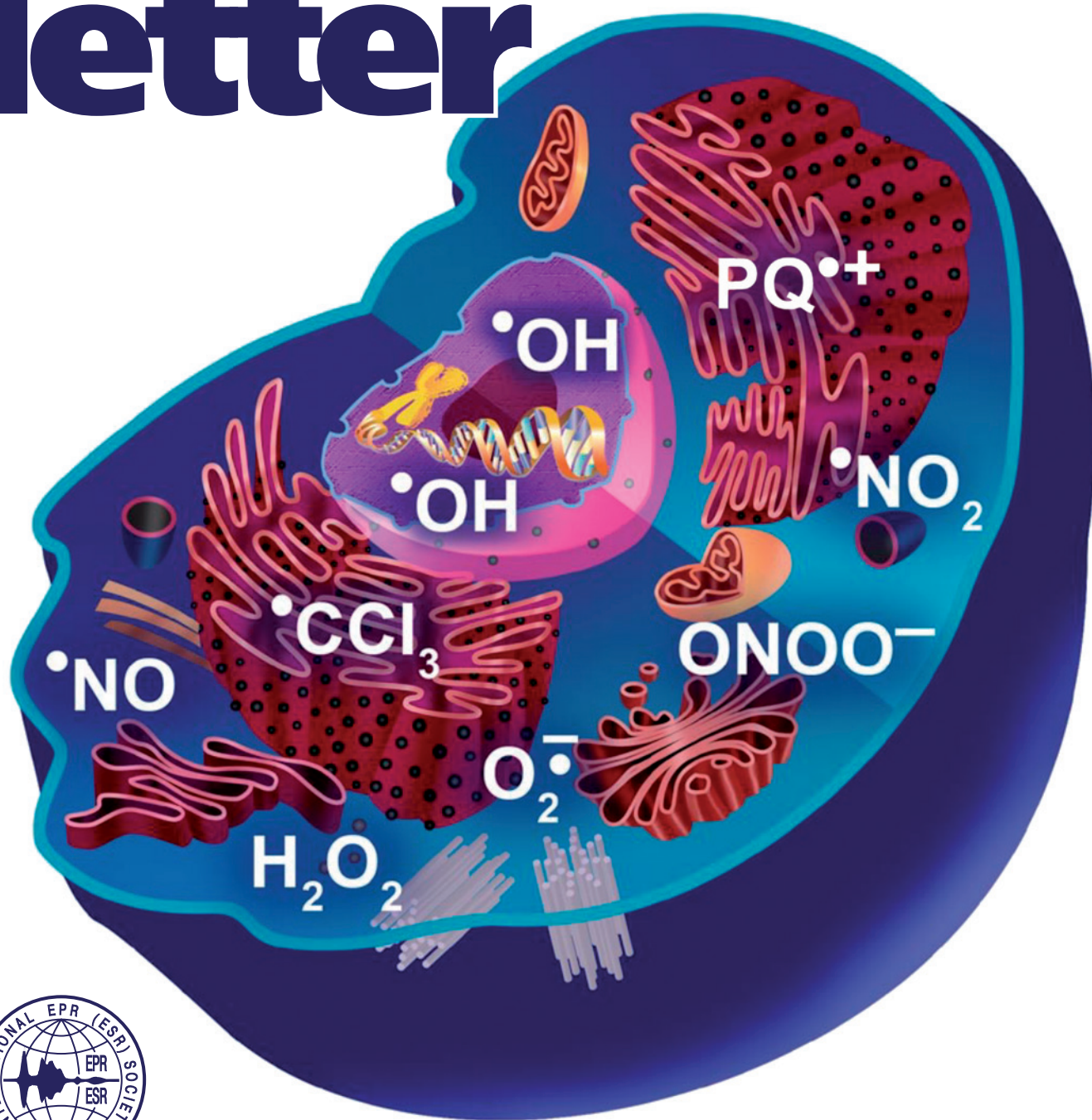


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The Publication of the International
EPR (ESR) Society



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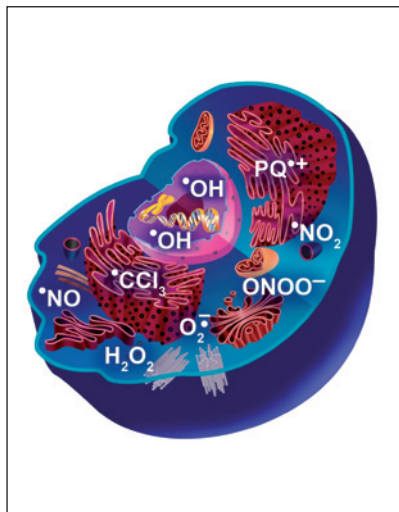
Please feel free to contact us with items (news, notices, technical notes, and comments) or ideas for the *EPR newsletter*.

The *EPR newsletter* is published quarterly by the International EPR (ESR) Society and is available in electronic and printed form to all members of the Society. The deadlines for submission of news for upcoming issues: Spring March, 15; Summer June, 15; Fall September, 15; Winter December, 15.

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The cover picture illustrates aspects of the research carried out by Ronald P. Mason, recipient of the Bruker Award 2010 and 2011 IES Gold Medal. It shows that under conditions of inflammation and oxidative stress all cellular biomolecules are potential targets for reactive species (H_2O_2 , ONOO^-) and free radical metabolites ($\bullet\text{OH}$, $\bullet\text{NO}_2$, $\bullet\text{CCl}_3$, etc). Free radical oxidative damage to cell lipids, proteins and DNA may lead to toxicity and disease.

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IES Annual Meeting

The 2012 Annual General Meeting of the IES will be held during the ESR Symposium at the 54th Annual Rocky Mountain Conference which will be held in Copper Mountain, CO, USA from July 15 to July 19 in 2012.

The Annual Meeting timing has yet to be confirmed. Please send any Agenda items to the IES Secretary Prof. Sushil K. Misra (skmisra@alcor.concordia.ca) as soon as possible.

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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Editorial

Dear colleagues,

I can imagine that the first thing you did when looking at the list of contents of the *EPR newsletter* was to search for the article by Alex Müller in the Guest of the Issue column on EPR in studying high-temperature superconductors that was announced in the previous issue. And yes, here it is on page 5! Please enjoy! However, I presume that we should consider Alex as a friend of the *EPR newsletter* because he generously contributes to the *EPR newsletter* (Lifetime of 28 years of a Bruker EPR spectrometer, 20/4, p. 10; Some words to the symmetry and symbolism of the number five, 15/4, pp. 6–8; An interview to the *EPR newsletter*, 14/1–2, pp. 21–22).

No articles in the Anniversary column in this issue seems strange. For sure some members of the IES had their 65th, 70th, 75th, etc. anniversaries. Please do not hesitate to inform Prof. Sushil Misra, IES Secretary, of relevant articles.

We heartily congratulate Kev Salikhov on the Bruker Prize 2012 and Alice Bowen on

the JEOL Prize 2012 (p. 3) and of course, it is a delight to let Alice tell us about her relevant research (pp. 3–4).

In my feeling, it is always interesting to read Another Passion articles, and Barney Bales, with his article “Working with Wood”, shows one other feature of his personality and describes the relevant relaxation processes that help him in solving problems in EPR.

We say farewell to Albert Overhauser. Charles P. Slichter’s In Memoriam article (pp. 9–10) gives the details of his biography and also demonstrates the warm feelings between two great researchers. Jason Sidabras (pp. 11–13) and Boris Dzikovski (pp. 14–15) nicely complement the instructive part of the *EPR newsletter*. Please pay special attention to the Readers Corner article. You must have read short articles in this column by Reef Morse. I quote his email message: “The purpose of the Steppingstone Magnetic Resonance Training (SMART) Center is to provide an opportunity for middle and high school students to have access to EPR spectroscopy as a tool for individual research. Students are taught how to use the instrument (a Bruker ESP300

kindly provided by Bruker BioSpin), how to prepare samples, and, most importantly, how to ask questions that EPR might help them answer. The result is often surprising – even students as young as 14 can begin to work on research ideas that arise from the literature as shown in the article (p. 19). The *EPR newsletter* offers an opportunity for Shreya Uppal to publish her work and have it read by an international audience. It is my hope that we as a community can attract more students to participate in the growth of the field of EPR and in the exciting opportunities it offers present and future scientists”. The enthusiasm of Reef found a good echo and understanding in the hearts of Jack Freed, Mike Bowman and Thomas Prisner (the then CEOs of the IES) when I discussed Reef’s proposal with them in Kazan during the “Spin Physics, Spin Chemistry and Spin Technology” conference in Kazan in the beginning of November, 2011.

So Shreya, the EPR community is getting acquainted with your poster presentation at the 53rd RMC 2011 (see also Reef’s article 21/4, p. 13).

Laila Mosina

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Awards

The Bruker Prize 2012 to Kev Salikhov

From left to right: Peter Höfer (Director for EPR at Bruker), Kev Salikhov (Kazan Physical-Technical Institute), Robert Bittl (Freie Universität Berlin) and Mark Newton (Chairman RSC ESR Group). Picture courtesy of Art Heiss.

For details, see the forthcoming newsletter



The JEOL Prize 2012 to Alice Bowen

Peter Meadows of JEOL (UK) Ltd presents the JEOL prize to Alice Bowen. Picture courtesy of Art Heiss.

For details, see the forthcoming newsletter

Alice Bowen:

I would first like to thank the RSC EPR committee and JEOL for providing me with the opportunity to present my work as part of the JEOL prize session at the 45th Annual RSC EPR meeting in Manchester. For the first time 5 JOEL talks were presented covering a wide range of EPR topics from applications driven work on solar cells through to method development measuring NMR spectra via triple resonance EPR. Having presented my own talk I was able to listen to those given



by the other students and there was one consistent factor, the quality of their talks was amazingly high and I would like to recognise the work of Ilia Kaminker, Tomasz Mazur,

Christoph Meier and Gunnar Reginsson; I feel very honoured to have been grouped with such exciting young scientists.

Secondly I would like to take this opportunity to thank my supervisor Dr Christiane Timmel who has been a wonderfully supportive presence throughout my doctorate. I must also acknowledge the help of Dr Jeffrey Harmer, Dr Kiminori Maeda and Dr Arzhang Ardavan in the work I presented during my talk.

My doctoral work thus far has seen me study a wide variety of systems using Double Electron Electron Resonance (DEER or PELDOR) and the mixed nature of these systems has made me aware of some of the problems inherent to the existing widely used 3- and 4-Pulse DEER techniques that can

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limit the quality of data that can be collected. 4-Pulse DEER has the obvious advantage over the 3-Pulse technique of being dead-time free, however the longer pulse sequence results in lower signal-to-noise for pulse sequences with the same evolution time compared to 3-Pulse data. The loss of the zero-time can result in an uncertainty in the distance measured and prevents the accurate measurement of the modulation depth. In terms of effect this has on systems studied; the longer length of the 4-Pulse sequence makes it less suitable for studying systems with short relaxation (T_m) times such as membrane proteins.

