EDITORIAL:

Editor: Swiss Neutron Scattering Society

Board for the Period June 2007 – June 2010:
President: Dr. P. Allenspach peter.allenspach@psi.ch
Board Members: Prof. Dr. S. Decurtins silvio.decurtins@iac.unibe.ch
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Dr. M. Zolliker, Paul Scherrer Institut
Address: Sekretariat SGN/SSDN
Paul Scherrer Institut
WLGA/018
5232 Villigen PSI, Switzerland
phone: +41-(0)56 - 310 4666
fax: +41-(0)56 - 310 3294
www: http://sgn.web.psi.ch

Bank Account: Postfinance: 50-70723-6
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ON THE COVER:
Schematic doping-field phase diagram for La$_2-x$Sr$_x$CuO$_4$. The ordered moment is given in false colors with red (blue) as the maximum (minimum).
More information is given in the article on ‘Tuning competing orders in La$_2-x$Sr$_x$CuO$_4$ cuprate superconductors by the application of an external magnetic field’ by J. Chang et al within this issue.
The original manuscript and the figure was published in PRB 78, 104525 (2008).
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DEAR MEMBERS

The Swiss actively shielded 16T-magnet for SNS (a joint project of SGN/SSDN with the Staatssekretariat für Bildung und Forschung [SBF], PSI, MaNEP and SNS) is presently being assembled at Bruker Biospin in Fällanden. It will be moved to PSI for neutron tests in April and thereafter shipped to SNS in Oakridge. Based on this collaboration, the following rules apply (quoted from the MoU):

Swiss researchers will be guaranteed access to SNS instruments generally described by a 2% allocation of an instrument, distributed across all operating instruments.

The guaranteed access to the SNS instruments for Swiss researchers will be provided for at least a ten-year period beginning when the magnet facility is fully commissioned at SNS.

Proposals from Swiss researchers will be reviewed and beam time will be allocated through the general user program as described in the SNS User policies. The allocation of beam time to Swiss researchers will be reviewed annually and adjusted if necessary. Adjustments to beam time allocation will be agreed upon by the SNS Experimental Facilities Division Director and the Chairman of SGN representing the Swiss research community.

Hence, ICNS 2009 in May, in Knoxville, is a good time to visit SNS and also to think about first proposals for experiments there.

On November 28, 20 years of Swiss membership at ILL was celebrated at PSI (see article in this issue). This partnership together with our own national source SINQ is the reason for the exceptional strength of the Swiss neutron user community. In order to assure continuity a prolongation contract has been signed with ILL for the years 2009 - 2013. Due to a favorable exchange rate the Swiss contribution increased by 11% compared to the previous contribution.

ESS is high on the agenda of the EU commission and ESFRI and was also discussed at the competitive council of the EU research ministers on December 2. However, no decision was taken up to now concerning its
siting by the European governments, which seems to be vital for a further progress of the project. The site priorities of the Swiss users, decided at the last general assembly on November 28, is, however, Lund followed by Bilbao.

After 20 years membership in the ILL Steering Committee Dr. Paul E. Zinsli participated for the last time as Swiss governmental representative. He was instrumental in setting up the original contract with ILL and all following processes. He also made the 16T-magnet project with SNS possible and in addition he was and still is extremely active in leading the ESFRI ESS-siting process. Let me take this opportunity to thank him very much for his invaluable support for the Swiss and European neutron scattering community.

Peter Allenspach

Paul E. Zinsli (Swiss State Secretariate for Education and Research)
Minutes of the SGN/SSDN General Assembly on 28/11/2008

1. WELCOME

The president of the SGN/SSDN, Peter Allenspach welcomes the participants to the general assembly 2008.

2. MINUTES OF THE GENERAL ASSEMBLY 2007

The minutes of the general assembly of the SGN/SSDN from 26/06/2007 published in Swiss Neutron News 31 (July 2007) are accepted without objections.

