persons at Bruker for their positive attitude to serve our small EPR community with innovations and new technologies that proved to be so important for applications in physics, chemistry, biology and even medical research. It was my pleasure to be present in Kazan (Russia) in 2000 when Dieter Schmalbein received the special Zavoisky Award on behalf of Bruker BioSpin, a high honor that showed how close the company is to the scientific community.

Congratulations, Bruker, to your 50th Anniversary.

Wolfgang Lubitz



Wayne Hubbell (left) and Christian Altenbach (right).

to Dieter Schmalbein) and returned with the news that Bruker would be willing to build it as part of the development of the new 580 instrument. I managed to find the money to order an instrument and we ultimately received a state-of-the-art saturation recovery spectrometer. There were a few issues regarding the newly designed DC-AFC lock, but there was never a moment when we did not have help to get us on the air doing experiments. There are few, if any, companies with which one can have this kind of productive and interactive relationship. Since that time, Bruker has been of enormous help to my laboratory, and the people involved, Dieter Schmalbein, Peter Höfer, Ralph Weber, Arthur Heiss and others, have been more like collaborators and friends than business relations. On more than one occasion, these people have gone far beyond expectations to enable us to get experiments done. I am sure that I cannot be alone in the sentiment that the EPR community owes much to this company. A warm and personal “thank you” is appropriate, and I look forward to a long and productive interaction with Bruker!

Wayne Hubbell

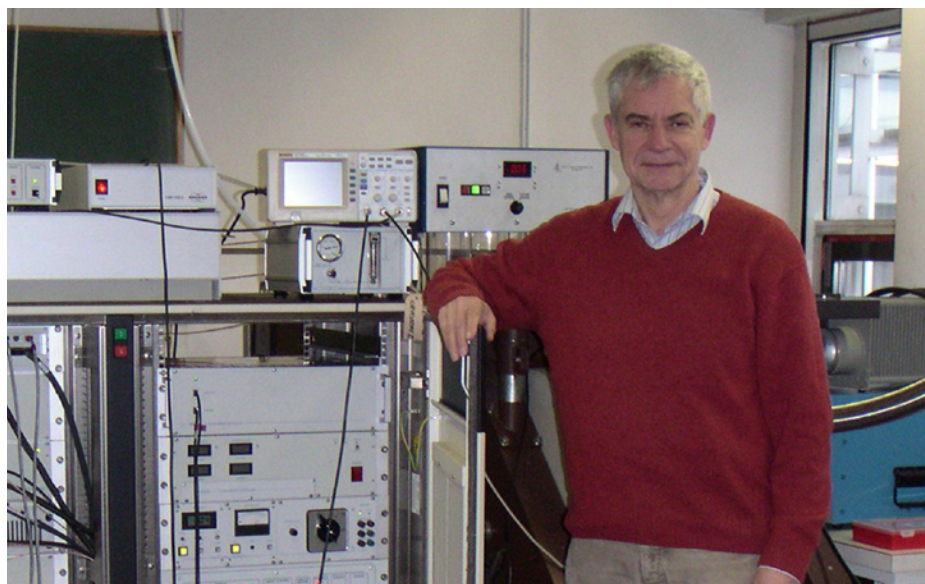
Bruker Biospin: a Partner in Science

My introduction to Bruker was via Karoly Holczner, a designer of Bruker instrumentation in an earlier life and now a Professor of Physics at UCLA. We were having coffee on a sunny afternoon (not unusual in Los Angeles) and discussing the future of time domain EPR for

biological applications. I was arguing that saturation recovery would be an important technology, but instrumentation capable of providing good signal-to-noise at the low concentrations typical of spin-labeled proteins was not commercially available. After some discussions, Karoly said that Bruker could probably provide an instrument that would fulfill the requirements. The same day he made a telephone call (I believe

Bruker and Scientists – a Personal Recollection

When setting up a first ENDOR spectrometer in the late 60's at the Free University Berlin in the lab of Klaus Möbius, I was only faintly aware of the existence of a company producing instruments in the “neighbouring” NMR world. But even then I heard that this company had a very direct wire to the scientists, allowing modifications of the equipment at short notice. There was some rumour, however, that sometimes this happened at the expense of reliable documentation. At that time I was more impressed by the performance of Varian EPR equipment, defining a standard of technology and engineering. The situation changed when the newly established EPR group of Bruker, managed by Dieter Schmalbein, also took advantage of direct contacts, and pushed the development of a commercial continuous wave ENDOR spectrometer, based on the design developed together with the late Reinhard Biehl in Berlin. It was only natural that Reinhard Biehl was offered a position at Karlsruhe, and he was subsequently in charge of the construc-



One of the first Bruker E680 spectrometers at its present location at the Free University Berlin. K.-P. Dinse enjoys ongoing research close to the place where he started as a young student. Generous support from the UniCat cluster of excellence and Robert Bittl with his group is gratefully acknowledged.

tion of the ENDOR/TRIPLE spectrometer, unsurpassed by any competitor.

The advantage of having good personal connections directly to the heart of the de-

velopment part of the company is clearly of mutual benefit, although Dieter Schmalbein always complained about “unfriendly”, or should I say “indecent”, demands from the

“good friends” with respect to delivery time and “uncounted” options.

Close contact to leading research groups based on mutual trust was probably also important for the decision to enter the cutting edge technology of 100 GHz EPR in the 80's. Here the company had to decide on a costly investment in new technology without really knowing about the market's demand. The enthusiasm of scientists in research labs had to be weighed against financial risks. I am convinced that the generous support from the Deutsche Forschungsgemeinschaft supported this move by guaranteeing the purchase of the first three spectrometers.

Having Peter Höfer in charge for exploration of future possibilities for advanced EPR, it was quite natural that the next step towards THz spectroscopy was undertaken. I remember lively discussions about the use of EPR in this frequency range with Dieter Schmalbein and Peter Höfer, in which demands of “freaky scientists” with expectations of “normal Lab people” had to be matched.

I think that the ongoing success of Bruker is partly based on the efforts of people in the company to fulfil scientific demands and not being mainly driven by financial considerations. I wish for the company in the coming years to be able to balance these contradictory goals!

Peter Dinse



My Bruker Memories and Expectations

EPR spectroscopy never has been and probably never will be a branch of science where cutting-edge results can be attained by pushing a button on a device that is considered as a black box. An EPR spectrometer is a

highly optimized and highly complex system. Experimental data may be unusable if measurement parameters are set wrongly or if an electronic problem in a spectrometer goes unnoticed. These arguments may suggest that you build your own spectrometer, so that you know for sure what you are doing. When I started my PhD studies in Arthur Schweiger's group at ETH Zurich back in 1993 this was how the group was operating. The approach worked well for me when I wanted to use an arbitrary function generator for some unusual ENDOR excitation and I could obtain information on any detail of the device and line of the control program from other people in the group.

Two years later the first commercial pulse EPR spectrometer, a Bruker ESP 380, was introduced into Arthur's group. My love for the home-built machines was known and thus it came as a surprise (and may even have dismayed some people) that from the very first day of installation I measured almost exclusively on the commercial machine, which I found was faster and very reliable.

When later leading a small group at MPI for Polymer Research in Mainz, I kept sticking as closely as possible to commercially available spectrometers, but now for another reason. I wanted to develop methodology that could be used in many other groups. Some of the very elegant techniques from Arthur's lab had never been taken up by others who shunned the effort of constructing specialized probe heads and other equipment.

Now being back at ETH I follow a mixed approach of using the engineering strength of the institute to do some things that even the best and most universal commercial spectrometer cannot (yet) do. Still it remains a concern that the methodology- once proven to be useful- can be integrated into a commercial spectrometer with minimal effort.

And this is why I hold the Bruker team in high regard- they are curious, science-driven people who try to push the limits of EPR spectroscopy, although they could probably still make money with less effort and a slower speed of development. If there is a new idea that significantly improves the art of measuring with high sensitivity and precision, Bruker is likely to take it up. This attitude has strongly contributed to the renaissance that EPR spectroscopy is now experiencing. Thank you very much Bruker and belated congratulations to your 50th birthday!

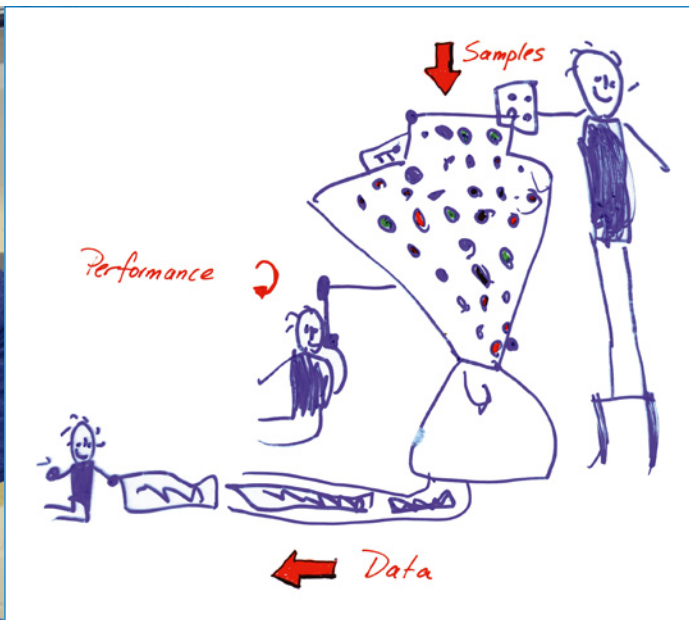
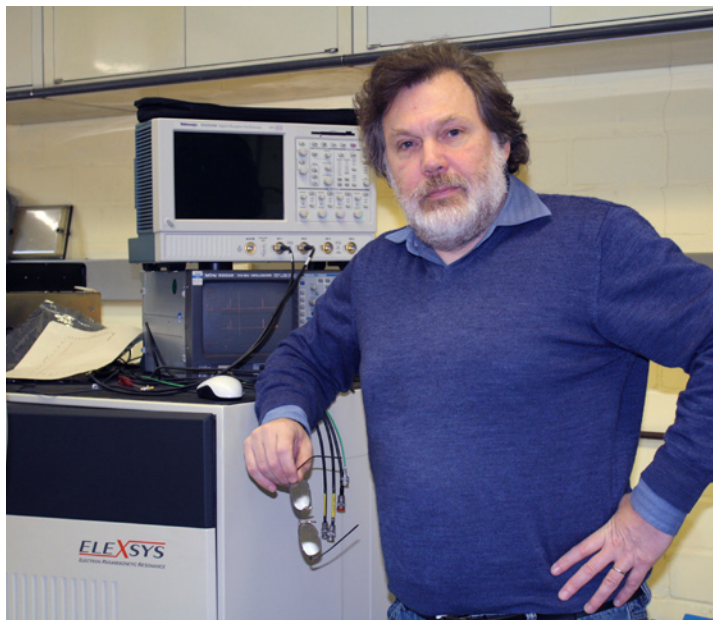
Gunnar Jeschke