For systems with broad EPR spectra compared to the width of the pulses used low modulation depth can pose a serious problem for the signal-to-noise ratio of the data collected as only part of the spectrum is excited by each pulse. A significant improvement may therefore be achieved by increasing the bandwidth of the pump pulse, this can be realised by applying multiple pump pulses at different frequencies across the spectrum.

For my JOEL talk I presented two variants of the existing DEER pulse sequences which may be used to improve the data collected (see insets). In each case the techniques involved the crossing of mw pulses of different frequencies. Therefore in order to be confident of the pulse turning angles during the pulse crossings it is important to work within the

Dead-time free 3-Pulse DEER

The discontinuity that obscures the zero-time in 3-Pulse DEER can be attributed to two effects, the non-linearity of the TWT amplifier and also a dynamic phase shift. The TWT non-linearity can be overcome by reducing the input power of the pulses either by increasing the pulse length or using a smaller resonator with a higher input power to B_1 conversion. We also examined the source of the dynamic phase shift and suggested how this could be overcome in some circumstances.

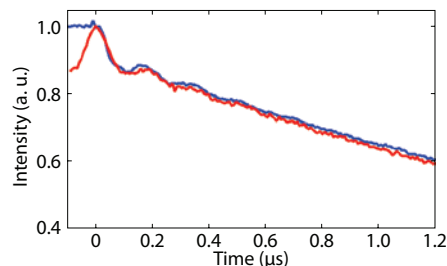


Figure 1. Plot showing a dead-time free three-pulse DEER trace (red) and a corresponding four-pulse DEER trace (blue).

linear regime of the mw amplifier. For a 1 kW TWT amplifier at X-band this meant that the data was collected using a 2 mm split-ring resonator, which has a higher B_1 field relative to the power input compared to larger resonators.

I have been very fortunate over the course of my doctoral studies to attend several conferences and thus meet many of those working in the EPR community at all levels from fellow students to leading scientists in the field. I feel I have benefited greatly from these experiences not only by listing to the presentations given by others but also by learning to present my own work both as posters and oral presentations. As the JOEL session chair Dr Fraser Macmillan stated at the beginning of this year's session, over a third of the attendees at the conference were

Repeated Excitations IN DEER (REINDEER)

Conventional DEER uses two frequencies, one to pump the spins and the other to detect. Even at X-band, pulses (typically tens of nanoseconds in length) do not excite the entire EPR spectrum for both nitroxides and metal centres; as a result the experimental sensitivity is lower than the theoretical maximum. We have addressed this shortcoming through the use of additional microwave sources to increase the frequency spectrum of the pump pulse. Data collected using multiple pump frequencies is shown to have a significant increase in modulation depth and corresponding signal-to-noise ratio.

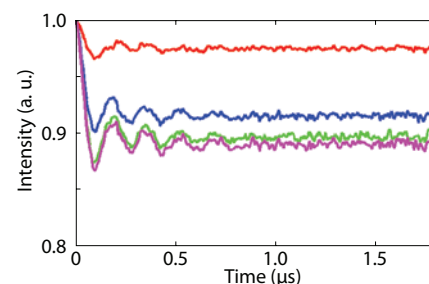


Figure 2. Graph showing the increase in DEER modulation depth achievable with the use of multiple pump pulse frequencies for a di-nitroxide system. Red and blue traces, single pump frequencies: detection on $m_1 = 1$ and pump on $m_1 = -1$ and $m_1 = 0$ respectively. Green trace, two pump frequencies: detection on $m_1 = 1$, pump on $m_1 = -1$ and $m_1 = 0$. Magenta trace: the sum of red and blue traces minus 1.

eligible to enter the JOEL contest, I would like to add my support to his call for those students to consider entering for a JOEL presentation next year. I believe that the experience is a very rewarding one and the process of writing a presentation very useful not only for honing your own ideas about your current research but presenting to an audience is also a vital skill to possess both in academia and beyond.

John-Weil Young Investigator Award

The family of late John Weil has established an award in his memory to be called John Weil Young Investigator award, to be given each year, in addition to the regular Young Investigator award. The nominations are to be sent to the President of the International EPR Society by November 15. The requirements are the same as those for the regular award, as follows: "A Young Investigator Award shall be made for outstanding contributions to EPR (ESR) Spectroscopy by a young scientist. Nominees should be un-

der the age of 35 years on the 1st July of the year of the award. The date of birth of the nominee must be included in the nomination. The nominee will ordinarily be at the post-doctoral level. Only in exceptional circumstances will either doctoral candidates or junior faculty members be considered for this Award. In the case of the Young Investigator Award, please provide copies of two recently published papers which, in the nominator's judgment, represent the nominee's best work."

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The Impact of ESR (EPR) on the Understanding of the Cuprates and Their Superconductivity*

The impact of nuclear magnetic resonance (NMR) to understanding the classical superconductors was substantial. At the phase transition temperature T_c a peak in the relaxation time of nuclei was observed by Hebel and Slichter in Al, and it could be understood later within the Bardeen-Cooper-Schrieffer (BCS) theory as resulting from the special phase coherence of quasiparticles at the transition [1]. The Slichter peak supported early the BCS theory. After the discovery of the superconductivity in copper oxides NMR was readily detected for the ^{63}Cu and ^{65}Cu nuclei, however no Hebel-Slichter peak was reported to date. This indicated that the superconductivity in these compounds might have a quite different origin. The observed NMR, NQR, their quadrupolar splittings, their relaxation times and intensities were analyzed mainly in terms of a single electronic band following the then popular resonating-valence-bond (RVB) and t-J models. Despite the fact that the Cu^{2+} ion carries an electronic spin as is evidenced by the antiferromagnetism (AFM) of the un-

doped materials, they remained ESR-silent. This behavior remained unsolved, despite the theoretical efforts of such great spirits as Orbach, Anderson, Chacharaverty and others. It became understood by the second EPR experiment to be described below.

Before the above advance an ESR line was discovered by J. Sichelschmidt during his thesis in Bruno Elschner's group in Darmstadt. This center with $S = 1/2$ and axial symmetry along the c-axis of LSCO, in which it was observed, had specific properties of the axial g-values shown in Fig. 1: as a function of temperature they cross near 40 K. It was Boris Kochelaev from the Kazan State University who used a three-spin model for an analytical description [2]: it consists of two Cu^{2+} spins of spin $S = 1/2$ each antiparallel to each other and to the rest of the lattice, plus a hole mainly located on the neighbor oxygens, also with spin $S = 1/2$. The center is stable because the oxygens move out of equilibrium as indicated in an exaggerated way in the upper panel of Fig. 1. Two conformations are possible and there occurs tunneling between them, thus there is a splitting between the energy levels. The two local distortions of the oxygens shown are those of the lifting of the doubly degenerate

$d(x^2-y^2)$ orbitals of the Cu^{2+} , the so-called Jahn-Teller (JT) effect.

From the three-spin center there is but one important step to the intersite bipolaron state as introduced by Mihailovic and Kabanov [3]. It occurs by adding a second hole on oxygen orbitals with the antiparallel spin to the first as shown in Fig. 2. The total spin is therefore $S = 0$, thus overcoming the difficulty to move in the AFM lattice which a single polaron with spin has. Bipolarons as such had been proposed earlier by a number of theoreticians but only the intersite Jahn-Teller bipolaron whose model is depicted in Fig. 2 is the true elementary quasiparticle occurring in the copper oxides. A large number of properties of the cuprates can be understood with it: for instance, a quasigap below $T^* > T_c$ occurs due to the formation of the JT bipolarons below T^* upon cooling entering the pseudogap phase. By further lowering the temperature the bipolarons become phase-coherent and T_c is reached.

The above description appears to belong to a homogeneous system. From the second EPR experiment to be presented hereafter this is not the case even at very low doping: below 6% no superconductivity is present. The EPR experiments were conducted in $\text{La}_{1-x}\text{Sr}_x\text{CuO}_4$, in which a small percentage of Cu^{2+} ions were substituted for Mn^{2+} ions as probes. The EPR spectrum in the latter was monitored as a function of temperature. Two EPR lines were detected: a broad line whose intensity is reduced on cooling and a narrow one which increased substantially. The broad line was shown to result from Mn^{2+} ions coupled magnetically to the AFM lattice. From the analysis the relaxation time of the AFM Cu^{2+} ions could be deduced. It was shown that the microwave energy absorbed by the Mn^{2+} is not directly flowing to the lattice but to the AFM Cu^{2+} ions. In NMR it is the well-known bottleneck effect. From this observation it was inferred that this Cu^{2+} relaxation time is so fast, i.e., the EPR lines of the Cu^{2+} are so broad, that it cannot be detected, thus solving the years-long quest for the "EPR-silent" cuprates [4].

The narrow line has a Lorentzian shape. Its width is independent of the Sr^{2+} doping (up to 6%) and shows no oxygen isotope effect. It was assigned to Mn^{2+} ions sited in metallic-type clusters or stripes, the latter being dynamic, i.e. deforming and moving in the lattice in an intrinsic way. The intensity of this line grows exponentially upon cooling. The activation energy ΔE is independent of the doping and is 460 ± 40 K (Fig. 3). It was concluded that

* This article is a slightly up to date extract from a Viewpoint by K. A. Müller, J. Phys. Cond. Matter 19, 251002 (2007)

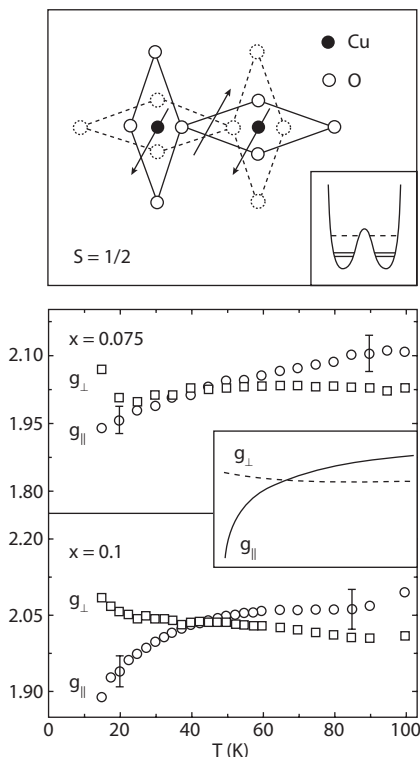


Fig. 1. Upper panel: Three-spin magnetic polaron which is regarded as the EPR-active center in the CuO_2 plane. The Jahn-Teller distorted polaron has two degenerate configurations as indicated by the dashed lines. The inset shows the corresponding double-well potential with the excited vibronic states (dashed lines) and the ground state split by tunneling (solid lines). Lower panel: Temperature dependence of the g -factors for two different doping concentrations. The inset shows the results obtained from model calculations based on the three-spin polaron (3SP) of the upper panel [2].