3. ANNUAL REPORT OF THE CHAIRMAN

P. Allenspach reports on the activities of the SGN/SSDN in the years 2007/08:

a) First he reminds on the late Walter Fischer, one of the major pioneers of SINQ, who died of cancer on March 17, 2008. The SGN dedicated the July 2008 issue of Swiss Neutron News to Walter Fischer.

b) The membership contract with ILL was signed in November for the period 2009-2013, (15.346 M€: increase of 11.1% compared to 13.816 M€ 2004 – 2008)

c) On December 4–5, 2008 Paul E. Zinsli will represent Switzerland at the ILL Steering Committee in Grenoble for the last time

d) The project of the actively shielded 16T Swiss magnet for SNS is going well and in time. First tests with neutrons are planned at SINQ for spring 2009

e) An ‘apero’ was again sponsored by the SGN/SSDN at the PSI Summer school in Zuoz, August 16–22, 2008 (Probing the Nanometer Scale with Neutrons, Photons and Muons)

f) Two new issues of Swiss Neutron News will appear in 2008 (December issue in preparation)

g) Actually the SGN/SSDN has 197 members
4. REPORT OF THE TREASURER

S. Janssen presents the annual balance sheet 2007:

Assets SGN/SSDN on 1.1.2007: $5,539.85

<table>
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<th>Revenues [SFr]</th>
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Net earnings 2007: $–1,553.94

Assets SGN/SSDN on 31.12.2007: $3,985.91

Balance sheet 2007:

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Assets on 31.12.07 $3,985.91
5. REPORT OF THE AUDITORS

Bericht der Revisoren

Die Rechnungsrevisor haben die Belege, die Abrechnungen und die Bilanz für das Jahr 2007 geprüft und für in Ordnung befunden!

Datum 24.1.08
Dr. W. Fischer, PSI

Datum 24.1.08
Dr. K. Krämer, Uni Bern

Both Auditors (W. Fischer, K. Krämer) have examined the bookkeeping and the balance 2007. They accepted it without any objections. The participants therefore unanimously vote for a release of the SGN/SSDN board.

6. BUDGET 2008 AND 2009

The treasurer presents the following proposal for the budget 2008 and 2009:

2008:

<table>
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<th>Receipts [SFr]</th>
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<td><strong>Total</strong></td>
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2009:

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<tbody>
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<td>member fees</td>
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<tr>
<td>interests</td>
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<tr>
<td>fees PC account</td>
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<td>Zuoz Apero 2008</td>
<td>700,–</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>605,–</strong></td>
</tr>
<tr>
<td><strong>balance 2009</strong></td>
<td><strong>– 135,–</strong></td>
</tr>
</tbody>
</table>

The participants accept the budget proposals unanimously.
7. NEWS FROM ENSA (P. ALLENSPACH)

a) 3 ENSA meetings were held since the last SGN annual assembly: Bilbao (October 2007), Delft (April 2008), Copenhagen (October 2008):

b) Greece is new member of ENSA

c) The ENSA/ESF European Neutron User Survey was published by the end of 2007.

d) The following new ENSA board members have been elected: vice-chairman A. Deriu (Parma), secretary A. van Well (Delft) (the whole board will be active close to the end of the ESS-PP project in spring 2010).

e) It has been decided to introduce a national weight of votes. Votes of countries with many users have more weight than those with less users (< 50 users: 1 vote; 50-500 users: 2 votes; > 500 users: 3 votes).

f) News on the ESS project will be treated in topic 8).

g) The call for the 2009 Walter Hälg prize has been announced in November 2008. The prize will be awarded during the International Conference on Neutron Scattering (ICNS) early May 2009. Together with the European Crystallographic Association (ECA) ENSA will also call again for the 2009 Lewy-Bertaut prize.

8. NEWS FROM ESS AND THE ESS-PP PROJECT

a) ESFRI process: In 2006 the European Strategy Forum on Research Infrastructures (ESFRI) published a ‘European Roadmap for Research Infrastructures’ with originally more than 200 projects, 35 of those were earmarked as mature, the European Spallation Source ESS was one of those 35: http://cordis.europa.eu/esfri

b) ESS Preparatory Phase project: Being among the 35 earmarked projects ESS was eligible for a EU ‘Preparatory Phase (PP)’ Project. The proposal was successful and a total of 5 M€ was allocated for a project duration of 2 years starting from April 1, 2008. The purpose of the ESS-PP project with 9 workpackages is to facilitate decision making for politicians, to investigate critical issues (strategic, financial, legal, governance, etc) and to conclude on an agreement about the ESS. 11 partners and 21 observers participate in the project, which is coordinated by PSI (P. Allenspach).