Bruker EPR Anecdotes

This issue is devoted to the EPR division of Bruker Biospin, the worldwide leader of EPR instrumentation. Especially with respect to modern pulse EPR techniques, Bruker is the only commercial supplier serving the scientific communities for many decades. It has substantially helped the advance of these methods tremendously.

I followed the development of a commercial pulsed EPR spectrometer at Bruker almost from the beginning. It started as my PhD supervisor Klaus Peter Dinse (at the University of Dortmund at that time) had purchased the first – hand wired – pulse programmer developed by the Bruker company in 1984. Software was almost non-existent at that time and the manual was written more for an electronic or computer engineer than a user. But interestingly enough it was possible to buy a stand-alone pulse programmer! Unfortunately, from the rather cryptic manual it was unclear how many pulses could be pulled out of this device, but problems like that were easily settled by one or more phone calls (I remember interesting conversations with Hans-Ulrich Schütze-Pallmann on this issue!). Finally, after writing and modifying some assembler code programs to drive the pulse programmer and connect it to our home-built spectrometer, we managed to do the first fast averaged ESEEM measurements with it. Photoexcited pentacene molecular crystals, chosen as the test system showed wonderfully deep and never ending oscillations. I was so happy and impressed by these wonderful oscillations that only after turning the crystal in the magnetic field and still getting the exact same modulation frequencies, I grew suspicious! It took me a while to realize that this modulation in signal intensity was rather a pulse length modulation as a function of pulse separation instead of a molecular ESEEM effect. We called it ‘Bruker spikes’, and I soon figured that it could be avoided by choosing only specific step lengths. I remember very stimulating scientific and technical discussions on the future and importance of pulse-EPR at Bruker in Rheinstetten with Dieter Schmalbein and Reinhard Biehl.

This was a long time ago and the pulsed EPR spectrometer at Bruker rapidly evolved and improved; especially as Peter Höfer, coming from Michael Mehrings group at the University of Stuttgart, joined Bruker EPR. Soon after having the pulsed X-band spectrometer in shape, Bruker EPR switched to W-band frequencies. The first commercial pulsed HF-EPR spectrometers were rapidly distributed in



Optimized EPR spectrometer: 1) Throw sample in, 2) Turn handle, 3) Enjoy data.
Drawing by Simon Prisner at the age of 4.

Germany by a special program of the DFG (German Research Society), which resulted in a priority program of the DFG called High-field EPR in Physics, Chemistry and Biology headed by Klaus Möbius from the FU Berlin. This strongly boosted the method and the whole EPR field in Germany, and Bruker EPR, contributed a good part to that.

As important is the expansion of the method into new fields as molecular biology or materials science; here the commercial X-band pulsed spectrometer (see Figure) opened up new avenues for example for structural investigations on macromolecular complexes. Bruker EPR expanded in manpower, just to mention Patrick Carl and Igor Gromov on the

pulse and high-frequency EPR development and application side. This leads to an impressive 'bandwidth' of pulse EPR spectrometers nowadays - covering the frequency range from 1 GHz up to 260 GHz! In many cases, new developments were inspired or started in collaboration with scientists working in the field, reflecting the very strong and successful connections with the scientific community. Different from most other companies, you can always be sure that you will find an expert at Bruker EPR helping to solve your problems or realizing your crazy ideas!

In this sense, I believe that a statement made by Sir Humphrey Davy (1778–1829) 200 years ago describes the success and achievements

of Bruker EPR very well: "Nothing tends so much to the advancement of knowledge as the application of a new instrument. The native intellectual powers in different times are not so much the causes of the different success of their labors as the peculiar nature of the means and artificial resources in their possession." (Elements of Chemical Philosophy). In this respect I hope very much that Bruker EPR will supply us, scientists, with new technology and further improvements in the future!

Thomas Prisner

The EPR community has available to it a list server. The address is epr-list@xenon.che.ilstu.edu. To subscribe to the list, send the words SUBSCRIBE epr-list to majordomo@xenon.che.ilstu.edu. That sends a message to Reef Morse who will then manually place you on the list. This honors only legitimate requests to join the list. Reef also moderates the list which keeps it spam-free.

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Fifty years of Bruker BioSpin! What would EPR be without this company?

It is truly remarkable, how Bruker fosters our research despite dominating the market of EPR spectrometers completely. In the early days of magnetic resonance, the communities of NMR and EPR were interacting a lot. Later, they separated more than I feel they should have done. Maybe, the fact that Bruker Biospin is active and highly successful in both areas made it possible to introduce concepts from NMR to EPR. Examples are two-dimensional EPR, such as HYSORE introduced by Michael Mehring and Peter Höfer, now in charge of the EPR division of Bruker Biospin, to measure electron nuclear hyperfine couplings and four pulse double electron-electron resonance (DEER) based on the ingenious approach introduced in Novosibirsk by Alexander Milov, Kev Salikhov and Yuri Tsvetkov to measuring dipole-dipole couplings between electron spins. Here, cross-fertilization was highly successful because using the concept of first generating an echo



to overcome the dead time of the receiver, a concept well-established in NMR, boosted the applications of this technique to measure distances in the nanometer range in macromolecular systems, including protein folding and protein complexes.

I remember the times when high field EPR required outstanding experimental skills of pioneers like Jan Schmidt, Klaus Möbius or Jack Freed, in particular when it came to

pulsed EPR. These techniques are now easy to use by students after some training, as the spectrometers are highly reliable these days and the quality of microwave pulses steadily increases. The most remarkable case of cross-fertilization is, of course, dynamic nuclear polarization, introduced in the early days of magnetic resonance by pioneers such as Anatole Abragam and recently boosted to high field applications by Bob Griffin. Needless to say that Bruker Biospin developed a commercial instrument that will lead to numerous applications to biopolymers and surfaces etc.

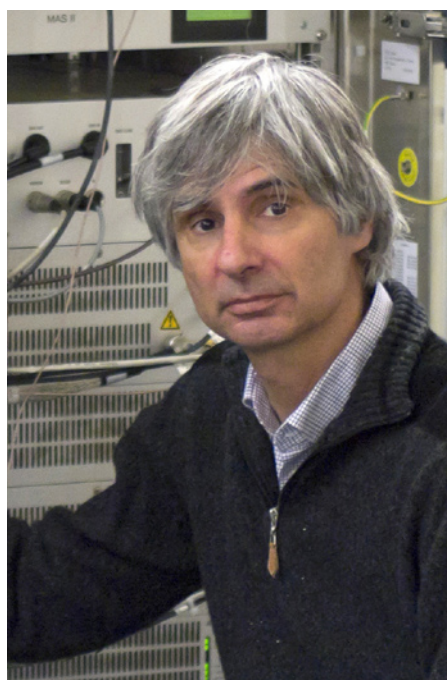
The 50th anniversary of Bruker Biospin also marks the transition from the generation of leaders of the company that followed the founder Günther Laukien, namely, Tony Keller in NMR and Dieter Schmalbein in EPR to the next generation. My warmest congratulations to you and my best wishes to Bernd Gewiese and Peter Höfer for the years to come for the benefit of our beloved field of magnetic resonance!

Hans Wolfgang Spiess
President of the International Society
for Magnetic Resonance
Max-Planck-Institute for Polymer Research,
Mainz, Germany

Groupement AMPERE

Magnetic resonance was proclaimed dead many times during its history over more than 65 years since the seminal papers by Zavoisky, Bloch, and Purcell, appeared. But regularly, new developments such as Fourier spectroscopy, coherent averaging, multi-dimensional spectroscopy, magic-angle sample spinning, dynamic nuclear polarization – to name only a few – have given the field new impetus. In addition to being indispensable as an analytical tool (85% of the publications of the Organic Laboratory at my home institution contain magnetic-resonance data), NMR and EPR have developed into premier structure-determination methods in structural biology and materials science. Clearly, an interesting future lies ahead of us!

Many of the developments, and all those explicitly mentioned above, have only become possible due to technical developments in the fields of computer science, electrical



engineering, superconducting magnet design and mechanical engineering. The field has been very fortunate to have – over 50 years – the support of Bruker that has worked in close partnership with the research scientists, and has provided the field with the advanced instrumentation that is the basis for much of the success of magnetic resonance.