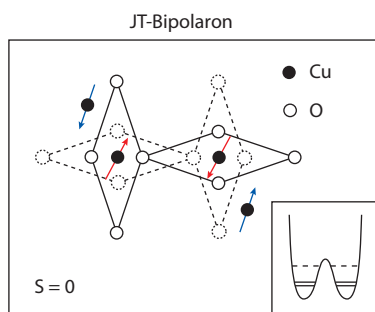


Fig. 2. Schematic representation of the bipolaron [3].

this energy is the one necessary to form the intersite JT bipolaron (Fig. 2). These bipolarons cluster to form metallic aggregates. Their size is limited because they repel each other due to the Coulomb interaction, as impressing simulations of the group of Mihailovic in Ljubljana has demonstrated [1]. With these experimentally obtained parameters the onset of superconductivity at 6% Sr^{2+} doping and the maximum of T_c near 15% were obtained in agreement with the experimental findings [5].

Furthermore, the formation energy of 460 K lies within that between 100 and 700 K of

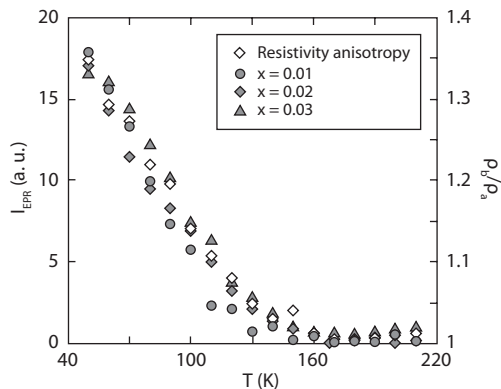


Fig. 3. Temperature dependence of the narrow EPR line intensities in $\text{La}_{2-x}\text{Sr}_x\text{Cu}_{0.98}\text{Mn}_{0.02}\text{O}_4$ [4] and the resistivity anisotropic ratio in $\text{La}_{1.97}\text{Sr}_{0.03}\text{CuO}_4$ [8].

ab initio calculations by Kochelaev and Safina at the Kazan State University [6]. This span is due to the not sufficiently known electronic correlation energy present in the bipolaron. The independence of E_p on the Sr^{2+} doping up to 6% follows the theoretical paper of Alexandrov, Kabanov and Mott, in which this formation energy was predicted to behave in this way [7]. Ando [8] measured the anisotropy of the magnetoresistance in monodomain LSCO as a function of temperature. He found an exponential increase upon cooling, and as Fig. 3 shows, the increase is the same as the intensity increase of the narrow Mn^{2+} EPR line. Ando concluded from his macroscopic measurements that they resulted from the anisotropy of the stripes present. From the agreement of the macroscopic magnetoresistance and microscopic EPR enhancement the clustering of the bipolarons to stripes follows.

The impact of the two EPR experiments described above on understanding the microscopic origin of the superconductivity in the copper oxides in terms of the intersite JT bipolaronic quasiparticles has been remarkable: The first experiment on the three-spin polaron [9] was leading in a direct way to the bipolarons present in the cuprates, and the EPR of the Mn^{2+} as a probe on the presence of metallic clusters or stripes with the aggregation of these

At all concentrations an intrinsic heterogeneity is present overlooked by many theories. Finally, it should be noted that this important advance was achieved by the experimental results at the universities of Darmstadt and Zürich on the one side and the deep theoretical insight of Boris Kochelaev at the Kazan State University explaining them on the other side. One might as well compare the advance of these but two experiments with the very large number of NMR results published, which were for a long time interpreted in terms of single band theories, and even more so regarding the expensive work in photoemission. In the latter dispersions of energies versus wavelength are measured. This is valuable in presence of large correlation lengths present as in classical superconductors. However in the doped cuprates with the bipolarons as quasi precursors of the Cooper pairs present, the coherence lengths are on the order of a lattice distance and a description in terms of local deformations and time is more appropriate, as is usually used in EPR.

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Bales looking at Mount Rainier from his deck at his Seattle home

I only remember two of my childhood gifts; a bicycle that my parents could never afford and was supplied by Santa and a wooden wagon handcrafted by my grandfather. He was a chiropractor, provoking yelps and groans until mid afternoon, and working in his simple shop afterwards. I still remember the yearning to work with wood as a youngster, a desire that I carried, unfulfilled, all through life. When I retired from teaching in 2004 and moved to Seattle, my chance to see if I had any artistic ability within came in the form of an advertisement from the local community college promoting various vocations, including Fine Woodworking and Cabinet Making. I investigated, thinking that it would be something like all of the other continuing education I had pursued, one night a week for six weeks. They offered that but also offered a serious 5-quarter program 4 days a week 7:00 AM to 3:30 PM.

Thus, in the winter 2006, I got up before dawn and rode my bicycle 42 min each way up and down the Seattle hills in the rain, to learn to build cabinets, furniture, and pretty wooden crafts. There were three tracts: Fine Woodworking, Boat Building, and Carpentry. At the time there was a two-year waiting list for the Fine Woodworking program; however, they allowed me in immediately because I did so well on the entrance exam! Life's not fair. They didn't weigh the fact that I was severely

overeducated and had taught in a university for 35 years, but I didn't complain.

Everyone in the three tracts spent the first quarter learning basic skills before branching out to their specialties. They did not allow us near a power machine for the first few weeks while we learned to handle and maintain hand tools. There were lectures and shop time covering every imaginable facet of wood together with endless discussions of safety. One is a fool to turn on a table saw or a jointer without proper instruction. Their instruction was anecdotal, mostly recounting what things (all bad) happen to people who got careless or did not follow the safety rules. All students were required to take a first aid course to get certified by the Red Cross.

Quarters 2–5 went so fast that they are now a blur. We received the same advice from all of the instructors: keep it simple, learn the particular skill, and move on. There were required projects and about the time most of the students were ready to move to the next one, there would be instruction on the next project. I took the instructors advice about keeping it simple and was considerably faster than my colleagues so I would be finished with a project long before it was discussed. In retrospect, it served me well. I wonder if there is a better way to learn than to find your way through a set of problems and then see how professionals would solve them. In those

discussions the instructors would point out a number of common mistakes to be avoided. I was amused to find that I made almost every one of those mistakes. Figure 1 shows one of the required projects, a file cabinet.

The required projects were supposed to occupy quarters 2–4 while quarter 5 was normally devoted to a project of the student's choice. By doing all of my design work at home and working efficiently, I was able to finish the require projects in two quarters leaving me two full quarters to pursue advanced projects under the watchful eyes of two of the best woodworkers in the US.

I was hesitant to set up a serious shop because of the large expense involved; however, I resolved to do that and to follow everyone's advice to buy the best tools that I could afford. Fortunately, one of the projects that I did while still in school paid for my shop. I built our kitchen cabinets in a remodel of a 1928 home and the savings from doing that work myself paid for the tools. Figure 2 shows bedside tables and some boxes. Figure 3 shows a desk that I designed and built for my wife who is a pianist and composer. Under the desktop is a sliding platform to support her piano keyboard that she pushes out of the way while doing other work. Figure 4 shows a writing desk that I built for my sailing buddy's wife, featuring a walnut stripe running at an angle through the desk front and



the drawers. I fabricated the front and drawers in one piece, sliced it up and reassembled it. There's a secret compartment housed in the space between the drawers.

1. A required project, a file cabinet. American oak with raised-panel door fronts.
2. Bedside tables with boxes. American oak and Peruvian walnut.
3. Desk with pull out piano keyboard support.
4. Writing desk with angular stripe through the desk front and drawers. Tissue box on top.

Since graduation 5 years ago, I have built full-wall bookshelves, numerous tables, chests, desks, shelves, boxes, and small decorative pieces, a deck and four sheds. There has been a surprise a day; however, two things stand out in my mind. First, when I used to go through showrooms with wood projects, I marveled at how high the prices were. Now I wonder how they keep them so low. For example, a tissue box (Figure 4) takes as long to build as a table. If I build them 10 or 20 at a time, I can do them in 3 hr each including applying the finish. Calculate the price I would have to command if I wanted to make any money on one! Second, it makes no sense to build anything that you can buy especially if a high quality second-hand piece is available. It's a tedious art form. A good painter can produce a beautiful piece in an afternoon; a woodworker cannot.

I was always curious how artists develop a style. I know that many woodworkers study the masters' work and evolve from there. I studied nobody and stumbled onto my style when I didn't have a board wide enough to do a project so I glued several together using different woods producing a stripe. The file cabinet does not have a stripe because I was keeping it simple then,

but the other projects in Figures 2–4 and virtually everything else that I have built do have them.

Working with wood provides relaxation after spending time solving problems in EPR. In recent years, I have used spin probe techniques together with careful fitting of EPR spectra to study micelles. I interrupted that work to study techniques to separate spin exchange and dipole-dipole interactions in liquids before getting back to micelles. I was surprised that the problem had not been solved satisfactorily and have been dedicating most of my research efforts to find a solution. Thus, what I thought would be a short period of study has turned out to occupy the past 11 years! I'm confident that we can separate the two interactions at a single temperature based solely on the shape of the EPR spectrum, but that was the same thing I thought two papers ago: they kept changing the theory!

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In Memoriam

Albert W. Overhauser (1925–2011)

Albert W. Overhauser, one of the best known and beloved pioneers in the development of magnetic resonance, passed away peacefully on December 10, 2011.

Born August 17, 1925 in San Diego, California, he attended high school in San Francisco. In 1942, he entered the University of California in Berkeley as a physics and mathematics major. He left college from 1942 to 1944 to serve in the United States Naval Reserve, training to be a radar repair specialist. Returning to college after the war, Overhauser graduated in 1948 and promptly entered Berkeley graduate school, also in physics. His thesis advisor, Charles Kittel, who was in the process of moving from Bell Labs to Berkeley, proposed as a thesis topic developing the theory of the spin-lattice relaxation time of the conduction electrons in metals. When Kittel finally arrived permanently at Berkeley in 1951, Overhauser presented him with the completed thesis. Kittel immediately placed a phone call to Frederick Seitz at the University of Illinois who offered Overhauser a post doctoral appointment doing experimental studies of radiation damage in solids working with Professor James Koehler. At this point Overhauser asked his fiancée Margaret Mary Casey whether she could imagine leaving Berkeley to move to Illinois, a subtle but successful way to propose marriage.