c) “Zinsli group” and group of wise persons: Official bids to host ESS came from Lund (SE), Bilbao (ES) and Debrecen (HU). An ‘ESRFI working group on ESS Siting, EW ESS’ (chaired by P.E. Zinsli) and an ‘ESS Site Review Group, SRG (group of wise persons) have been put together. The SRG reported to EWESS by Sep 15, 2008 on their inspections of the three sites. The SGN also has been asked by the Staatssekretariat für Bildung und Forschung (SBF) on it’s site preference. The SGN priorities were: 1-Lund, 2-Bilbao, 3-Debrecen with Lund and Bilbao being on almost equal level. On Nov 27, meetings of the site contenders and of the ‘group of the willing’ countries to support ESS took place in Brussels. There is still a certain chance to get a site decision during an ECRI meeting in Versailles on Dec 9–10, 2008.
9. NEWS FROM THE INSTITUT LAUE LANGEVIN ILL

The ILL director R. Wagner reports on recent news from the ‘Institute Laue Langevin’. The main statements can be summarized as follows:

a) The ‘Reactor Seismic Refit Programme’ was officially signed off in October 2007. The next meeting of the ‘Groupe permanent’ to check the integrity of the reactor key components will only be in 2017. From a technical point of view the HFR can be operated at least until 2030.

b) The reactor operation 2008 consisted of 4 cycles with the last one to end on December 19. Between December 20, 2008 and March 30, 2009 a long winter shutdown is scheduled to enable the installation of new guides and instruments.

c) The Millennium Programme (Phase M-0) will be completed by the end of 2008 with a total budget spent of €38.2 M. In total five new instruments were built (VIVALDI, SALSA, Flat Cone Detector, BRISP, MINIBALL) and six instruments were upgraded (D3C, IN20, D19, D22, D7). Three more instruments have been completed and will be commissioned soon:
   - D11 (SANS, new detector and new collimator system)
   - IN5 (TOF, new detectors, largest array of detectors (30 m²) ever built for neutron scattering)
   - FIGARO (Fluid Interfaces Grazing Angles Rectrotractor)

d) ILL and ESRF plan for the installation of several new infrastructure on the campus. 17 M€ have been approved for this project: A building for scientific partnerships and laboratories will be built close to the ILL main building. Furthermore a new restaurant, a new site entrance and an exhibition hall are planned.

e) R. Wagner then addresses the future of the ILL and summarizes the plans within the Upgrade Programme Phase M-1 (2007-2013). The available investment budget for that period will be €43 M provided Russia will rejoin the ILL as a scientific member. The following measures are envisaged:
   - Five new instruments: D33 (SANS), IN16B (Backscattering), THALES (cold three axis), WASP (Wide Angle Spin Echo) and SuperADAM (Rectstrotractor, CRG)
   - Three instrument upgrades: D17 (Rectrotector), IN1-LAGRANGE (hot three axis), IN4 (thermal TOF)
   - Several instruments will be phased out: D1A, DB21, IN3, IN10, IN11, IN14, IN16 and ADAM
   - The instruments D16, Cryo-EDM, IN12 and LADI will be re-sited
   - Guide projects: new guides H14 and H112 in guide hall ILL 7 and H5 in hall ILL 22
   - Finally investment will be made into the ILL sample environment devices

f) Finally R. Wagner remarks that the Swiss success rate of ILL proposals is significantly high: In 2007 Swiss proposers requested a total of 246 days out of which 186 were accepted. That success rate of more than 75% is the highest of all member countries. In 2007 3.9% of the ILL beamtime was used by Swiss users,
whereas the official budget is 3.1%. Most of the users come from PSI and ETH Zürich, Fribourg, Bern, Lausanne and Geneva.

10. SGN/SSDN ACTIVITIES 2008 AND 2009

P. Allenspach reports on planned future activities of the SGN/SSDN:

a) Various SGN members participate actively (presentations) in today’s (November 28) symposium on the occasion of 20 years of Swiss partnership with the ILL, Grenoble.

b) The next ENSA meeting will be organised on April 1, 2009, Zürich (after NMI3 general meeting at PSI).

c) The SGN/SSDN will again sponsor the welcome reception during the Summer School Zuoz 2009 (preliminary title: Functional Materials, date: August 1—7, followed by practical sessions at SLS/SμS, SINQ on August 8—9).

d) The activities within the ESS/ESS-PP projects will be continued.