It is a particular pleasure to congratulate Bruker on the occasion of their 50th birthday and to wish them all the best and success for the years to come. Despite the strong growth of Bruker Biospin, the company has maintained a close partnership with the scientific community and is seen much more as a partner than as a vendor. It would be wonderful if the company could keep its open and collaborative spirit for at least another 50 years.

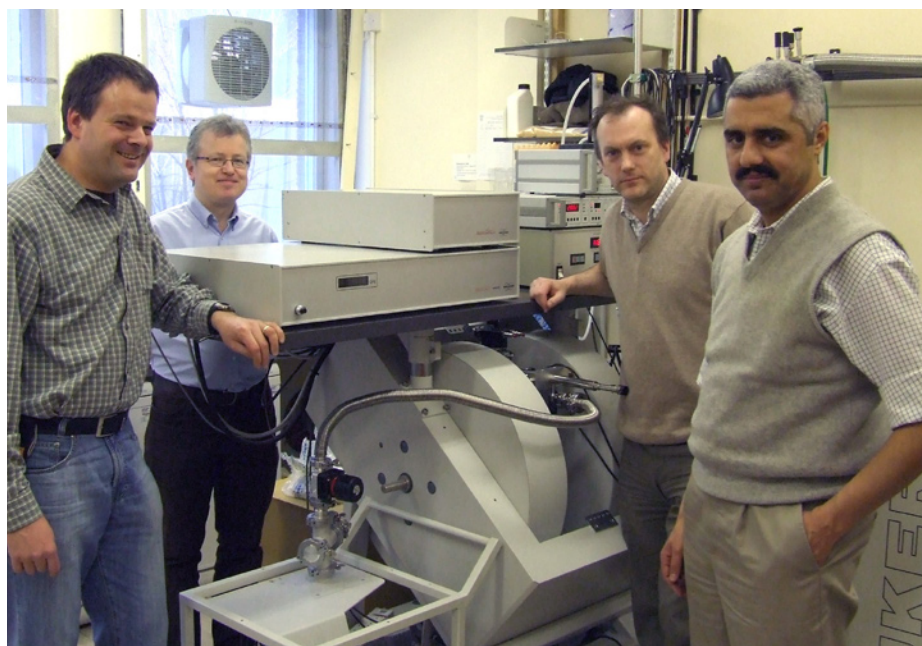
Beat Meier
President of the Groupement AMPERE
ETH Zurich, Switzerland



It has been said that if Bruker EPR is doing well, then the entire international EPR community is doing well, and rumours have it that Christmas bonuses for the Bruker EPR group have recently been exceeding those of their NMR counterparts. I remember twenty years ago a Bruker EPR representative telling me that the challenge for the company was not really persuading people they wanted to buy systems (as quality and reliability were largely taken for granted) but it was more about helping the research community justify their science to major funding bodies and being responsive and forward looking to their technical and scientific requests.

The last 50 years of Bruker has been characterised by substantial investment into research and innovation, whilst simultaneously supporting multiple training and dissemination activities. Today we all take for granted the exceptional point sensitivity provided by the cw systems, the flexibility and relative ease of use of all the pulse systems and the range of different spectrometers and accessories available for multi-frequency EPR. And yet it should be recognised that each of these initial investment decisions represented both significant technical and financial risks for the company. At the time, it was not necessarily so obvious that there were substantial markets for both pulse EPR and high field EPR beyond the research groups pioneering these fields.

However, it is now these very initiatives that have succeeded in both substantially growing the EPR market whilst simultaneously creating new opportunities for both the company and the entire EPR research community. And this strong emphasis on research and development continues, with recent important initiatives on quantitative EPR, very high field EPR and DNP amongst many others. Today they also run application centres, with measurement facilities that can provide preliminary results to support major new grant applications.



From left to right: Bruker engineers Peter Maerz and John Carter with Graham Smith and his colleague Hassane El Mkami.

Bruker have also always been quick to recognise new and important opportunities and activities, whilst acknowledging those people that have significantly advanced the field. The Bruker prize remains one of the highest honours that the EPR community bestows on its members. This is given at the annual Royal Society of Chemistry conference held in the UK, which is the longest running EPR conference series in the world. It is a prize decided by the RSC EPR committee, following advice and nominations from past winners. The 26th winner in 2011 is Prof Thomas Prisner from Frankfurt University, recognising his outstanding contributions to instrumentation, applications and methodological development in both pulse EPR and DNP.

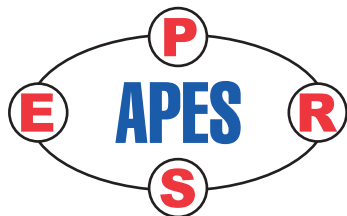
It is also widely recognised that EPR can be a difficult and challenging field for young scientists and Bruker have been highly supportive of long term training and dissemination initiatives to support new entrants to the field. They support major conferences including both the annual RSC and Rocky Mountain Conferences. And on behalf of the European EPR community I would particularly like to thank and acknowledge Bruker for the tremendous support they have given to the European COST Action initiative, and both the European Federation EPR summer schools and conferences.

They have made both direct and indirect financial contributions, which have been key to the leverage of further funding and have contributed greatly to training initiatives. Peter Höfer has taught at every EPR Summer School and Bruker volunteered to run and host a full multi-day hands-on workshop on pulse instrumentation and techniques for the COST initiative. All their courses, lectures and indeed instrumentation manuals have been characterised by outstanding clarity, quality, professionalism and high educational value.

Bruker instrumentation now underpins much of the present EPR research activity across the world – and their presence and influence undoubtedly represents a win-win situation for everyone involved in EPR. So next time you are at one of those splendid wine receptions hosted by Bruker, I would invite you all to raise a glass to both the last and the next 50 years of partnership between Bruker and the EPR community.

Graham Smith
President of the European Federation
of EPR Groups
School of Physics & Astronomy,
University of St Andrews, UK

Congratulations



On behalf of the Asia-Pacific EPR/ESR Society (APES) Council I would like to express our appreciation of the achievements of Bruker BioSpin in developing EPR facilities in countries of the Asia-Pacific region. Bruker EPR equipment is installed in Australia, China, India, Japan, Russia, South Korea, and other countries of the region.

APES was created in 1997 with the aim to promote EPR (ESR) studies in countries of the region. The most important activity of APES is organization of biennial conferences, which also are attended by many scientists from Europe and USA. Bruker BioSpin supports these conferences, and each time its representatives make very useful and interesting presentations and distribute important information about their products among the participants. We are very grateful to Bruker BioSpin for this activity.

In 1992 I had a lucky opportunity to perform experiments on one of the first Bruker pulse ESP 380 machine sold abroad. It was in Japan in the laboratory of Professor Asako



From left to right: Hideyuki Hara, Sergei Dzuba and Hiroyuki Mino.

Kawamori (Kwansei Gakuin University, Nishinomiya). At that time this machine seemed to be a breakthrough in EPR equipment, it was very convenient and flexible. This is true for all series of spectrometers developed by Bruker. Also, Bruker EPR spectrometers proved to be very reliable, even after long time in operation. As I know, this machine at the Kwansei Gakuin University (later transported to other place) is still operational.

We wish Bruker BioSpin further prosperity and many successes. And not only to the company but also to their people who are very nice and very kind!

Sergei Dzuba
President of the Asia-Pacific
EPR/ESR Society
Institute of Chemical Kinetics and
Combustion, Russian Academy of Sciences,
Novosibirsk, Russia

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Multi-frequency pulse-EPR

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and
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The concept of multi-frequency EPR is not new – the continuous wave version has been used since the early days of EPR. In addition to the most popular X-band frequency, microwave systems at other bands like L-, S-, K- and Q-band have been developed very early. Already with the ER 200D series Bruker offered the full range of microwave frequencies from L- to Q-Band and in the mid 90's the first high frequency system at 94 GHz was added to the commercial line. With the recently introduced ELEXSYS E 780 Bruker has now extended the range of commercial EPR frequencies up to 263 GHz. This long history of commercial multi-frequency developments shows on one hand the scientific demands and on the other hand Bruker's commitment to fulfill them.

The main focus of multi-frequency CW-EPR is naturally the frequency dependence of the EPR spectrum as other parameters are often not accessible. The frequency dependence of the EPR spectrum can be used to differentiate features related to the g -factor, hyperfine and zero-field parameters. Increasing the MW frequency emphasizes g -factor features while minimizing hyperfine features. Conversely, lowering the MW frequency leads to a hyperfine dominated EPR spectrum. For large zero-field splitting, increasing the MW frequency allows observation of transitions containing the zero-field splitting parameters.

Since many EPR parameters are not directly accessible from the CW-EPR spectrum, we rely more on line shape fitting and spectral simulations to extract relevant parameters related to electronic and molecular structure. Multi-frequency CW-EPR is a valuable tool for probing line shape changes and for cross-checking the extracted parameters.

Molecular motions impact both the overall EPR spectrum and the observed line shape through the correlation time of the motion. Since the ratio of the microwave frequency to the correlation time governs the observed spectral changes, multi-frequency techniques

are well suited to the study of mobility phenomena.

Another important aspect of a multi-frequency measurement is the consistency check of the analysis. When a given set of Hamiltonian parameters reproduces the spectrum at various frequencies through simulation, we can be more confident about our analysis. When this is not the case, the additional information available from the multi-frequency experiments allows refinement of the analysis.