At that time, Illinois was a hotbed of NMR research. Erwin Hahn had gotten his PhD at Illinois in 1949, and stayed on for a year as a post doc after discovering spin echoes. Herbert Gutowsky had joined the Chemistry Department in 1948, a fresh PhD from Harvard where he had begun NMR research with Purcell's student George Pake. I had obtained my PhD in 1949 with Purcell, and joined the Physics Department at Illinois that fall. When Overhauser arrived, my first



student, Dick Norberg, was just finishing his PhD thesis studying the ^1H NMR of hydrogen adsorbed in Pd metal. Overhauser got to know the resonance groups and learned about their studies of relaxation times in the alkali metals. In January 1952 he attended a talk by Norberg about his thesis. Overhauser reminisced to me: *"what Norberg said in his seminar was: the free induction decay contains information. I believed that, during the decay, the system is out of equilibrium (of course). So what I did in the next two days was to find out what happens when the system is held (steadily) out of equilibrium. (The discovery followed quickly.)"*

The discovery, now known as the Overhauser effect and also as dynamic nuclear polarization, was that one could increase the nuclear polarization in a metal one thousand fold if one excited the resonance of the conduction electron spins sufficiently strongly. My students and I were amazed at this prediction and were eager to test it. As yet, no one had observed the magnetic resonance from conduction electrons in metals. In his thesis, Overhauser predicted a very narrow (0.1 G wide), intense electron spin resonance (ESR) signal. So we immediately started searching various metals looking for such a narrow ESR signal using an NMR apparatus at 10 MHz and a correspondingly low magnetic field. In late 1952, Thomas W. Griswold, Arthur F. Kip, and Charles Kittel discovered the resonance, much broader than predicted, in metallic Na using 3 cm microwaves. Immediately thereafter, Thomas R. Carver and I found the ESR signal (5 G wide) in powdered Li metal, and quickly embarked on an effort to verify Overhauser's predicted effect.

Albert Overhauser pointed out that at low temperatures and in strong magnetic fields, large nuclear polarizations would shift the frequency of the ESR signal. He proposed looking for this frequency shift to verify his prediction. However, my group lacked the microwave and low-temperature equipment needed to carry out this method. Instead, we proposed a double resonance experiment in which we observed the effect on the ^7Li nuclear magnetic resonance (NMR) of powdered Li metal produced by exciting the conduction electron ESR. This experiment could be done at room temperature and without microwave equipment. We required that the diameter of the metal particles be smaller than the electromagnetic skin depth for both electrons and nuclei, limiting the maximum frequency of ESR to approximately 100 MHz, requiring that the static magnetic field be about 30 G, and the NMR frequency near 50 kHz.

Albert Overhauser presented his idea in a ten minute talk at the April 1953 meeting of the American Physical Society to an audience containing Felix Bloch (Nobel Prize in Physics 1952), Edward M. Purcell (Nobel Prize in Physics 1952), Nicolaas Bloembergen (future Nobel Prize in Physics 1981), Isidor I. Rabi (Nobel Prize in Physics 1944), Norman F. Ramsey (future Nobel Prize in Physics 1989), and Anatole Abragam. They were highly skeptical, perhaps suspecting that his idea violated the second law of thermodynamics. In June, Overhauser left Illinois to become assistant professor of physics at Cornell. He submitted a manuscript to Physical Review in late June. On August 12, Carver and I first observed the enhancement (100-fold) of the ^7Li NMR signal. We sent a telegram to Overhauser telling the happy news and quickly submitted a paper. It was received at Physical Review on August 17, Overhauser's 27th birthday.

Carver and I realized that the Overhauser effect required three elements: that the relaxation time involve matrix elements of the spin-spin interaction between nucleus and electrons in which both spins were simultaneously flipped in going from the initial to the final spin states, that there were degrees of freedom that could absorb the Zeeman energy difference between the initial and final spin states, and that there be an electron spin resonance signal that could be saturated. Thus the Overhauser effect might be possible in a non-metallic liquid. In 1954, we demonstrated this, achieving a 100-fold enhancement of the polarization of protons in liquid ammonia in which we

provided unpaired electron spins from dissolved Na atoms. Much of the present day dynamic polarization uses these principles. In 1955, Ionel Solomon demonstrated an Overhauser effect for a system whose spins consisting solely of nuclei (^{19}F and ^1H in the molecule HF). The nuclear Overhauser effect became very important in determining the structure of large biomolecules, as is evident in the Nobel Prize lecture of Kurt Wüthrich.

At Cornell, Overhauser was promoted to associate professor in 1956, but in 1958 he was lured by the physicist Jack Goldman to leave Cornell to join the research laboratory

at Ford Motor Company. After Goldman left Ford to join Xerox in 1969 (and founded the Xerox Palo Alto Research Laboratory), Overhauser remained at Ford just until 1973 when he became Professor of Physics at Purdue, a position he held until his death.

Throughout his career, he was deeply interested in simple metals. His last publication, in 2011, was a book titled "Anomalous Effects in Simple Metals" (Wiley-VCH), a compilation of the 65 papers he wrote on this topic.

Overhauser's many important contributions were honored by election both to the American Academy of Arts and Sciences and the

National Academy of Sciences. He received the Oliver E. Buckley Solid State Physics Prize in 1975, the Alexander von Humboldt Senior Scientist Award (1979–1980), an Honorary Doctor of Science from the University of Chicago (1979), and an Honorary Doctor of Laws from Simon Fraser University in 1998. In 2009, he was awarded the Russell Varian Prize. In 1994, President William Clinton presented him the United States National Medal of Science.

Charles P. Slichter,
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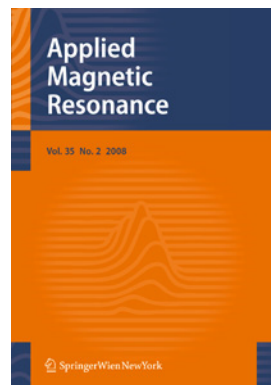
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Custom Design of Microwave Probes for EPR Using Numerical Analysis Techniques

Jason Sidabras

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Milwaukee, WI USA

With the progression of computer technology to multi-core processors, it has become increasingly efficient to use computer simulation models to test experimental ideas. Through these virtual experiments, intuition is gained and theory refined to better describe these models. This especially holds true in resonator development, where interactions between electromagnetics and the sample play a crucial role in optimizing probes for specific experiments or sample types.

While analytical methods have laid the groundwork for theoretical advancement, practical solution space is not always solvable in a closed-form solution. To solve these problems, numerical methods are used. Many numerical methods have been developed, such as the finite-difference time-domain (FD-TD), the finite-element method (FEM), and the method of moments (MoM). Each method has its strengths and weaknesses and is valid for many different boundary-value problems. Here, the focus will be on finite-element modeling.

Finite-Element Modeling

The finite-element method was developed as a way to solve complex structural analysis problems and can be traced back to Alexander Hrennikoff [1] and Richard Courant [2]. Both developers created a discretization of a continuous domain by developing a mesh of sub-domain elements. The solution is then solved on the sub-domains and later extrapolated to the whole domain. The method by Richard Courant, where finite triangular subregions are used to solve partial-differential equations (PDE), is more widely used. A more detailed history can be found in Refs. [3], [4], and [5].

As an example, a two-dimensional object is created as a solvable domain, as shown in Fig. 1a. The domain is then split into an arbitrary number of sub-domains by way of meshing (Fig. 1b). The trade-off in the finite-element method is between the number of sub-domains and the total error of the solution. As the number of sub-domains increases, the

number of unknowns increases, using more memory and CPU time to formulate and solve the solution matrix. With too few sub-domains, the irregular object would not have an adequate approximation to its actual shape. Each sub-domain is connected via its vertices, and each connection is called a node. Each node is assigned a number, and a connectivity array is created describing the interlacing of the sub-domains to each other. Nodes are either described as open or fixed. An open node represents a node that requires a solution, while a fixed node represents either a boundary or source value.

Commercially available electromagnetic finite-modeling software creates a suite in which boundary conditions, sources, and dielectric properties are available in a CAD-like environment. ANSYS High Frequency Structure Simulator (HFSS) and Computer Simulation Technology (CST) Microwave Studio are two such commercial electromagnetic three-dimensional FEM solvers.

Both employ “driven-mode” and “eigenmode” solving domains, which are primarily used for the development of EPR resonators. The “eigenmode” solver uses Maxwell’s equations in their variational form to find the lowest energy states of a structure given its boundary and electromagnetic material prop-

erties. This lowest energy state, or eigenvalue, is then used to calculate the eigenvectors of the structure, yielding a wave solution. No sources are needed in this mode, and, typically, solutions are normalized by the electric field to 1 V/m. The “driven-mode” solver uses Maxwell’s equations with the addition of a source-forcing function. For “driven-mode” coupling, considerations are devised in order to maximize power transfer to the resonator. The “driven-mode” provides outputs similar to network analyzers and is typically normalized to an input power of 1 W.

Signal Calculation and Resonator Comparison

A method to obtain EPR signal intensities from numerical modeling has been devised [6]. This method uses parameters calculated in post-processing field calculators to determine a normalized EPR signal intensity under saturating or nonsaturating conditions. This calculation can be done using eigenmode or driven-mode methods. For a matched reflection cavity and a voltage-sensitive detector, Feher [7] expressed the microwave EPR signal as

$$S = \chi'' \eta Q P^{1/2} [V],$$

where χ'' is the imaginary part of the magnetic susceptibility, η is the filling factor, Q is the unloaded Q_0 -value with sample, and P is the incident microwave power. In comparing resonators, we assume the sample has the same concentration for an arbitrary volume. With this assumption, the magnetic susceptibility, χ'' , simply becomes proportional to frequency. This incorporates the Boltzmann factor to resonator comparisons.