11. ELECTIONS

The Swiss representative in the ILL scientific council as well as those in the ILL proposal evaluation colleges 1, 5b and 9 have to be elected. In addition the late Walter Fischer has to be replaced as revisor of the SGN finances. The candidates partly act already as substitutes, but must be confirmed by the SGN General Assembly. The following people are now elected unanimously by the attending members of the society:

ILL scientific council:
Kurt N. Clausen, Paul Scherrer Institut
(replacement P. Schurtenberger)

ILL college 1:
Alex Evans, Paul Scherrer Institut
(replacement E. Lehmann)

ILL college 5b:
Vladimir Pomjakushin, (replacement M. Medarde) Paul Scherrer Institut

ILL college 9:
Peter Fischer, ETH Zürich
(replacement F. Scheffold)

SGN financial auditor:
Markus Zolliker, Paul Scherrer Institut
(replacement W. Fischer)

12. MISCELLANEOUS

K. Clausen asks the participants to deliver input to P.E. Zinsli for the scientific council meeting of the ILL on December 4-5, 2008.

S. Janssen, SGN secretary
December, 2008
Doping dependence of orbital order in A-site ordered manganites, a combined resonant x-ray- and neutron-powder diffraction approach

M. García-Fernández¹, U. Staub¹, Y. Bodenthin¹, V. Scagnoli², V. Pomjakushin³, E. Pomjakushina³-⁴, K. Conder³-⁴ and S.W. Lovesey⁵.

¹Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland
²European Synchrotron Radiation Facility, BP 220, 38043 Grenoble Cedex 9, France
³Laboratory for Neutron Scattering, Paul Scherrer Institut & ETH Zürich, 5232 Villigen PSI, Switzerland
⁴Laboratory for Developments and Methods, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland
⁵Diamond Light Source Ltd. and ISIS Facility, Rutherford Appleton Laboratory, Chilton, Oxfordshire OX11 0QX, United Kingdom

The close interplay between spin, charge, orbital and lattice degrees of freedom in doped manganites can lead to a variety of electronic and magnetic ground states ranging from states with colossal magneto resistance to charge- and orbital- ordering (CO and OO respectively) [1]. Due to coexistence and competition between different types of ordering, the properties of the system can be modified by small changes of chemical compositions, either leading to structure (chemical pressure) or electronic (doping) changes. The balance between competing phases is often subtle, and small changes may significantly affect the material properties, for example, inducing temperature driven metal-insulator (MI) type transitions combined with CO and OO [2].

Recently it has been proposed that other phases than the checkboard charge and orbital ordering pattern, which is characterized by the alteration of Mn³⁺ and Mn⁴⁺ sites (Mn-centered charge ordering), might be present in manganites, close to half doping. Another “charge-ordering” pattern may exist where the charge is localized, but on the bonds (bond-centered charge ordering) [3]. From the crystal structure of Pr₀.₄Ca₀.₆MnO₃ [4] and the magnetic structure of YBaMn₂O₆ [5] determined by neutron diffraction, a bond-centered charge-ordering pattern was proposed. These phases are of Zener polaron type, dimers or
tetramers of spins with ferromagnetic intra-cluster exchange interaction caused by shared electrons. In the later study, the authors also claim that the magnetic scattering is essentially the same in YBaMn$_2$O$_6$ and in TbBaMn$_2$O$_6$, as shown by their neutron powder diffraction experiments. This implies that the ground state of YBaMn$_2$O$_6$ and TbBaMn$_2$O$_6$ are the same and it is expected that this holds for all RBaMn$_2$O$_6$ compounds where R (rare earth) is heavier than Nd. Besides the pure charge order / Zener polaron states, an intermediate phase that combines both features may exist and would lead to the existence of different magnetic states such as simple ferromagnetism (F), antiferromagnetic (G-type) and more complicated A-, C- and CE-type antiferromagnetic order [3].