From a technical point of view, multi-frequency CW-EPR, at least up to Q-Band, can be done with just one magnet system. The development efforts are mainly focused on the microwave bridges and probeheads.

All the concepts of CW-EPR multi-frequency techniques apply equally well to pulse-EPR – but the pulse technique has a lot more to offer.

Multi-frequency pulse-EPR at Bruker started with the introduction of the ELEXSYS series and the E 680 W-Band spectrometer in 1996. The intermediate frequency concept used for W-Band laid out the foundation for further developments. In the IF concept the X-band CW/FT bridge is used as a transmitter and receiver base frequency which is combined with a local oscillator and an up-converter to generate the new working frequency. The EPR signal of the new frequency is down converted back to X-band and then further processed in the X-Band bridge. A major advantage of the IF concept is the extensibility to other frequencies and the possibility of having a multi-frequency instrument. A quite common setup is, for example, an X/W dual band system. The frequency range was extended in 2002 with the Q-Band accessory, in 2006 with L-Band, in 2007 with S-Band and in 2009 with 263 GHz. Today up to three frequencies can be combined in one instrument, e.g. X/Q/W. Inherent to the IF concept is that all features of the X-Band bridge are transferred to the other operating frequencies. This means, for example, that just a single ELDOR source at X-Band is used to provide the ELDOR capability at the second or third operating frequency.

B_1 and Bandwidth

The outcome of many pulse EPR experiments hinges upon the available B_1 , detection sensitivity and bandwidth of the pulse resonator. For example, when the B_1 is less than

the transition frequency, the ESEEM effect will be diminished or not even be observed. Similarly, when the resonator bandwidth is insufficient the ELDOR detected NMR spectrum can fail to detect the nuclear transitions. In the frame of multi-frequency EPR, a balance between the available MW amplifiers for excitation and resonator bandwidth is the key development criterion.

With increases in available MW power, the resonator construction must often be refined. To provide the maximum flexibility, the resonator coupling range should vary from critically coupled (CW and ENDOR experiments) to over coupled (ESEEM, ELDOR and Relaxation experiments). In most cases, design changes must be implemented to increase the bandwidth at over coupling.

Orientation Selection

One of the most well known advantages of multi-frequency EPR is the exploitation of the MW frequency dependence of the g -factor. By increasing the MW frequency, the g -factor resolution is increased, while decreasing the MW frequency leads to a hyperfine dominated EPR spectrum. The increased g -factor resolution permits the collection of quasi-single crystal pulse EPR spectra. These orientation specific spectra are then used to gain insight into the molecular structure (ENDOR, ESEEM, and ELDOR) or into the motions of the molecule (T_1 , T_2 , and T_m).

While the increase in g -factor resolution at higher frequencies is advantageous, this often comes at the price of limited B_1 and limited resonator bandwidth (Fig. 1).

Sensitivity

Another well known advantage in multi-frequency EPR is the signal to noise dependence on microwave frequency, $SN \propto \omega^{3/2} Q_{1/2}$ (for constant filling factor). This gain in SN upon increasing the MW frequency is beneficial for cases where the sample amount is limited as is often the case for biological species and species on the surface of materials. The price for the SN gain at higher frequencies is the increased difficulty in sample handling. For the W-band resonator, the sample tube has an inner diameter of 0.5 mm for non-lossy samples while for lossy samples the inner diameter is 0.1 mm. At lower MW frequencies, the resonators can be constructed to accept larger samples and the penetration depth of

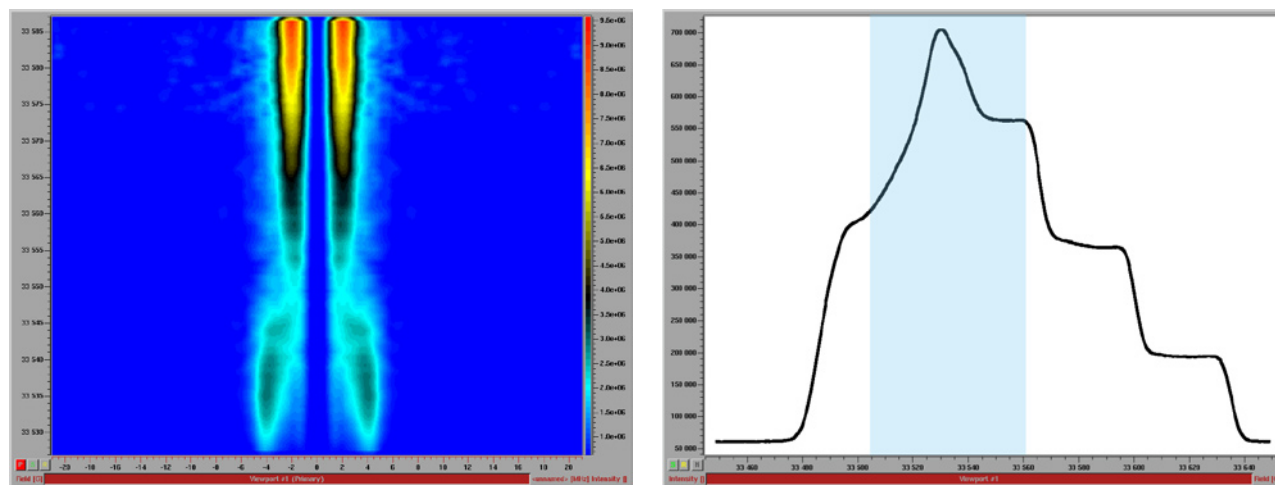


Fig. 1. Left: W-band 2D DEER spectrum of nitroxide biradical showing selective dipolar coupling at lower field edge of EPR spectrum. Right: W-band field swept echo detected EPR spectrum of nitroxide biradical where the highlighted region indicates the orientation selective DEER was acquired.

the microwaves increases for lossy samples. This opens up the possibility to conduct pulse EPR and pulse EPR imaging measurements on small animals.

Relaxation and Motion

Multi-frequency EPR is an essential tool for disentangling the mechanisms contributing to the unpaired spin’s relaxation. By matching the microwave frequency to the rate of motion (vibrations or rotations) involved in the relaxation, the relaxation process is enhanced and dominates therefore allowing identification of the different processes taking place. The matching condition is typically at lower frequencies like S-band and L-band where orientation selection due to *g* anisotropy is less problematic. At higher frequencies when *g* anisotropy is present, the relaxation measure-

ments can be more involved due to orientation selection. The extraction of the relaxation times requires several measurements across the EPR spectrum, however such measurements are advantageous since they provide insight into the relaxation processes in the frame of the molecular structure. Again the disadvantage to working at the lower frequencies will be the loss in SN requiring longer acquisition times and large sample amounts.

ESEEM

Multi-frequency Electron Spin Echo Envelope Modulation (ESEEM) offers promising benefits as both the MW frequency is increased and decreased. Increasing the MW frequency results in a higher nuclear frequency resolution through the nuclear Larmor frequency’s increases with magnetic field. At X-band fields,

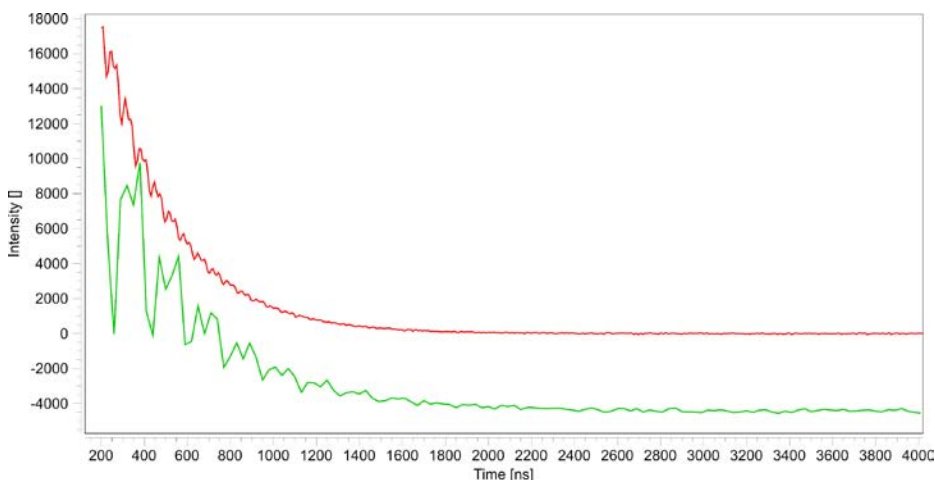


Fig. 2. 2-pulse ESEEM spectrum of powder BDPA sample at X-band and S-band. ¹H ESEEM modulation depth at X-band = 16% and at S-band = 75%.

95% of the nuclear isotopes lay within the 0-5 MHz range (including the most common ¹³C, ¹⁷O, ¹⁴N, ²H). By increasing the MW frequency to Q-band, a threefold increase in nuclear frequency resolution is achieved. The drawback is that the modulation depth tends to decrease with increasing MW frequency, leading to a considerable reduction in ESEEM signal amplitude. The available MW *B*₁ and resonator bandwidth at higher frequencies also limits the practical use of ESEEM at higher frequencies. If the available *B*₁ is less than the nuclear transition frequency, the ESEEM will not be detectable, for example ¹H at Q-band ($\nu_L = 52$ MHz). Similarly, limits in resonator bandwidth at higher frequencies often prevent the excitation of the ESEEM transitions.