The filling factor is defined as the ratio of the magnetic field in the sample (that gives an EPR signal) to the magnetic field in all space. Using the FEM program, this can be calculated as

$$\eta = \frac{\int H_r \cdot H_r^* dV_s}{\int H \cdot H^* dV},$$

where H is all three rectangular magnetic field components integrated over all space (dV), and H_r is the clock-wise (or counter clock-wise) rotational component of the linear magnetic field components perpendicular to the static magnetic field integrated over the sample volume (dV_s). Assuming H is linearly

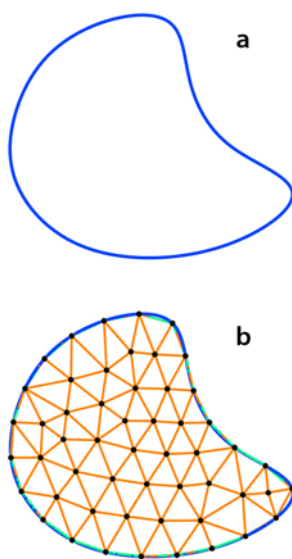


Fig. 1. Two-dimensional finite-element method taking an arbitrary domain (a) and breaking it into sub-domains (b) using a mesh. The mesh becomes a numerical representation of the object.

polarized and the static magnetic field is in the x -coordinate,

$$H_r = \frac{1}{2}(H_y + H_z) \text{ [A/m]}.$$

The Q -value of a circuit is classically described as the ratio of the stored energy and power loss of a system per cycle,

$$Q = \frac{\omega\mu}{2P_l} \int H \cdot H^* dV,$$

where power loss, P_l , is the sum of the power losses on sample walls, defined as

$$P_{lw} = \frac{\sigma}{2} \int \mathbf{n} \times \mathbf{H} \cdot \mathbf{H}^* dS_w \text{ [W]},$$

where σ is the skin depth and $\mathbf{n}$ is the normal vector of the resonator walls (dS_w), and power loss in dielectric materials, defined as

$$P_{ld} = \frac{\omega\epsilon_0\epsilon''}{2} \int \mathbf{E} \cdot \mathbf{E}^* dV_d \text{ [W]},$$

where ϵ'' is the imaginary part of the dielectric constant of the volume, dV_d . Multiple dielectrics or conducting surfaces are summed to create the total power loss, P_l .

Two CW experiments are typically performed: the experimental microwave power is held constant or the experimental microwave field at the sample is held constant. The first experiment is considered for unsaturable samples, where increasing the microwave power increases the EPR signal intensity. The second experiment is considered for saturable samples, where the sample is held at the same microwave field. In this case, it is convenient to introduce the microwave efficiency parameter, [8]

$$\Lambda = \frac{\mu 10^4 \max(H_r)}{P_l^{1/2}} \text{ [G/W}^{1/2}\text{]}.$$

The microwave efficiency parameter, Λ , assumes a uniform magnetic field over the sample; for nonuniform fields, an average microwave efficiency parameter can be introduced as

$$\Lambda_{ave} = \frac{\mu 10^4}{P_l^{1/2} V_s} \int H_r dV_s \text{ [G/W}^{1/2}\text{]},$$

where V_s is the sample volume and dV_s is the integration over the sample volume. A saturable sample can be calculated by normalizing the magnetic field and computing

$$S_s = \frac{\chi'' \omega}{10^4 P_l^{1/2} \max(H_r)} \int H_r \cdot H_r^* dV_s \text{ [V]}.$$

Conversely, by normalizing the input power, the unsaturable sample can be calculated by

$$S_s = \frac{\chi'' \mu \omega}{P_l} \int H_r \cdot H_r^* dV_s \text{ [V]}.$$

These calculations can be inserted into post-processing field calculators, or the fields can be exported to MATLAB for further analysis. The numbers obtained from these calculations are proportional to the voltage signal and are used as ratios in comparing different simulations of resonator geometries. The microwave efficiency parameter can be directly compared to experimental calculation.

Tailoring Resonators for Specific Experiments or Samples

As software-defined bridges (SDB) (where components that are typically implemented in hardware [e.g., mixers, filters, oscillators, and detectors] are replaced by digital counterparts after direct acquisition of the carrier frequency) and sources replaced by ultra-low phase noise DAC cards (arbitrary waveform generators) become more common, so will the need for specific resonators (optimized for the experiments) to replace general purpose probes. It is no longer adequate for a resonator to be suitable for spin labels and Cu complexes. Instead, optimizing frequency and volume constraints can yield improvements a fixed frequency general probe could not obtain. This is also the case in experiments where uniformity of magnetic field

sweep at multiple frequencies is the driving design criteria and analysis of eddy current effects are required. These niche resonators follow the same design development, as outlined in Fig. 2.

One such example is an Lband (2 GHz) loop-gap resonator designed for Cu complexes and optimized for high uniformity B_1 , and to minimize stray fields that give rise to forbidden transitions (Fig. 3). This resonator was designed with the steps outlined in Fig. 2.

The frequency was chosen specifically because of spectral crossovers that occur at 2 GHz. This frequency was confirmed using computer simulations of the spin system. The resonator was selected to be a two-loop-one-gap resonator so that the sample does not go through the coupling loop. The coupling loop was fixed to a PTFE holder to minimize vibrations, a common source of noise. Coupling was adjusted using a variable transmission line. A solid 0.99999 silver design was used in the fabrication of the resonator – both for its thermal stability and purity.

In order to allow 100 kHz field modulation penetration, modulation slots were cut perpendicular to the sample loop. Finally, sample “shields” were placed above and below the sample loop to reduce the magnetic field in the coordinates perpendicular to the

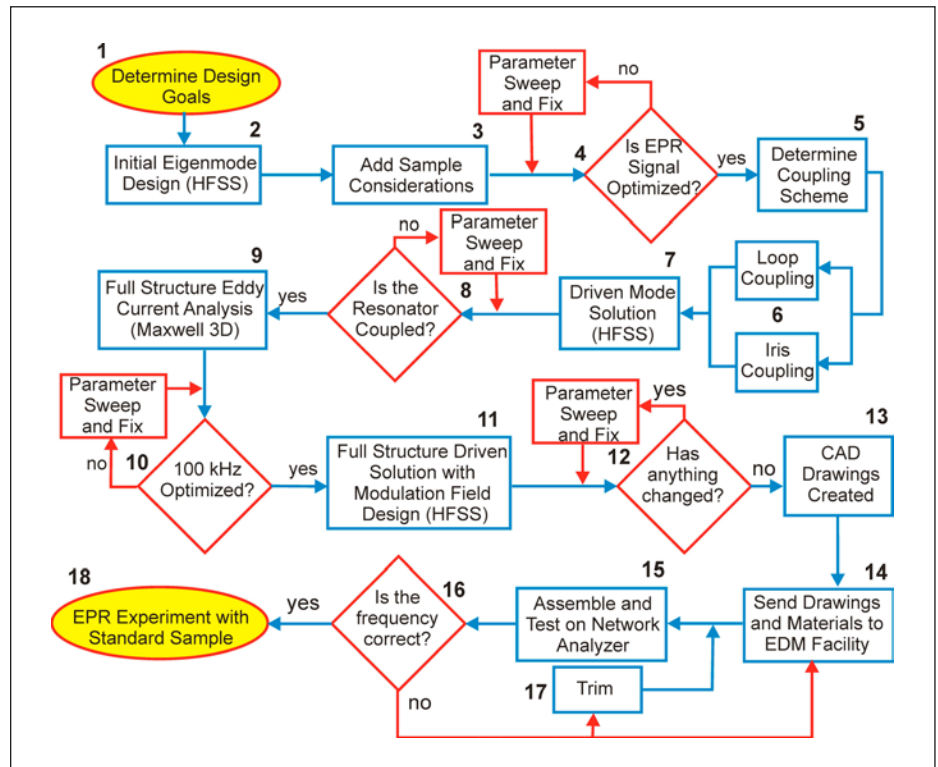


Fig. 2. Flowchart for resonator development.

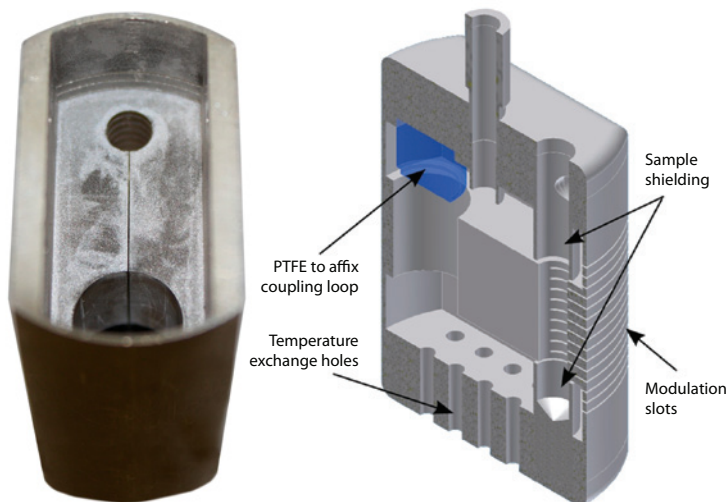


Fig. 3. New two-loop-one-gap L-band LGR fabricated with electric discharge techniques (left). This resonator provides many advances (right) to previous one-loop-one-gap designs.

sample axis. The shields forced the flux and reduced the non-axis components by 30%.

Such specific goals and intuition could only have been accomplished by computer-aided numerical designs. By optimizing resonators to specific experiments or samples, sensitivity

gains and/or quantitative gains are numerous. Additionally, by combining analytical methods, which couple approximations to numerical data, parameter spaces can be narrowed down and insights into the physical properties of samples and resonators can be made.

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Sample Preparation for Quasioptical High-Field ESR

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Advanced Center for ESR Technology (ACERT), Cornell University, Ithaca, NY, USA

In recent years, the quasioptical technique became a standard for ESR at high and very high frequencies [1]. For lossy samples a semi-confocal Fabry-Perot resonator is often used. It provides more convenient sample geometry, i.e., relatively large flat, disk-shaped samples compared to samples that must fit into fundamental mode resonators with sizes in all dimensions dramatically decreasing with an increase in the microwave frequency. Moreover, for non-lossy samples the quasioptical technique is not size-limited and can accommodate samples of various size and geometry. Non-lossy samples can also be studied via the 'bucket' non-resonant structure developed by the St. Andrews group [2].

However, handling lossy samples in the Fabry-Perot resonator is a more challenging proposition. To minimize dielectric losses, a thin flat sample must be precisely located at a B_1 maximum and E_1 minimum near the center of the resonator in the plane perpendicular to the incident far infrared (FIR) beam. The thickness of the flat aqueous layer depends on the microwave frequency. For example, at 240 GHz (1.27 mm) it is only 10–25 μm ; for high viscosity biological samples with high water content the thickness can be slightly greater. Also, increasing microwave frequency imposes additional requirements on the material of the sample holder. It should (1) have very low dielectric losses, (2) be free from minor paramagnetic impurities, since some of them (Mn, Fe trapped in glass etc.) show a strong increase in the ESR frequency.