The A-site ordered manganite (R$_{1-y}$Ca$_y$)BaMn$_2$O$_6$, where the R/Ca and Ba are located on planes alternating along the c axis, is an ideal candidate to study the long range orbital and charge order in detail. The crystal structure of the cation-ordered material is of 2$a_p$x2$a_p$x2$a_p$ type with $a_p$ being the cubic perovskite unit cell parameter, a configuration of the crystal structure is shown in Figure 1. The charge and orbital threshold temperature $T_{CO/OO}$, which corresponds with a MI type transition, depends strongly on the size mismatch of the R/Ba ions.

A previous electron diffraction study on SmBaMn$_2$O$_6$ [7] found $T_{CO/OO}=360K$ and an antiferromagnetic transition at $T_N=250K$ followed by a reorientation of the orbital order at $T_{CO2}=200K$. High-resolution neutron powder diffraction [8] found that this transition is accompanied by a structural transition lowering the symmetry to P-1. These studies also propose a ferro-orbital ordering for R=Y in the temperature region $T_{CO} < T < T_{CO2}$.

A direct study of the orbital and charge ordered ground state is achieved with resonant x-ray diffraction. Experiments performed in the vicinity of the Mn K edge are mainly sensitive to the Jahn-Teller distortion [9], while experiments in the vicinity of the Mn L edge directly probe the transition metal 3$d$ states and are most sensitive to charge, orbital and magnetic order [10]. These soft x-ray resonant diffraction studies have directly observed the OO but so far no agreement on its type, i.e. $x^2-z^2/y^2-z^2$ versus $3x^2-r^2/3y^2-r^2$, has been achieved for the single layer manganite [11-14]. However, these studies showed the significance of Mn-O hybridization and its influence on the spin correlations [12-14]. In addition, the electronic orbital order and the associated Jahn-Teller distortion demonstrate an individual temperature dependence distinguished via their specific resonant energies [15].

Here we present a study on the ground state of A-site ordered manganites for half-doping (x=0.5) using resonant soft x-ray powder diffraction and neutron powder diffraction on the systems SmBaMn$_2$O$_6$ and Tb$_{1-y}$Ca$_y$BaMn$_2$O$_6$ for doping contents of x=0.55, 0.66 and 0.7 (where $x = 1 + \frac{1}{2}y$), corresponding to Ca contents of y=0.1, 0.33 and 0.4, respectively.

The sample preparation is described elsewhere [6]. Resonant soft x-ray diffraction experiments were performed on the RESOXS endstation [16] at the SIM beamline of the Swiss Light Source of the Paul Scherrer Institut, Switzerland. A polycrystalline pellet of 10 mm diameter was glued onto a copper sample holder mounted on a He flow cryostat, which
achieves temperatures between 10K and 370K. Experiments were performed using linear horizontal or vertical polarization light leading to $\pi$ or $\sigma$ incident photon polarization in the horizontal scattering geometry, respectively. Two dimensional data sets were collected with a commercial Roper Scientific CCD camera mounted in vacuum. Neutron powder diffraction measurements were carried out at the high-resolution HRPT diffractometer [17] at SINQ neutron spallation source PSI, Switzerland. The normal intensity mode of HRPT was used with the neutron wavelength = 1.49 Å. The refinements of the crystal structure parameters were performed using the FULLPROF program [18].

Figure 1. Crystal structure of the $\text{RBaMn}_2\text{O}_6$

An image of a section of the powder ring of the (1/2 1/2 0) reflection of SmBaMn$_2$O$_6$ at the Mn $L_3$ edge at $T=14K$ is shown in Figure 2a and a one-dimensional integration of the image is shown in Figure 2b [6]. The integrated intensity is obtained with a fit to a Lorentz function representing the (1/2 1/2 0) reflection and a linear background accounting for the fluorescence background (see Figure 2b).