Decreasing the MW frequency leads to deeper modulation depths (Fig. 2) resulting in increased sensitivity in the FT ESEEM spectrum (more intense peaks). This comes at the expense of decreased nuclear frequency resolution with the most common nuclei (¹³C, ¹⁷O, ¹⁴N, ²H) lying below 2 MHz. Due to the lower nuclear Larmor frequencies, spectral interpretation may be more complicated as most hyperfine couplings of interest will be larger than the nuclear Larmor frequency giving rise to ESEEM spectra where the peaks are centered at *A*/*2* and have a splitting of $2\nu_L$. *B*₁ and bandwidth limits seldom limit the detection of ESEEM at lower frequencies due to the availability of high power amplifiers and resonators with large over coupling ranges.

ESEEM at lower MW frequencies is also limited by the echo decay. Due to the lower ν_L , two-pulse ESEEM may be impossible since the echo has decayed before the modulation is sufficiently sampled. Alternative ESEEM

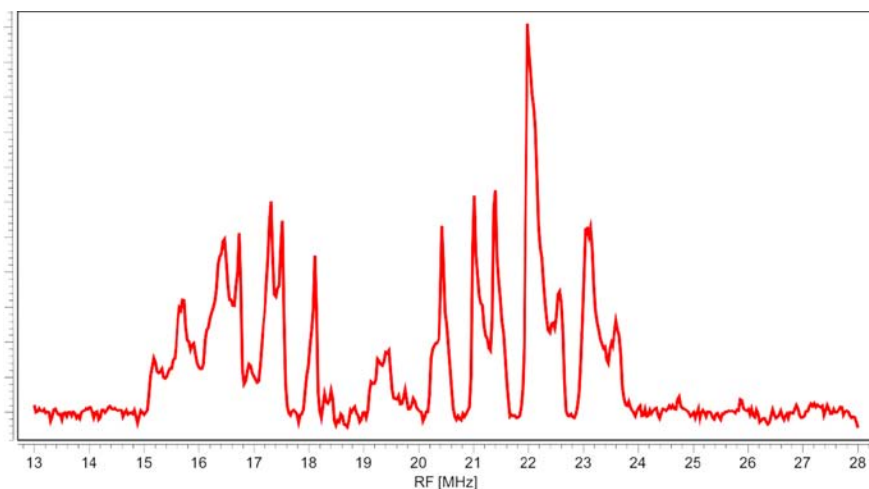


Fig. 3. Q-Band pulse Sn-ENDOR spectrum of V/SnO₂ (in collaboration with D. Murphy). The improved resolution of both isotopes of Sn (¹¹⁷Sn and ¹¹⁹Sn) at Q-band ($\nu_L = 19$ MHz and 20 MHz) facilitated assignment whereas at X-band ($\nu_L = 5.3$ MHz and 5.6 MHz) unambiguous resolution of the isotopes was not possible. (ref: D. Murphy, R. Farley, J. Marshall, D. Willock, Chem. Phys. Lett., 391, 1, 2004).

experiments (three pulse, four pulse, and HYSCORE) allow sufficient sampling times, however the blind-spot behavior may impose experimental limits on the experiment. For example, a blind-spot free ¹⁴N ESEEM (HYSCORE) spectrum at X-band requires a τ of 480 ns (for maximum modulation depth), while at S-band a τ of 1300 ns gives the maximum modulation depth with no blind-spots. Thus for fast decaying echoes, the S-band ¹⁴N ESEEM spectrum will show amplitude distortions that would not be present in the X-band spectrum.

Multi-frequency ESEEM also provides a unique tool for extracting the quadrupole parameters for $S > 1/2$ nuclei. When the MW frequency matches the hyperfine coupling, more information other than hyperfine may be easily obtained from the ESEEM spectrum. A typical example is ¹⁴N couplings at X-band, at exact cancellation or near exact cancellation the ESEEM spectrum exhibits peaks corresponding to single quantum and double quantum nuclear transitions and more importantly peaks corresponding to the nuclear quadrupole resonance frequencies (ω_+ , ω_- , and ω_0).

Pulse-ENDOR

Similar to ESEEM, pulse-ENDOR also benefits from the resolution increase with frequency. The technical challenges which arise are due to the increased frequency spread of the ENDOR signals from various types of nuclei and the reduction of the hyperfine enhancement effect. The larger frequency spread requires a more broadband ENDOR coil which can still generate enough RF field strength (B_2) to drive the nuclear transition with a short pulse. As long as the resonator design allows scaling of the ENDOR coil size with the sample size, the requirement of large bandwidth and strong B_2 can be fulfilled to a large extent. This is demonstrated by the ENDOR resonators in X-, Q- and W-Band where a 250 W amplifier generates a π -pulse for ¹H nuclei of typically 10 to 25 μ s.

ENDOR at lower MW frequencies suffers the same resolution problems as ESEEM. In addition, the closer an ENDOR line is at zero frequency the smaller is its transition moment. Consequently more power and/or longer RF pulses are required to drive low frequency ENDOR lines. Another complication arises due to the strong hyperfine enhancement of

the nuclear spin transition moment. At low fields (frequencies) the hyperfine enhancement can result in strongly varying ENDOR amplitudes across the spectrum. This effect can be partially compensated by the design of the ENDOR coil. At present the demand for low frequency ENDOR is minimal.

In complicated situations like spectrum overlap from different nuclei, various isotopes and powder lines, it may still not be sufficient to go to the next available higher MW frequency to fully disentangle the spectrum. However, the field/frequency dependence of ENDOR lines is easily analyzed and an ENDOR experiment at a second MW frequency will help to solve the puzzle (Fig. 3).

Pulse-ELDOR

Pulse-ELDOR techniques like distance measurement, ELDOR detected NMR and hyperfine selective ENDOR have found wide spread use in the last 10 years. In the context of multi-frequency pulse-EPR, the ELDOR technique is mainly used for improved orientation selection with higher frequencies. The main technical demands for an ELDOR setup are a large resonator bandwidth and sufficient MW power to generate short pulses. In this respect the design considerations for the resonator have changed with the availability of a second broadband microwave source for ELDOR. For a single frequency instrument the resonator bandwidth should be on the order of the inverse pulse length. This requirement is not sufficient for pulse-ELDOR and the resonator bandwidth should exceed the single frequency excitation bandwidth and should ideally allow using the full frequency range of the ELDOR source. In X-Band this goal has been achieved for example with the MS3 resonator which provides a bandwidth of up to 1000 MHz and still allows generating $\pi/2$ pulses with less than 10 ns length. At higher frequencies like Q- and W-band the available microwave power sets limits to the useable resonator bandwidth.

Frequency Band	Power / W	Bandwidth / MHz	B_1 / MHz	$t_p = \pi/2$ / ns	Coupling
W	0.4	110	15	16	critical
Q	3	146	18	14	over
X	1000	1000	38	7	over
S	30	70	10	25	over
L	200	60	15	16	over

Conclusion

The choice of optimum MW frequency for pulse EPR measurements is not a straightforward decision. A great deal of information on a wide range of sample classes can be extracted from pulse EPR experiments at single

frequencies, though there are limits inherent to each frequency band for each pulse experiment. While it is not possible to say any one frequency is the best for a given study, it is clear that the availability of more than one frequency will improve and enhance the over-

all analysis. With a multi-frequency approach, the benefits of each frequency band can be exploited to provide a more complete analysis of the molecular and electronic structure as well as the molecular motions present.

Software

EPR Simulation at Bruker EPR

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The first task in an EPR experiment is to acquire the EPR spectrum of the sample. This is then followed by the second task of extracting the spin Hamiltonian parameters. These parameters offer insight into the identity and structure of the paramagnetic species. In simple cases, simply measuring a few line positions and knowledge of the microwave frequency yield the desired spin Hamiltonian. Often matters are more complicated, hence the need for EPR simulation software with which one can compare experimental spectra with theoretical predictions. The optimal algorithms and methods for the simulations are highly dependent on the sample studied, resulting in many different simulation programs. A universal EPR simulation program is a very difficult goal to achieve. This article presents some of the history and evolution of EPR simulations at Bruker.

The use of computers at Bruker started in 1974. Art Heiss was a post-doc with Bruker and was tasked with writing acquisition, analysis, and simulation software for a Nicolet B-NC12 computer. This state of the art computer boasted 4 kWords (20 Bit) RAM and about 10 m of paper tape storage. Given the hardware limitations, simulations were limited to first order perturbation theory liquid solution simulations. Perturbation theory is an approximation that is used to calculate line positions efficiently in simulated EPR spectra.

The successor to this unnamed simulation program was

EPRCALC. This simulation software simulated isotropic solution spectra with multiple nuclei. It not only calculated splittings using second order perturbation theory (a more accurate approximation than first order theory), it also calculated the extra lines that one expects for multiple equivalent nuclei in which the hyperfine couplings are becoming large relative to the Zeeman interaction. The favorite example was the L-band EPR spectrum of the perinaphthényl radical. The software was implemented for the Aspect 2000 computer and the ESP300 and ESP300E EPR spectrometers. Figure 1 shows a photo of the program display.

Starting in 1991 it was evident that we also needed a simulation program for powder EPR spectra. Thus work on developing the SimFonia simulation program was started. I already had experience writing simulation and analysis software at University of Chicago, Leiden University, and MIT for both powder and single crystal samples. There were a number of articles that described a third order perturbation theory treatment of the spin Hamiltonian. After about 70 pages of hand scribbled algebraic derivations, I convinced myself that

I had the correct formulae for the anisotropic simulations. The next task was then to write the simulation algorithm in C. Bruker was kind enough to supply me with an OS-9 computer that I could take home. After several months working evenings and weekends in my study, I was able to get the code written and tested. The next step was to implement an interface. Philippe Printz was with us as a programmer and he had found a windowing system for the OS-9 operating system called G-Windows. He was able to build a GUI for the simulation program to aid in the entry of the parameters.