A convenient way to meet these requirements is to etch plates of fused silica with hydrofluoric acid. The depth of the etched concave can be adjusted by changing the high-field (HF) exposure time. Routinely, a round plate of fused silica is submerged into a shallow layer of liquid paraffin and cooled down. To make a concave depression, an area of the quartz plate with desired size/shape is then cleaned up from solid paraffin and treated with 48% hydrofluoric acid. The sample holder consists of an etched plate covered with an unetched one (Fig. 1). The ESR sample is placed in the

concave etched area and the assembly is sealed with vacuum grease. Sometimes, in particular for oxygen-sensitive samples prepared at anaerobic conditions, additional sealing using epoxy or Norland UV adhesive might be necessary.

Since such a typical sample holder can contain only a very small sample volume (<1 μL), a high signal-to-noise ratio (SNR) of the spectrometer is required. However, in some cases SNR can be improved by using multiple-layer samples or "sandwich samples". Such a "sandwich" usually consists of two or more layers of etched quartz sample holders held together by vacuum grease. Ideally, each next lossy layer containing sample is located in its own node at a B_1 maximum and E_1 minimum. This should multiply the signal (and SNR) by the number of layers. The distance between lossy layers to fit into the consecutive nodes of the B_1 field is λ/n , where λ is the wavelength and n is the index of refraction between the lossy regions. Because of the limited precision of etching and the heterogeneity of the space between the layers (quartz, grease), it takes usually a bit of trial and error to make a well working multilayer sample.

HF ESR spectroscopy can be considered as g -resolved ESR spectroscopy, wherein different orientations of the radical relative to B_0 resonate at different field values. The principal g -tensor values g_{xx} , g_{yy} , and g_{zz} can be determined by HF ESR from the corresponding features of the powder spectrum with high precision, often eliminating the need to determine these values using a single crystal, as in ESR at lower frequencies.

However, obtaining spectra of oriented samples, e.g., single crystals, aligned membranes etc. corresponding to different orientations of the magnetic field B_0 relative to the principal axes of the sample remains a useful and in many cases indispensable tool in ESR, also for higher frequencies. For example, in lipid research utilization of well-aligned membrane samples not only dramatically improves spectral resolution, but also provides valuable information on the orientation of the nitroxide moiety relative to the membrane normal. Such information, particularly in the slow-tumbling regime, is difficult, and often impossible to extract from the spectra obtained from vesicles.

For non-lossy samples, such as some single crystals and dried or frozen biological samples, obtaining angular-dependent HF ESR spectra in principle is not much different from ESR at lower frequencies. At 9 GHz one can get EPR spectra corresponding to different orientation relative to the magnetic field direction merely by rotating the sample in the resonator. Similarly, for HF ESR one can place a non-lossy sample in different orientations relative to the B_0 vector which is collinear with the direction of the incident FIR beam. To provide exact tilt position of the sample relative to B_0 , one can use wedges or even miniature makeshift goniometers from a non-lossy material, polyethylene for example.

There is a challenge, though, in using macroscopically aligned membrane samples in HF ESR studies at biological temperatures. As mentioned above, higher frequencies require for lossy materials very thin, flat samples with

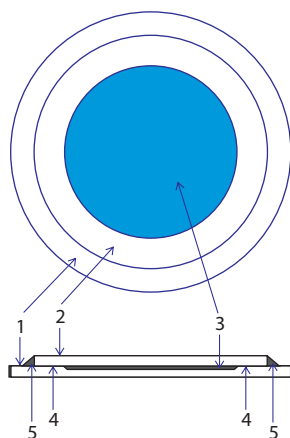


Fig. 1. Sample holder for lossy samples. (1) etched quartz plate (2) unetched quartz plate (3) etched concave depression filled with sample (4) vacuum grease applied (5) epoxy sealant applied if necessary.

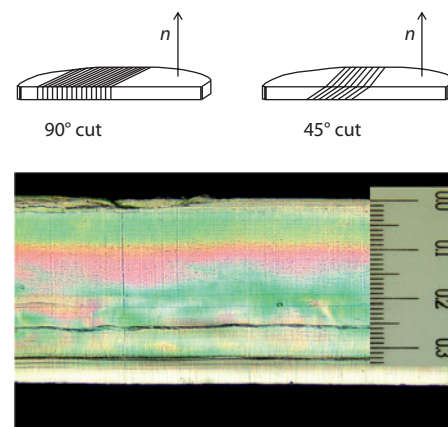


Fig. 2. Schematic graphic representation of the microtome cuts of aligned membrane samples at 90° and 45° and a microscopic view of one of these cuts.

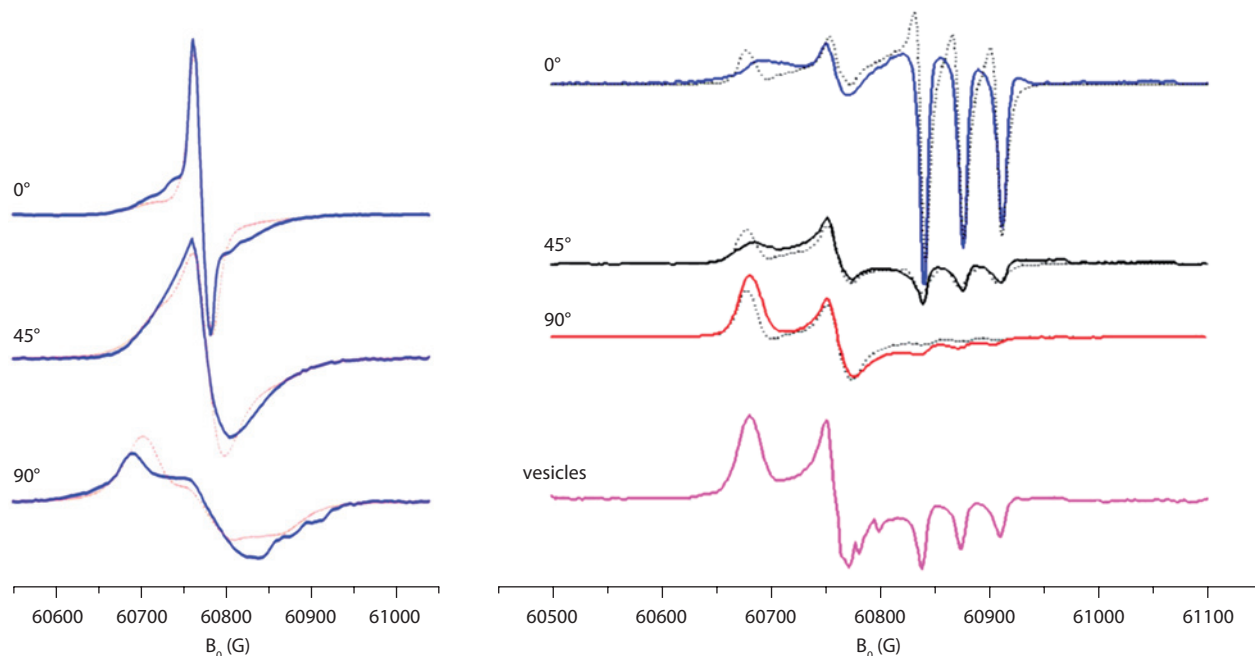


Fig. 3. Example angular dependent ESR spectra taken at 170 GHz in aligned membranes using microtome cuts. A) 0.4% mol. CSL in aligned DPPC membrane at 22 °C. Dotted lines show simulations for a simplified model of ideal Y-ordering and axial symmetric diffusion. B) GAsI (0.6% mol) in aligned DPPC membrane and vesicles at 16 °C. Dotted lines show simulations for ideal Z-ordering. The spectrum in vesicles contains a small fraction of free spin label.

B_0 directed strictly perpendicular to the plane of the sample in order to minimize dielectric losses in the resonant structure. It makes recording spectra for any tilted membrane orientation very difficult.

In 1998 in an elegant study by Barnes and Freed [3] a special “shunt” Fabry-Pérot resonator for a 250 GHz EPR spectrometer was designed to solve this problem and to accommodate a thin sample that must rest with its flat surface perpendicular to the optical axis of the incident FIR beam.

Recently, another method to record spectra from various membrane orientations in the magnetic field for HF ESR has been developed in ACERT [4]. It involves microtome cutting of thick, ISDU-aligned [5] membrane samples. This simple technique allows for any director tilt value, does not need special instrumentation, and can be used on EPR spectrometers at any frequency. A schematic graphic representation of the microtome cuts of aligned membrane samples at 90 and 45° and a microscopic view of one of these cuts is shown in Fig. 2. To obtain these cuts, a piece of hydrated aligned membrane, usually DMPC or DPPC, is embedded in ice in a fixed position. Then a cryostat microtome is used to cut through the ice at a chosen angle. The slice thickness setting usually varied between 40 and 80 μm . After the cutting procedure, 3–4 slices of the membrane are put with a small amount of water into a sample

holder of etched quartz. EPR spectra at 9 GHz for the microtome cuts of spin-labeled membranes at 90 and 45° match well with correspondent orientations obtained by rotating a thin aligned (“0° angle”) sample in the resonator. Figure 3 shows some example spectra taken at 170 GHz in aligned membranes using this microtome technique. Since at this frequency the effect of the g -tensor overwhelms the A -tensor splitting to a great extent, there are three distinct spectral regions attributed to g_{xx} , g_{yy} , and g_{zz} . Changing the orientation of the principal magnetic axes of the nitroxide relative to B_0 manifests itself as a shift of the spectral intensity between these regions. In aligned membranes, this visualizes the orientation of the magnetic

axis of the nitroxide moiety relative to the membrane normal, and substantially simplifies the spectral analysis.

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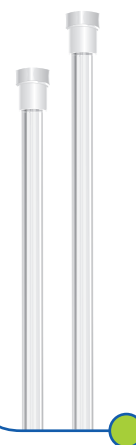
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The 40th Annual Southeastern Magnetic Resonance Conference (SEMRC) Atlanta, Georgia USA, November 4–6, 2011

For forty years, the SEMRC has provided an opportunity for scientists to share research developments and techniques in NMR, EPR, and MRI. Each year the conference is held at a different location in the southeastern United States. For the 40th Southeastern Magnetic Resonance Conference, 133 scientists (including graduate students and international guests) gathered at Georgia State University in Atlanta, Georgia. Georgia State University (GSU), as a major research university in the

region, has active research activities in all areas of magnetic resonance spectroscopy. The 40th SEMRC was organized by Drs. Aimin Liu, Jenny Yang, and Markus Germann of GSU in Atlanta.