The energy dependence of the fluorescence and the integrated intensity of this orbital reflection can be found in reference [6], measured at the Mn $L_{2,3}$ edges. By comparison of this energy dependence with theoretical simulations [14] it was proposed that the OO of the e$^g$ electrons is of $x^2$-$z^2$/$y^2$-$z^2$ type in the layered SmBaMn2O6 while a 3$x^2$-$r^2$/3$y^2$-$r^2$ type of orbital ordering is present in the single-layer manganite. The spectra taken with $\sigma$ and $\pi$ polarization are equal within experimental accuracy, indicating that the scattered radiation is rotated ($\sigma$-$\pi$ or $\pi$-$\sigma$), because signals in the unrotated channels ($\sigma$-$\sigma$ and $\pi$-$\pi$) are different form each other.
The \( q \) vector of the orbital reflection has dependence with the doping content as shown in reference [7]. The energy dependence of the fluorescence and the integrated intensity of the orbital \((0.45, 0.45, 0)\) reflection of \( \text{Tb}_{0.9}\text{Ca}_{0.1}\text{BaMn}_2\text{O}_6 \) at the Mn \( L_{2,3} \) edges are shown in Figure 3(a), the spectra was taken with \( \sigma \) and \( \pi \) incident polarization. In Figure 3(b) the energy dependence of the fluorescence and the integrated intensity of the orbital \((0.3, 0.3, 0)\) reflection of \( \text{Tb}_{0.6}\text{Ca}_{0.4}\text{BaMn}_2\text{O}_6 \) at the oxygen K edge collected for both incident polarizations is also shown.

The spectra taken with \( \sigma \) and \( \pi \) polarization are equal within experimental accuracy at both O K- and Mn \( L_{2,3} \)-edges as shown in Figure 3. This behavior is the same as in the half doped case [6]. The polarization dependence of the \((\delta, \delta, 0)\) reflection contains inherent information on the orbital ordering, and the occurrence of possible Zener polaron ordering. For a Zener polaron ordering, the diffraction amplitude at resonance is given by:

\[
F(\theta) = \sum_{Q} e^{-iQ\cdot r} \left( 1 - e^{iQ\cdot r} \right) [1 - V Q e^{i\theta} e^{-i\theta}] d^{4}_{QQ'}(\theta) \]  

(1)

With \( K=2 \), and \( Q= \pm 1, \pm 2 \), \( \langle T_{Q}^{2} \rangle \) represents the quadrupole, \( \chi_{Q}^{2} \) the properties of the beam (polarization) and \( d^{4}_{QQ'} \) a rotation of axis between the crystal axis and the axis of the experiment [19]. Developing this expression we can obtain the diffraction amplitude for the four polarization channels:

\[
F_{\sigma}(\theta) = \sqrt{6} \left( -\frac{1}{\sqrt{2}} \langle T_{\sigma}^{2} \rangle \sin(2\theta) + \frac{1}{2} \langle T_{\sigma}^{2} \rangle (1 - \cos(2\theta)) \right) \]  

(2)

\[
F_{\pi}(\theta) = -\sqrt{2} \langle T_{\pi}^{2} \rangle \sin^{2} \theta \sin 2\theta - \langle T_{\pi}^{2} \rangle (1 + \cos^{2} \theta + \sin^{2} \theta \cos 2\theta) \]  

(3)

Figure 3. (a) Energy dependence of the integrated intensity of the orbital reflection \((\delta, \delta, 0)\), with \( \delta=(1-x) \), measured at the Mn \( L_{2,3} \)-edge for \( x=0.55 \) doping and the fluorescence. (b) Energy dependence of the integrated intensity of the orbital reflection for \( x=0.7 \) doping and fluorescence measured at the O K-edge. The signals are collected for \( \sigma \) and \( \pi \) incident polarization and at \( T=55K \).
For a Zener polaron ordered ground state, we therefore should see significant different intensities for the $\sigma$ ($F\sigma'\sigma + F\sigma'\pi$) and $\pi$ ($F\pi'\sigma + F\pi'\pi$) polarization channels, which is not observed in our experiment.

The temperature dependence of the orbital (1/2 1/2 0) reflection for SmBaMn$_2$O$_6$ taken at the maximum of the L$_3$-edge (642.25 eV) is shown in Figure 4a [6]. The orbital reflection appears at $T_{CO} \approx 355$K and its intensity is constant between 330 K and 220K. Below $T_{CO2} \approx 210$K a sharp increase in intensity is observed and the intensity at 180 K is twice that of the intensity above $T_{CO2}$, indicative of the orbital stacking reorientation transition [6, 7]. The intensity increases further below 180K but with a smaller gradient. The integrated intensity reflects the orbital order parameter. For x>0.5 we have no doubling of the intensity, indicating an absence of orbital stacking transition, as can be seen in Figure 4 (b) for the case x=2/3. The intensity follows a smooth curve until the signal disappears at the MI transition. Interesting is that at the same temperature as the restacking is observed for the half-doped case (x=0.5), for x=2/3 the orbital ordering wave vector gets temperature dependent. A temperature dependence was also observed for the case of Bi$_{0.31}$Ca$_{0.69}$MnO$_3$ [20] and Bi$_{0.53}$Sr$_{0.47}$MnO$_3$ [4].