Another desire was to incorporate some instrumental parameter effects such as time constant and modulation amplitude into the simulations. This feature could also serve a pedagogical purpose when training new users. I wrote an algorithm to simulate solution spectra using FFTs and convolution theory. This method made it easy to incorporate the two instrumental parameters into the simulation via a convolution with the transfer functions of the two parameters. The first order time constant response is easy to derive. The field modulation response is much more difficult.

After many pages of derivations and consulting the integral tables of Gradshteyn and Ryzhik, I was able to derive the transfer function for phase sensitive detection as well. Alas to my dismay, I found out a week later that G.V.H. White had already done this in Australia in 1961.

Microsoft Windows® was starting to become more popular in 1994. Thus started the work on WinEPR SimFonia. The al-

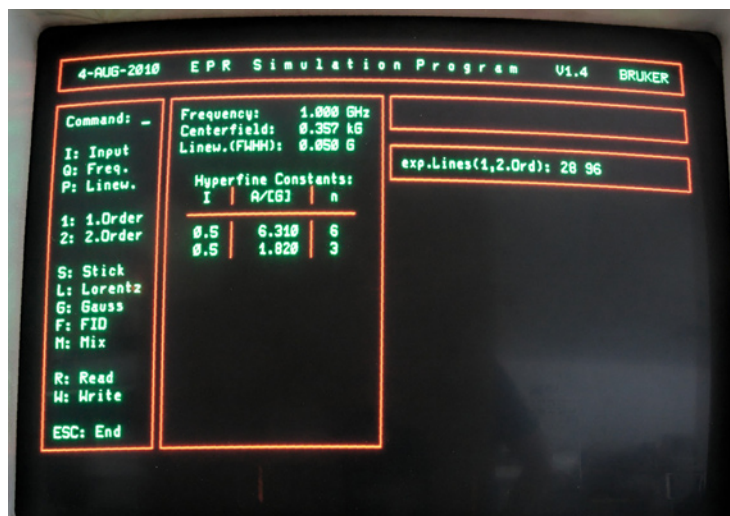


Fig. 1. User interface for EPRCALC running on an ESP300E spectrometer.

gorithms were already there; it just needed a GUI. Juergen Erstling implemented an interface including a periodic table for isotope selection and cursors for hyperfine splitting measurement. SimFonia had incorporated Kivelson theory for m_I -dependent linewidths but determining the polynomial coefficients could be difficult. Cursors for measuring the linewidths and a least-squares routine made measurement of the coefficients easy. Peter Such, an application scientist in Karlsruhe at the time, was particularly happy that without entering any parameters, a single click of the Run button would directly give a simple spectrum. Figure 2 shows some of the displays as well as an overmodulated EPR signal simulation.

SimFonia was written for much slower processors and therefore a perturbation theory approximation was used and also no automatic parameter optimization was implemented. While perturbation theory is a very efficient approximation for many EPR simulations, the approximation is not sufficient for high-spin systems with large zero field splittings, metal clusters, or other systems with large interactions. An exact diagonalization method is required to simulate such spectra. As computers were becoming more powerful, such calculations were now feasible. Without automatic parameter optimization you needed to make successive guesses for the parameters until your simulated spectrum matched your experimental EPR spectrum. As with the exact diagonalization technique, the added power of the newer computers made optimization possible. An initial guess is made for the parameters and the software then varies the parameters to find the best fit to the experimental spectrum. To fulfill these two requirements, we started collaborating together with Graeme Hanson and his group at University of Queensland in order to release XSophe in 1995.

XSophe is particularly good for more complicated systems such as dimers and trimers of transition metals such as copper in metalloproteins interacting via exchange coupling. Often metalloproteins do not have a single set of g -values and hyperfine couplings, but instead have a distribution of values. XSophe can calculate the effect of these distributions in the simulated spectrum. There is also the capability to calculate energy levels and transition surfaces to aid in the analysis of complicated iron spectra that may exhibit looping transitions. Figure 3 shows some of the displays for parameter entry and a transition surface display.

Over the past two years, we have been developing software for quantitating the concentration or number of spins in a sample, otherwise

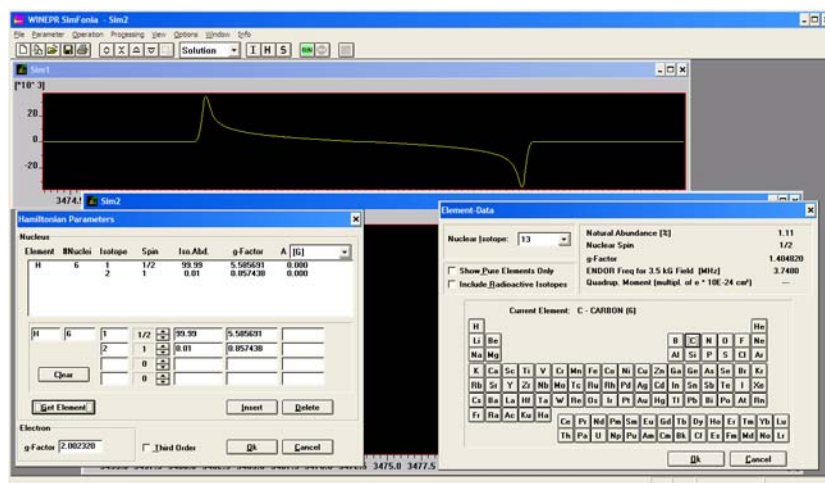


Fig. 2. User interface for WIN SimFonia. Also shown is a simulated overmodulated EPR spectrum.

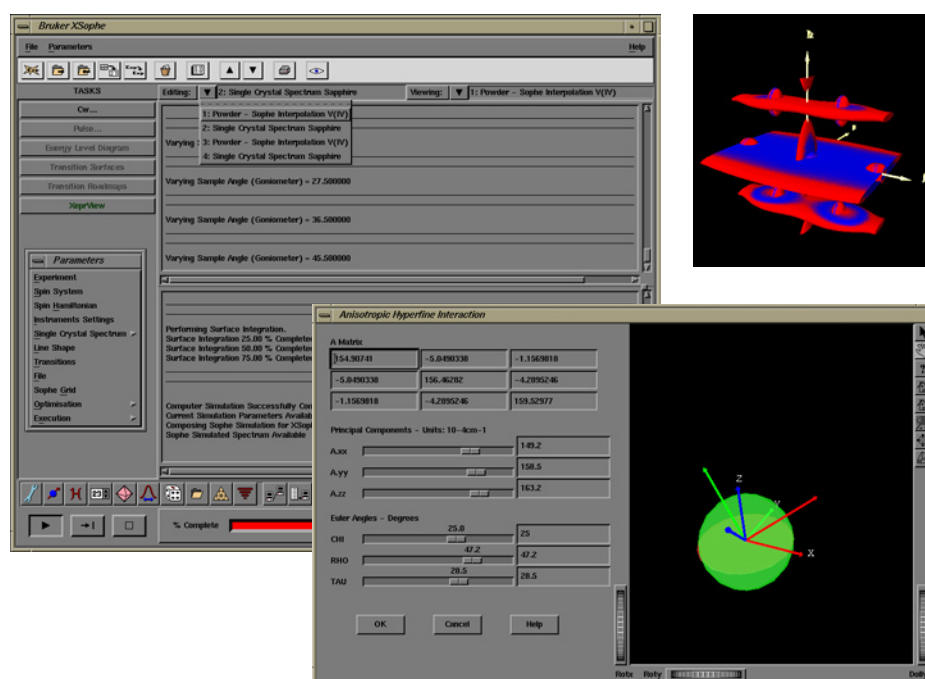
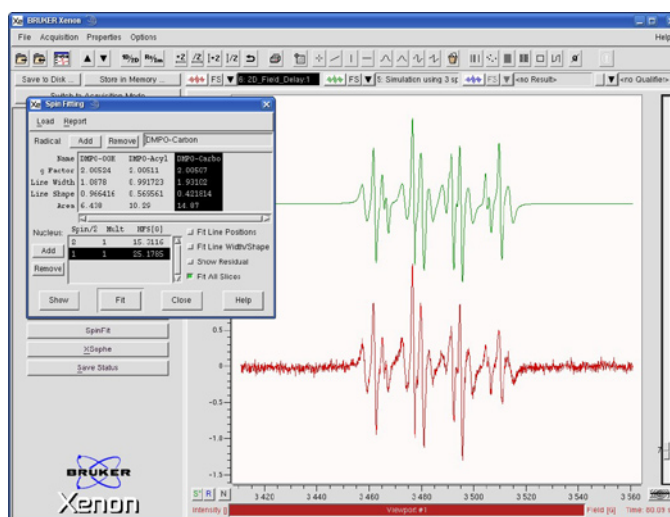


Fig. 3. User interfaces for XSophe and a transition surface plot.