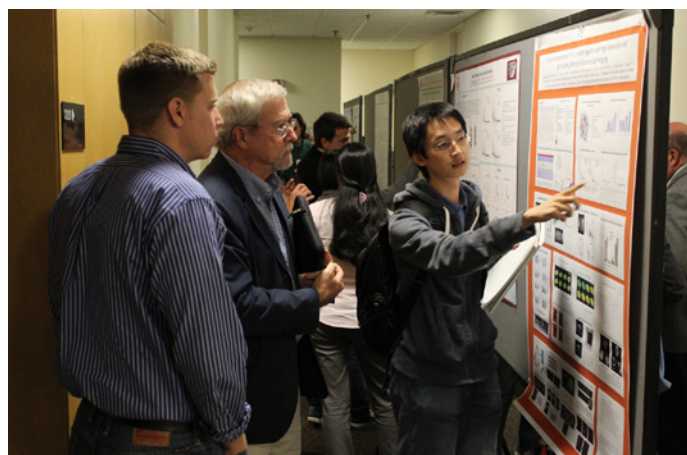
In total, there were 34 oral presentations separated into nine sessions spanning three days. The event kicked off with a welcome reception on Friday night before opening remarks by GSU President Dr. Mark Becker. The first session, which was held Friday night, consisted of talks from each of the three major areas of interest, EPR, NMR, and MRI. The following Saturday was kicked off with the first two sessions focusing on EPR and NMR. Dr. David

Close (East Tennessee State University) was invited to speak in memoriam of the late Dr. William H. Nelson (GSU) and gave an overview of selected studies they had done together on radical species in irradiated single crystals of nucleotides. The day continued with sessions focused on MRI and contrast agents thereof. A special session comprised of selected student and postdoctoral researchers was included in the conference. The Quantum Spin Dynamics Lecture was given by Dr. Irinel Chiorescu (Florida State University) and covered recent advances in spin detection and manipulation.

Saturday closed with poster presentations. In total, 38 posters were presented and prizes



Georgia State University President, Dr. Mark Becker, gives some opening remarks.



Ph.D. Students present their research work.

notices of Meetings

VIII Voevodsky Conference "Physics and Chemistry of Elementary Chemical Processes" (VvV-2012) & Satellite School "Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics" Novosibirsk (Akademgorodok), Russia July 15–21, 2012

www.kinetics.nsc.ru/vvv2012/index.html

Scope:

Elementary stages of chemical and biochemical reactions
Magnetic and spin effects in chemistry and biology
Correlation between structure, dynamics and function at molecular level
Electron transfer in chemistry and biology
Reactivity of excited states and intermediates

Advisory Committee:

Gleb A. Abakumov (Institute of Organometallic Chemistry, Nizhnii Novgorod), Sergey

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Marianna V. Voevodskaya (Presidium of the Russian Academy of Sciences, Moscow).

Organizing Committee:

Renad Z. Sagdeev – Co-chairperson, Sergey A. Dzuba – Co-chairperson, Elena G. Bagryanskaya – Vice-chairperson, Leonid V. Kulik – Vice-chairperson, Petr A. Purto – Vice-chairperson, Ivan P. Pozdnyakov – Scientific Secretary, Victor A. Bagryansky, Alexei V. Baklanov, Elena V. Boldyreva, Igor A. Grigor'ev, Nina P. Gritsan, Alexander I. Kokorin, Igor V. Koptuyg, Nikita N. Lukzen, Victor F. Plyusnin.

Contact:

Dr. Ivan P. Pozdnyakov, Scientific Secretary of the Conference

vvv2012@kinetics.nsc.ru

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Institute of Chemical Kinetics and Combustion, Novosibirsk

were awarded to outstanding presenters. Two \$100 gold prizes were given to Hsiau-Wei Lee of University of Georgia for his poster "Structural Characterization of the α -2,6-sialyltransferase and Fucosyltransferase III and IV Using Solution NMR" and Adonis Bovell of Emory University for his poster "Site Directed Spin Labeling Studies of the Dynamical Roots of Radical Catalysis in B12-Dependent Ethanolamine Ammonia-Lyase"; two \$60 silver prize were awarded to Jin Zhang of Georgia State University and Tihami Qureshi of the University of Tennessee for their posters. Other prizes were given to Garrett Astary and Luis Colon-Perez from the University of Florida and Shenghui Xue of GSU.

The conference resumed Sunday morning with selected speakers whom were chosen from submitted abstracts. The final session of the conference opened with Dr. Astrid Gräslund of Stockholm University sharing her work on the amyloid peptide involved in Alzheimer's disease and featured NMR, EPR, and a talk on coherent spin manipulation of single-molecule magnets. The conference was closed with presentation of the poster awards and a few closing remarks from the conference chair, Dr. Aimin Liu of GSU. The 41st annual SEMRC will be held at North Carolina State University and will be organized by Dr. Alex Smirnov (aismirno@ncsu.edu).

The conference was generously sponsored by Bruker BioSpin, the National High Magnetic Field Laboratory, Applied Photophysics, Wilmad Lab Glass, Cambridge Isotope Laboratories, Resonance Instruments Inc., NEW ERA, the Georgia State University Research Foundation Inc., the Molecular Basis of Disease (MBD) Program at Georgia State University, the Center for Diagnostics and Therapeutics (CDT) at Georgia State University, the Center for Inflammation, Immunity & Infection at GSU, and the GSU Departments of Biology, Physics & Astronomy, and Chemistry.

Aimin Liu



From left to right: Conference Co-Chair, Dr. Marcus Germann, Conference Chair, Dr. Aimin Liu, Conference Co-Chair, Dr. Jenny Yang, and poster award winners, Shenghui Xue, Jin Zhang, Hsiau-Wei Lee, and Adonis Bovell.



Cake!

ICMRBS 2012: XXVth International Conference on Magnetic Resonance in Biological Systems

Lyons, France, August 19–24, 2012

www.pasteur.fr/infosci/conf/sb/ICMRBS

The ICMRBS conference, held biennially, is widely considered one of the leading meetings in the rapidly growing field of magnetic resonance in biology, covering important new developments and biological applications using high-resolution liquid and solid-state NMR, EPR, in vivo NMR, metabolomics and MRI.

The XXVth ICMRBS conference will gather a broad range of experts from around the world with interests in all aspects of magnetic resonance in biology, offering opportunities to improve communication and cooperation between researchers. The challenge of this major event is to provide an in-depth panorama of the current state of the art in the field as well as to assess the directions where magnetic resonance could have the greatest impact on

addressing biologically important problems.

Topics:

Biological EPR • Biological solid state NMR • Computational NMR • Disordered proteins, folding and aggregation • Drug Development / Dynamics • Glycoproteins and carbohydrates • High resolution MRI and MRS • Hyperpolarisation/DNP • In cell NMR • Integrative structural biology • Labelling techniques • Large macromolecular complexes • Membrane proteins and lipids • Metabolomics • New methodologies (liquid, solid, MRI) • Nucleic acids • Paramagnetic NMR • Protein-DNA/RNA interactions

Plenary lectures:

Baldus Marc (University of Utrecht, The Netherlands), Banci Lucia (CERM, University of Florence, Italy), Bax Ad (National Institutes of Health, Bethesda, USA), Dalvit Claudio (University of Neuchâtel, Neuchâtel, Switzerland), Griffin Robert G. (Massachusetts Institute of Technology, Cambridge, USA), Gronenborn Angela (University of Pittsburgh,

USA), Hubbell Wayne (University of California, Los Angeles, USA), Jeschke Gunnar (ETH Zürich, Switzerland), Kay Lewis (University of Toronto, Toronto, Canada), Nicholson Jeremy (Imperial College, London, UK), Shimada Ichio (University of Tokyo, Tokyo, Japan), Shirakawa Masahiro (University of Kyoto, Japan), Ugurbil Kamil (University of Minnesota, Minneapolis, USA), Wright Peter (The Scripps Research Institute, La Jolla, USA)

Chairpersons:

Muriel Delepierre, Institut Pasteur (CNRS, Paris, France), Anne Lecroisey, Institut Pasteur (Paris, France)

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notices of Meetings



Michael Bridges became an Assistant Professor of Chemistry at California State University – Fullerton in August 2011. Mike received his undergraduate degree in physical chemistry and Master's degree in nuclear chemistry from the University of British Columbia (Vancouver, Canada) in 2004 and his PhD in physical chemistry from the University of California – Los Angeles in 2010. His doctoral and postdoctoral work focused on saturation recovery EPR and protein conformational exchange in Wayne Hubbell's laboratory. Dr. Bridges' current research focuses on the study of small, intrinsically unstructured proteins and the changes to

their motional dynamics upon binding, activation, phosphorylation, etc. by SDSL EPR spectroscopy. In particular, he is studying the configurational and dynamical changes that the cytoskeletal regulation protein stathmin undergoes upon binding to microtubules and free tubulin to elucidate the mechanism of microtubule destabilization by stathmin as a function of phosphorylation level.



notices of Meetings

SFRRI 2012 – 16th Biennial Meeting of the Society for Free Radical Research
London, UK, September 6–9, 2012
www.sfrriemeeting.org/index.html

The 16th biennial meeting for the Society for Free Radical Research International (SFRRI) will be held at Imperial College London in the heart of South Kensington in London. This meeting will be a premier forum for the latest advancements in free radical research. International experts from a broad range of disciplines including chemistry, biology and medicine will gather in 2012 to discuss the impact of current research, concepts and applications of free radicals and antioxidants in medicine and pharmaceutical industry.

The exciting scientific programme features an extra day of Satellite Meetings on Wednesday, 5 September followed by the Main Meeting from Thursday, 6 – Sunday, 9 September which will include morning plenary lectures, followed by afternoon parallel themed sessions as well as early evening poster presentations. The meeting will bring together over 800 of your peers giving you a unique chance to network and interact with your international colleagues.

Chairmen:

Professor Giovanni E. Mann, Secretary General SFRRI Meeting Chairman

Professor Malcolm Jackson, President SFRR International

For all enquiries regarding your submitted symposium and abstracts and programme please contact: Heidi Ma, Publishing Content Co-ordinator, e-mail: h.ma@elsevier.com, phone: +86 10 8520 8697

XI Convegno Nazionale GIRSE & 1st Joint Meeting ARPE-GERPE-GIRSE
Hotel Citta del Mare-TERRASINI, Palermo, Italy, October 3–6, 2012
www.fisica.unipa.it/girse2012

The Meeting of the Italian EPR group (GIRSE) is organized in cooperation with ARPE and GERPE, the French and Spanish groups, respectively. During the Meeting the opportunity to extend the cooperation of the three Groups with periodical joint activities and programs will be discussed.

Scientific Committee: E. Giamello (Torino), Coordinator; P. Alonso Gascon (Zaragoza), A. Barbon (Padova), M. Lucarini (Bologna), M. F. Ottaviani (Urbino), M. Marrale (Palermo), D. Gourier (Paris), B. Guigliarelli (Marseille), B. Tuccio (Marseille), H. Vezin (Lille), J. Vidal Gancedo (Barcelona).