![Figure 4](image_url)

Figure 4. a) Temperature dependence of the integrated x-ray intensity of the (1/2 1/2 0) reflection, taken at the Mn L$_3$ edge (643.25 eV) with $\pi$ incident radiation of polycrystalline SmBaMn$_2$O$_6$. The vertical lines indicate the various phase transitions as discussed in the text. b) Temperature dependence of (1/3 1/3 0) reflection measured with $\pi$ incident radiation of polycrystalline Tb$_{0.66}$Ca$_{0.33}$BaMn$_2$O$_6$ at the O K-edge together in the same plot it's shown the change of the $q$ vector as a function of temperature for (1/3 1/3 0) measured with resonant scattering $\pi$ and the temperature dependence of the $q$ vector of the (2 2 0) reflection, calculated from the unit cell parameters, obtained from the neutron powder diffraction refinement. $q_0$ is taken as the value of $q$ for the lowest measured temperature.
[21], but occurring much closer to $T_{\text{OO}}$. The origin of this anomalous incommensurable melting remains still unclear.

We have complemented these results with neutron powder diffraction experiments to determine the temperature dependence of the crystal structure. The evolution with temperature of the orbital $\mathbf{q}$ vector expected from the temperature change of the unit cell parameters, was calculated using the values of $a$ and $b$ obtained from the powder neutron data refinement and is plotted also in Figure 4(b). It can be seen that the change of the $\mathbf{q}$ vector of the orbital reflection as a function of temperature, observed in the resonant scattering experiments, cannot be explained simply in terms of changes of the $2a_p \times 2a_p \times 2a_p$ unit cell as a function of temperature, and that its origin must be related to changes in the electronic state of the Mn ions, rather than having structural origin, even though a structural change could drive the electronic change. A possible explanation could come from the loss of 3-dimensionality of the system as a function of temperature, due to the random stacking along the $c$-axis. The orbital ordering in this compound is formed by the $x^2-y^2$ orbital on the $e_g$ state which interact not only in plain but also along the $c$-axis. As a function of temperature the unit cell size increases as can be seen in the Figure 5(c). Two crystalline transitions can be observed in the

Figure 5. (a) Unit cell parameters as a function of temperature for $x=2/3$. (b) Variation of volume with temperature for $x=2/3$, the inset shows the deviation of the unit cell volume from a linear fit. (c) Variation of unit cell parameters for $x=0.5$, (d) variation of volume with temperature for $x=0.5$. 
plot; the first one happening at $T=210K$, the same temperature at which the orbital reflection becomes incommensurate and the second one at $T=380K$ corresponding to the temperature at which the OO disappears.

In Figure 5 we show the temperature dependence of the lattice constants of $x=0.5$ and the $x=2/3$ doped samples and for $x=0.5$. Nd$_{0.4}$Tb$_{0.6}$BaMn$_2$O$_6$ was chosen in replacement of SmBaMn$_2$O$_6$ due to the elevated absorption of neutrons by the Sm. The data was refined between 20 and 480K with orthorhombic (Cmmm) crystal symmetry, but the lattice constants undergo dramatic changes. The temperatures above room temperature were achieved using a closed cycle refrigeration setup, leading to a large temperature gradient over the sample volume for $T \geq 320K$.