Fig. 4. The SpinFit interface as well as an EPR spectrum of three species. The upper trace is the fitted simulated spectrum.



known as spin counting, without the use of an external standard. This procedure requires double integration of the EPR signal. Alas, double integration can be very sensitive to background signals, particularly when the signals are weak. This technique would also not work for overlapping spectra of multiple species. If one could simulate the individual EPR spectra of the mixture and determine the contribution of the individual species, both problems could be solved. Double integrating the simulated individual species eliminates the background problems as well as enabling one to quantitate the individual species. SpinFit was developed to fulfill these needs. Peter Hofer and Pat Carl started with some ideas and Christoph Albers produced the extensions for Xepr and Xenon softwares. Dave Barr and I made further suggestions for the interface and capabilities. SpinFit is particularly amenable to spintrapping applications where noise, background and multiple species can be problematic. Another feature that is added to SpinFit is the ability for the user to build a spectral library based on

Tips & Techniques

An FAQ for EPR

EPR is an extremely valuable technique in studies of structure and dynamics, but it can sometimes be difficult to determine the optimum conditions under which experiments should be performed. In addition, part of the 'art' of experimental design is in knowing what your existing equipment is capable of. If your current setup is not up to the job, it is extremely helpful to obtain guidance as to what solutions are available (either from a commercial vendor, or otherwise) in order to make your experiment feasible. The special thematic issue "EPR at Work," Concepts in Magnetic Resonance, 28A(1), 2006, is a useful retrospective on the practical side of EPR going back to the days of strip charts and vacuum tubes. Much of the advice in that collection is still relevant today with useful updates and modern references. However, the broad range of applications of contemporary EPR and the technical advances that have occurred since 1974 are outside the purview of the "EPR at Work" series. In this fiftieth anniversary year of Bruker in EPR it is an appropriate time to take stock of what the capabilities and challenges for EPR and its applications are. Steps

the spin Hamiltonian parameters. In fact much of the utility was inspired by Dave Duling and Ron Mason in their development of the Spin Trap Database and WinSim.

Dave Barr was investigating the photochemistry of flavor components of hops used in beer brewing. Several different species of radicals were trapped upon UV illumination and the kinetics of the individual species could be followed. These characteristics made the study an excellent test of SpinFit. Figure 4 shows the SpinFit interface and one of the slices exhibiting the spectra of three species and its fitted simulation.

As computing power increases, the simulation techniques will evolve and improve. Also as the EPR applications change, new simulation software optimized to the new problems will be needed. At Bruker we strive to supply the users with the best tools for analyzing their EPR data precisely and efficiently.



in that direction were provided by a presentation at the 52nd Rocky Mountain Conference on Analytical Chemistry, 1–5 August, 2010, Snowmass, Colorado, that was very much in the spirit of a comprehensive overview of the field of EPR. In particular, the presentation "Frequently Asked Questions in EPR" contained a wealth of practical information on resonators, data handling and experimental design, both for time-domain and frequency-domain experiments, including DEER and pulse ENDOR. When approached, Peter Höfer of Bruker BioSpin was enthusiastic about making this material more widely available. Although the Bruker FAQ presentation (www.bruker-biospin.com/epr_workshopbooklets.html) is much more terse than the "EPR at Work" pieces, it does contain much food for thought and can certainly be used as a starting point for conversations with Bruker personnel or with colleagues in the field. It will be interesting to see what further transformations EPR will undergo in the coming years.

Keith Earle

The 12th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena (SCM-2011)
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5th Training School on Advanced EPR of the European Federation of EPR Groups
Konstanz, Germany, September 5–12, 2010

European Summer Schools on EPR Spectroscopy have been growing in size and duration since 1999 when the first such school was held in Caorle, Italy. The schools in Retie, Belgium in 2002, in Wiesbaden, Germany 2005, and St. Andrews, Scotland, 2008 assembled about 80 students and 20 lecturers each. Due to the triannual schedule some PhD students could attend such a school only towards the end of their studies. In a test run, the 5th EF-EPR school was held in 2010, only two years after the one in St. Andrews, to reach the students earlier in their scientific career. The attendance of 78 students demonstrates that our field is now sufficiently large to sustain such schools on a biannual schedule. Most students were from Europe, but a few came from as far as Brazil.

The school was jointly organized by the University of Konstanz, Germany and ETH Zurich, Switzerland. All lectures and tutorials and most spectrometer practicals were held in Konstanz, with eight students taking part in a specialized lab course in Zurich on September 5th. The 22 lecturers, also mostly from Europe, represented all currently active areas of EPR research. With Prof. Kay Diederichs and Prof. Elke Deuerling from University of Konstanz the application field of protein structure and dynamics was also treated from a non-EPR view. Seven tutors from the organizing groups taught the lab courses and held afternoon tutorials on special topics. Further tutorials were offered by eight lecturers and two co-workers of Prof. Frank Neese. The opening lecture on EPR and protein dynamics was held by Prof. Jack Freed (Cornell University) and a special lecture on metalloproteins by Prof. Brian Hoffman (Northwestern University).



Session at the Symposium Hall.

At the banquet.

Altogether 29 lectures (45 minutes + 15 minutes discussion) were given, among them 14 on basic aspects of EPR theory, instrumentation, and experimental techniques, four advanced lectures on quantum chemical computation of EPR parameters, dynamic nuclear polarization, high-field EPR instrumentation, and seven lectures on important application fields. Students could deepen their knowledge and abilities by choosing from 27 tutorials on 12 distinct topics (75 minutes each) and 15 lab courses on 5 distinct topics (150 minutes each, 3-4 participants). A general question session and a feedback session were also organized.

Lectures were based on the idea that as little as possible previous knowledge of stu-

dents should be supposed. This principle was deemed necessary because of the expected heterogeneity of the students, with experience varying from master level to PostDoc and the main field being almost evenly distributed between physics (35.3%), chemistry (38.2%), and biol-

ogy (26.5%). Students graded difficulty of the lectures as 3.30 (standard deviation 0.72) on a scale where 1 was too easy and 5 too difficult – a small deviation from the ideal result of 3.00.

To ensure a lively discussion of each lecture by the students, questions by other lecturers were strictly forbidden and moderators of the discussion waited until the first student came forward with a question. After this procedure had been established on day 1 and the ice was broken, students did not need further encouragement to ask.

Tutorials were given with typical group sizes of 10-12 people, although limitations were not strictly enforced. The format differed between demonstrations on the black board, work of students on exercises, and 4 different computer-based tutorials (altogether 11 sessions) with explanation and hands-on experience. The concept caught on so much that Brian Hoffman and Stefan Stoll spontaneously offered extra tutorials on advanced topics. Most tutorials were running slightly overtime.

Most students did have the opportunity to take part in one lab course and up to seven tutorials, in addition to the 29 lectures and the poster session on Tuesday evening. This made for a fairly condensed program. Many students took some time off on tutorial afternoons for

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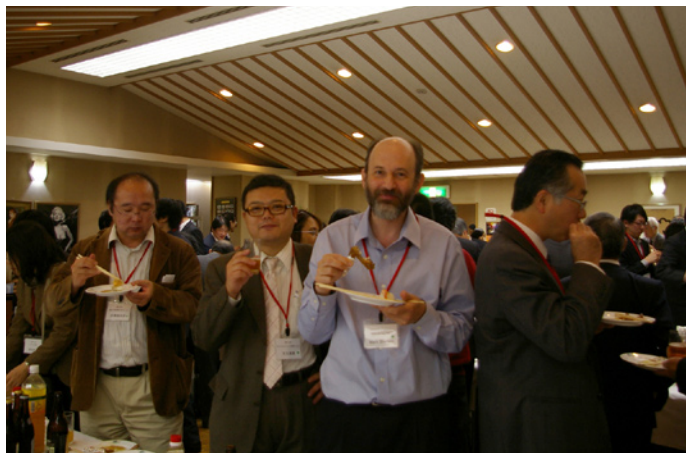
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The 49th Annual Meeting of the Society of Electron Spin Science and Technology (SEST2010)
Nagoya, Japan, November 11–13, 2010

The 49th Annual Meeting of the Society of Electron Spin Science and Technology (SEST2010) took place at the Symposium Hall of Toyoda Auditorium, Nagoya University November 11 to 13, 2010 (see photo). The meeting is dedicated to all aspects of research in the electron spin science and technology and its advanced detection and theory. This covers areas such as materials science, chemical reactions, life sciences and environmental concerns. It was organized by SEST, and was cosponsored by the Chemical Society of Japan, the Physical Society of Japan, the Japan Society for Analytical Chemistry, the Pharmaceutical Society of Japan, Society for Free Radical Research Japan and the Society for ESR Applied Metrology. It attracted 199 participants (including 69 students), and we had one plenary lecture, 3 award lectures, 13 invited talks, 60 oral talks and 59 poster presentations.

Following the opening address by the chairperson, the scientific session started with the

plenary lecture entitled “Free-electron laser-based pulsed EPR at 240 GHz and beyond” by Prof. M. Sherwin (University of California, Santa Barbara), followed by an invited talk entitled “Electron spin control by using the high-power far-infrared electromagnetic radiation” by Prof. S. Mitsudo (Fukui University). After the plenary and invited lectures, two parallel sessions followed. They included Young Scientists Presentation Award talks by 6 candidates.

The second day started with the Mini-Symposium on “Organic electronics and spin science” organized by Prof. T. Nakamura (Institute for Molecular Science) and Prof. T. Ikoma (Niigata University). There were 6 excellent presentations starting with an overview by Prof. Ikoma entitled “Recent organic spintronics”. The General Meeting of SEST was held in the afternoon. Then SEST Awards were presented to Prof. M. Kohno (Tohoku University), and Young Investigator Awards were presented to Prof. E. Ohmichi (Kobe University) and Prof. K. Kanemoto (Osaka City University). The three award lectures followed, and the poster presentations took place. In the evening we had a banquet (see photo) at “Hananoki” at Nagoya University and 141 participants gathered.