Organizing Committee: M. Brai (Palermo), Coordinator; P. Astolfi (Ancona), M. Cannas (Palermo), P. Fattibene (Roma), A. Longo (Palermo), C. Macaluso (Palermo), M. Marrale (Palermo), M. G. Santangelo (Palermo), P. Stipa (Ancona).

Topics of the Meeting belong to all areas of modern EPR. In particular the following areas will be covered:

- Bio systems (proteins, spin labelling, DEER, photosynthesis ...)
- EPR and radicals (organic and inorganic radicals, nitroxides and spin trapping, free radicals in medicine, radiation produced radicals, excited states, dosimetry ...)
- Material science (solid state, defects, magnetic materials, catalysis, polymers, cultural heritage ...)

- Soft matter (membranes, micelles, organic materials ...)
- Experimental aspects and theoretical techniques (novel experimental approaches, high field EPR, modelling ...)

The Meeting will be based on 6 Key-note lectures (KL, 45'), 6–8 Short Invited talks (SIT, 25'), 14–16 Oral presentations (20') and Posters. The official language of the meeting will be English. The annual social meeting of GIRSE will be held on October 4 in the late afternoon and it will be open to all ARPE and GERPE members present in Terrasini. A social event with banquet will be organized on Friday October 5.

In order to favor the presence of young researchers to the meeting, GIRSE will provide 10 Scholarships (covering Registration and Hotel fees) to PhD students and Post docs. Further scholarships are planned by ARPE. People interested in the GIRSE scholarships (open to Italian, French and Spanish young researchers) are invited to submit their candidature together with a Supervisor Statement, by e-mail to Pierluigi Stipa (p.stipa@univpm.it) before May 31, 2012.

Deadlines in 2012:

- 31.05 Registration and abstract submission
- 31.06 Communication of acceptance and Oral-Poster distribution
- 15.07 Payment of the Registration fees (early registration)
- 03.10 Registration in Terrasini (afternoon)

Contacts:

elio.giamello@unito.it and maurizio.marralle@unipa.it

Free Radical Generation during Roasting of Coffee Beans from Panama

Shreya Uppal

Steppingstone MAGnetic Resonance Training Center, Farmington Hills, MI 48336, USA

Free radicals generated during roasting or charring of coffee beans have been studied for over half a century [1] but Nebesny and Budryn showed that free radical formation during roasting is highly dependent on initial water content of the beans while Goodman *et al* saw large changes in free radical concentrations during roasting which depended on how the coffee was roasted, how it was cooled,

(Coffee Express, Plymouth, MI). Samples were taken every minute during the roasting process. These samples were roughly ground so that they would fit in a 5 mm quartz EPR tube.

EPR studies were carried out on a Bruker ESP300 using the program, EWWIN 2011 to gather data. Spectrometer settings were: magnet field center-3520 G, field sweep 100 G, modulation amplitude 1 G and microwave power 15 db. Each spectrum was taken over one minute with a time constant of 0.1 seconds. The integrated intensity of each sample was determined by simulating the spectrum,



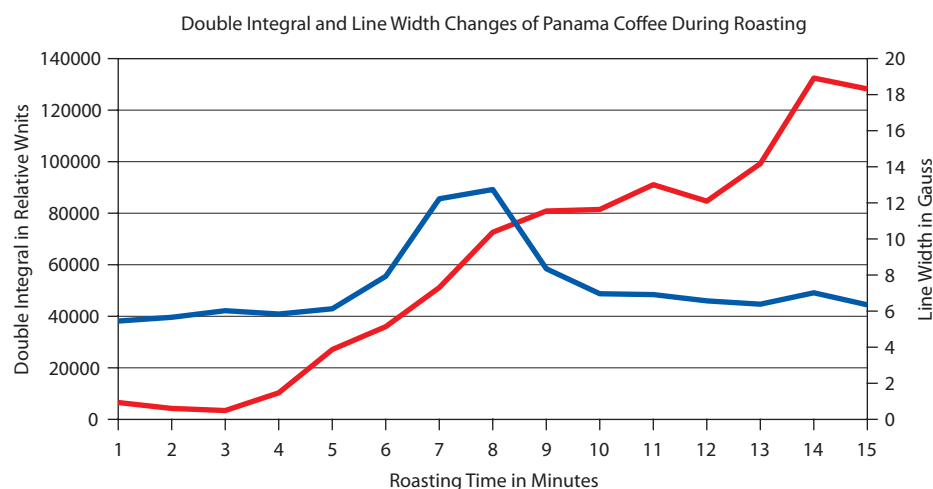
still increasing. I believe that the chemical changes that occur during roasting continue even after the coffee is removed from the roaster and the beans are cooling.

The increase in line width between 5 and 7 min of roasting suggests that chemical changes begin at this time. This is also the time at which the coffee begins to turn brown. Further roasting causes a decrease in line width. I hypothesize that this is a result of higher numbers of free radicals which could cause the line to narrow or interference from metal ions present in coffee beans. This result should be studied further.

Supported in part by grants from Toyota Tapestry and Bruker Bio-Spin to RM and the SMART Center. SU gratefully acknowledges support by Reef Morse and her parents.

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and the type of coffee [2, 3]. Roasting other products like peanuts, almonds, walnuts, and apricots leads to free radical signals at two different magnetic fields [4].

Because of the controversial nature of this topic, I decided to study the production of free radicals in coffee during more traditional roasting methods as may be encountered by a common consumer.

The coffee beans used in this experiment (Panama) were roasted by a commercial roaster

calculating the double integral then dividing by the sample weight and the spectrometer amplitude. The line width was obtained from the simulation as well. The integrated intensity was plotted as a function of roasting time. The data are shown below.

The data clearly shows that the free radical concentration in coffee beans increases during the roasting process and beyond. The beans were removed from the roaster after 12 minutes yet free radical concentration was

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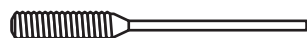
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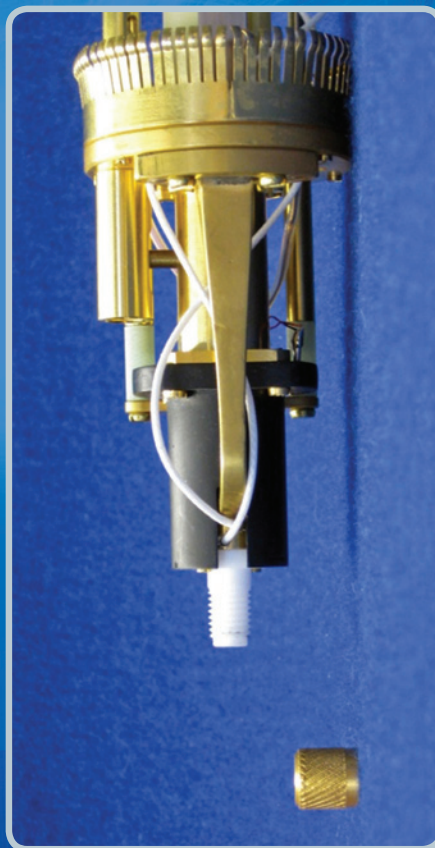
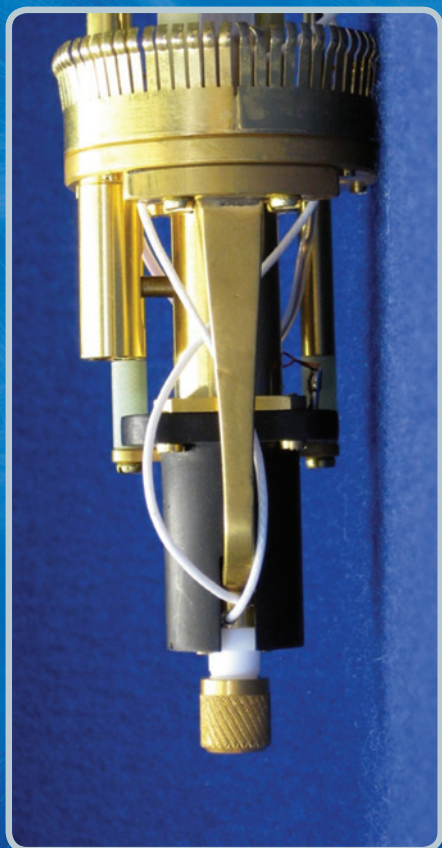
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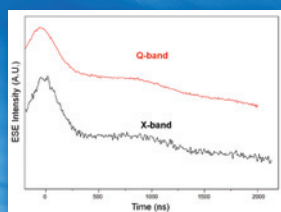


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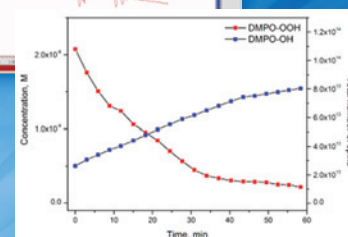
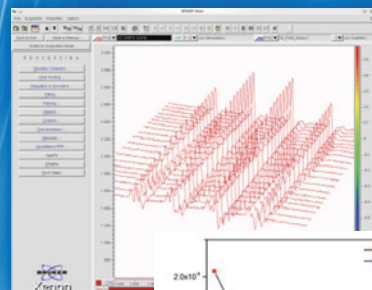
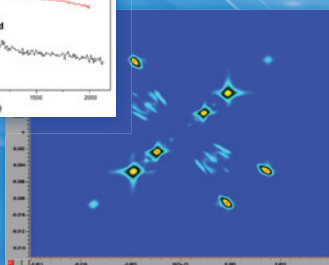
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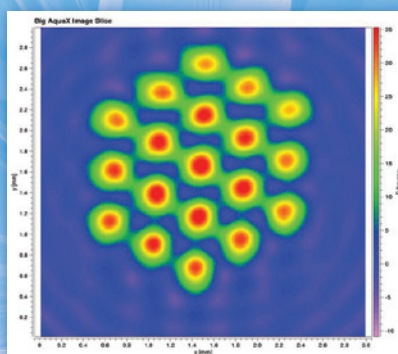
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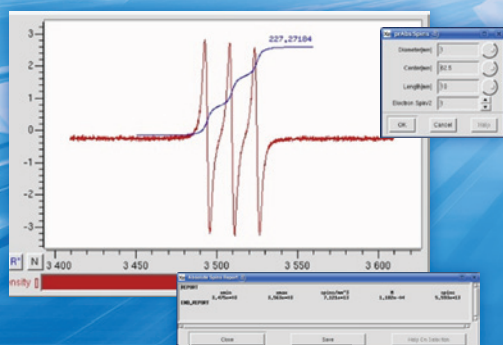
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