The final day started with the Mini-Symposium on “New development on measurements of oxidative stresses” organized by Prof. K. Ichikawa (Kyushu University) and Dr. K. Matsumoto (National Institute of Radiological Science). There were 5 excellent presentations starting with “A recent progress in EPR imaging for the measurement of oxidative stress” by Prof. H. Hirata (Hokkaido University). Following the Mini-Symposium, an invited talk was given entitled “The background radiation doses of tooth enamel of Japanese residents measured by ESR” by Prof. S. Toyoda (Okayama University of Science).

Finally it was announced at the banquet that the next SEST2011 Annual Meeting will be “A Joint Conference of the 2nd International Symposium on Electron Spin Science & the 50th Annual Meeting of the Society of Electron Spin Science and Technology (2nd ISESS-SEST)”, organized by Prof. S. Yamauchi (Tohoku University) and held November 16–19, 2011 at Hotel Matsushima Taikanso, Miyagi, Japan.

Shin-ichi Kuroda
Chair of SEST2010

informal discussions, often in front of their posters. The relatively short time assigned to poster discussion (one evening) made for the worst average grade given by students in the evaluation (“Time for poster discussion was sufficient”, grade 3.43, 12.5% assigned the worst grade 1). Poster discussions were observed even in the morning before lectures and during lunch breaks. This may explain why another 30% of the students awarded the best grade 5 in this question. The poster prize was awarded to Philipp Spindler from

Thomas Prisner’s group at Goethe University Frankfurt/Main, Germany. Students also voted for “Best Lecturer”. This prize went to Dr. Stefan Stoll, who is a graduate of the 1st European EPR Summer School 1999 in Caorle, Italy.

To avoid burn-out, the school also featured a conference trip with options for canoeing and hiking. After the last lecture there was some time for exploring the medieval town of Konstanz on a very sunny final day. Then students and lecturers embarked on a small

ship to beautiful flower island Mainau for the conference dinner. According to our impressions during this dinner, participants had as much fun at this school as we had. We want to express our thanks to all lecturers, tutors, and students who contributed to the success of the school.

Malte Drescher and Gunnar Jeschke
Organizing Committee

RELAXATION TIMES REVIEW

Extensive reviews of electron spin relaxation times are in:

- K. J. Standley and R. A. Vaughan: Electron Spin Relaxation Phenomena in Solids. Plenum Press 1969.
- I. Bertini, G. Martini, and C. Luchinat: Relaxation data Tabulation, chapt. IV in Handbook of Electron Spin Resonance (C. P. Poole, Jr. and H. A. Farach, eds.) AIP Press 1994.
- S. S. Eaton and G. R. Eaton: Relaxation Times of Organic Radicals and Transition Metal Ions. Biol. Magn. Reson. **19**, 29–154 (2000)

We are gathering relaxation times to update these prior reviews. Many electron spin relaxation times are buried in papers deeply enough that they are not found by computer searches. Sometimes we find them only serendipitously. Some papers contain information that suggest to us that the lab might have measured relaxation times but did not actually put a numerical result in the published paper. We will appreciate having relaxation time values brought to our attention, so that our review can be more complete than in the past.

Gareth R. Eaton (geaton@du.edu)

Magnetic Test and Measurement Equipment

- Fluxgate Nanoteslameters for measurement of environmental fields with 1 nT (10 μ G) resolution.
- Hall effect Teslameters for magnet field measurement and control with resolution to 0.1 μ T (1 mG)
- NMR Teslameters with field measurement from as low as 1.4 μ T (14 mG) up to 23.4 T.
- Digital Voltage Integrators for flux change measurements.
- Precision Current Transducers and Electromagnet Power Supplies.
- Laboratory Electromagnet & Helmholtz Coil Systems for spectroscopy and imaging.

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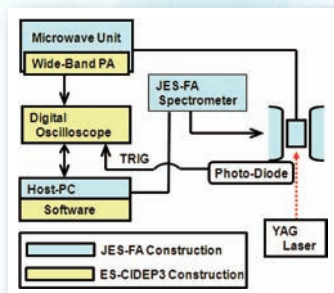
ES-CIDEP3 for JES-FA Series ESR

Chemically Induced Dynamic Electron Polarisation (CIDEP) facilitates sub-microsecond detection of spin-polarized paramagnetic intermediates as produced by laser excitation. This can yield unrivalled information on the spin dynamics and the chemical reaction.

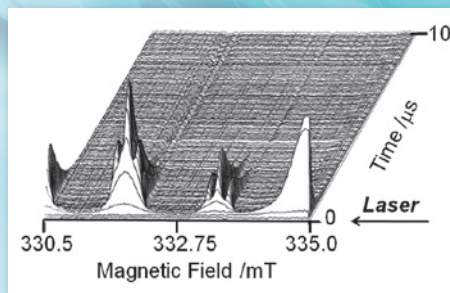
The high sensitivity and high speed of the JEOL FA series ESR spectrometers fitted with a CIDEP attachment ensures simple and reliable measurements.



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Block diagram of CIDEP attachment



2D TR-ESR of photo-polymerization process

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POSITIONS

Positions available immediately at Dartmouth

Job description: The Electron Paramagnetic Resonance (EPR) Center for the Study of Viable Systems at the Dartmouth Medical School is developing instrumentation and methodology to enable after-the-fact characterization of individual personal radiation exposures following a large-scale radiation accident or attack. This research is supported by several major grants from federal agencies. Our approach focuses on the use of EPR spectroscopy to detect radiation induced radical species in tooth enamel and keratin in nails.

Requirements for the instrumentation include high sensitivity to radicals present in the tissues, full automation of measurement procedures, compatibility for use with human subjects, ease of transport, and reliability and robustness under field conditions.

Activities within our engineering lab include the development of surface-loop and other novel resonators for detection of in vivo EPR signals, the design and fabrication of RF bridges, and the incorporation of these components into optimized systems capable of automatic tuning, coupling, and phase adjustment.

We are seeking several well-prepared, highly motivated individuals to join our international team pursuing this research. The persons hired for this position will assist in the design and construction of the instrumentation for EPR spectroscopy and will service the prototype instruments being evaluated within clinical studies. More specifically, they will be working with a team of local RF engineers, as well as national and international collaborators, to design, fabricate, and optimize RF bridges and resonators and to incorporate them into fully functional and automated instrumentation, to

enable EPR techniques to address an important national security concern.

The candidate should have experience in the design and manufacture of RF systems for frequency conversion and signal demodulation. The candidate should have practical knowledge in digital electronics systems and proficiency in Matlab based analyses. Familiarity with simulation software such as HFSS, ADS, and/or Pspice is desirable. Prior experience with EPR is desirable but not essential. An advanced degree in engineering is desirable. A strong work ethic and willingness to work hard and learn new areas is essential.

Qualifications: BS or more advanced degree in RF engineering or Physics. Experience with at least one and preferably several of the following: (1) EPR experience, (2) microwave circuit and/or system design experience, (3) modeling experience with either HFSS, ADS, Pspice or other circuit software design packages, (4) knowledge of Matlab, (5) digital electronics experience.

Contact:

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Multiple positions available – will consider varying degrees of expertise.

Postdoctoral position at Physics Department, National Dong Hwa University, Taiwan

A postdoctoral position is available in the laboratory of Prof. Shyue-Chu Ke at the Physics Department, National Dong Hwa University, Taiwan.

The research will involve the application of EPR and pulsed EPR spectroscopy to understand the fundamental questions related to adenosylcobalamin-dependent enzymatic reactions.

Additional information about the laboratory is available at: www.phys.ndhu.edu.tw/teachers/ke/ke.htm.

The position is available this summer and appointments are for up to 3 years.

If interested, please send a CV and summary of previous research experience to ke@mail.ndhu.edu.tw.

EQUIPMENT

Design and construction of EPR electronics

The University of Denver can supply electronic design and construction services for EPR applications. Low-noise pulse amplifiers, low-noise 100 kHz preamplifiers, boxcar integrators, and pulse timing systems are available. We also supply a conversion kit to convert Varian field-control units to voltage-controlled scan operation. A 6-digit 1-ppm frequency counter is available in X-, C-, S-, L-band, or MHz versions. Complete microwave/RF bridges from 150 MHz to L-, S-, or C-band are available from designs previously built and tested at the University of Denver.

Please contact: Richard W. Quine,
 e-mail: rquine@du.edu,
 phone: 1-303-871-2419

For sale: Varian and ESR equipment

Resonance Instruments has available: (1) Replacement klystrons for Varian EPR bridges and some Bruker bridges (at reduced prices) and other klystrons; (2) Resonance Instrument's Model 8320A is a general purpose Hall-effect based magnetic field controller that provides direct control and precise regulation of the magnetic field between the pole pieces of an electromagnet. Its high resolution permits precise adjustment of the magnet's field either through the front panel keyboard or through an RS232 serial interface with your PC.

Please contact: Clarence Arnow, President, e-mail: 8400sales@resonanceinstruments.com, phone: 1-847-583-1000, fax: 1-847-583-1021.

Available: Used Varian EPR equipment

(1) Varian E-104 EPR spectrometer with vertical style bridge and e-line fieldial. (2) Varian E-9 EPR spectrometer. Both available with warranty and continued service support. (3) Varian TM cavity with flat cell holders and flat cells. (4) Varian E-257 variable temperature controller with heater sensor and insert holder. (5) Varian E-272B field/frequency lock accessory.

Please contact: James Anderson, Research Specialties, 1030 S. Main St., Cedar Grove, WI 53013, USA.
 phone/fax: 1-920-668-9905
 e-mail: janderson36@wi.rr.com

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Applicants should have experience in analytical techniques and continuous or pulsed EPR methods and data analysis. Experimental physical chemists with experience in cell culture or synthesis would be beneficial, but is not essential.



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