We can distinguish two different regions: the region on the vicinity of $T_{\text{MI}}$ $T=380K$ for $x=2/3$ and $T=410K$ for $x=0.5$, and the restacking/incommensurate temperature that takes place at around 210K in both samples. For $x=0.5$ and increasing temperatures the unit cell parameters $a$ and $c$ show sharp positive jumps at $T_{\text{MI}}$ of 0.127% and 0.812% respectively, while $b$ drops by -1.046%. For $x=2/3$ the unit cell parameters $a$ and $c$ show sharp positive jumps of 0.967% and 0.302% and $b$ drops by -1.414% for $T>380K$. Those anisotropic changes of the crystal unit cell result in an abrupt negative drop of the unit cell volume at $T_{\text{MI}}$ of -0.106% ($x=0.5$) and -0.156% ($x=0.665$). In the vicinity of $T_{\text{MI}}$, a coexistence of the low- and high-temperature structures has been clearly observed in the diffraction data, providing evidence for the first-order type of the MI transition. A similar volume collapse effect was also observed at the MI transition in HoBaCo$_2$O$_{5.5}$ [20], A-site ordered cobaltate.

For the second region, a change in the unit cell parameters and correspondingly in the unit cell volume takes place at $T=210K$ for $x=0.5$. This change in the crystal structure, occasions a change in the charge and orbital ordering at this temperature leading to a different stacking of the orbitals along the c axis. For $x=2/3$ doping this change is not as pronounced. In addition the presence of Ca ions introduces extra Mn$^{4+}$ ions that alliterate the charge ordering introducing more disorder in the system and possibly leading to a more 2D character of the ordering as schematized in the inset in Figure 4 (b), causing finally the anomalous melting of the orbital order.

In conclusion, we have studied the doping dependence of orbital order in A-site ordered manganites by means of resonant soft x-ray scattering and neutron powder diffraction. The formation of a Zener polaron order can clearly be excluded in these systems. The MI transition is accompanied by a drop in the unit cell volume as clearly shown in the neutron data. A restacking of the orbitals along the c-axis at $T=210K$ was observed for the half doped case, accompanied by a change in the unit cell volume while for the higher doped samples no restacking could be detected but an anomalous incommensurable melting of the orbital order starts at the same temperature. This anomalous orbital order melting can not be simply explained by means of unit cell variations as a function of temperature.

We would like to thank the beamline staff of X11MA for their excellent support. This
REFERENCES:


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Tuning competing orders in \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) cuprate superconductors by the application of an external magnetic field

J. Chang\(^1\), Ch. Niedermayer\(^1\,*\), R. Gilardi\(^1\), N.B. Christensen\(^1\), H.M. Rønnow\(^2\), D.F. McMorrow\(^3\,4\), M. Ay\(^1\), J. Stahn\(^1\), O. Sobolev\(^5\), A. Hiess\(^6\), S. Pailhes\(^1\), C. Baines\(^7\), N. Momono\(^8\), M. Oda\(^8\), M. Ido\(^8\) and J. Mesot\(^1\)

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1 Laboratory for Neutron Scattering, ETH Zurich and Paul Scherrer Institute, 5232 Villigen PSI, Switzerland
2 Laboratory for Quantum Magnetism, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland
3 London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, London, UK
4 ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot OX11 0QX, UK
5 BENSC Hahn-Meitner-Institut, 14109 Berlin Wannsee, Germany
6 Institut Laue-Langevin, BP 156, F-38042 Grenoble, France
7 Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland
8 Department of Physics, Hokkaido University – Sapporo 060-0810, Japan
(Dated: December 2, 2008)

We report the results of a combined muon spin rotation and neutron scattering study on \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) (LSCO) in the vicinity of the so-called 1/8-anomaly. Application of a magnetic field drives the system towards a magnetically ordered spin-density-wave state, which is fully developed at 1/8 doping. The results – discussed in terms of competition between antiferromagnetic and superconducting order parameters – demonstrate the enormous strength of having a combined neutron and muon facility at the same site.

1. INTRODUCTION

Competing order parameters are a central theme in condensed matter physics. This is especially true for the study of high-temperature superconductors (HTSC), where superconductivity occurs upon hole doping of an antiferromagnetic Mott insulator. As a consequence of the competition between superconductivity (SC) and antiferromagnetism (AF) different ground states have been identified in the underdoped regime of La-based cuprates. Among those are (i) d-wave SC, (ii) a disordered spin glass like state, which coexists
with SC over a broad range of doping, (i) a spin density wave (SDW) state with suppressed SC around a specific hole concentration \( x \approx 1/8 \). This so called 1/8-anomaly was first observed in \( \text{La}_{15/8}\text{Ba}_{1/8}\text{CuO}_4 \) \(^2\) and later in \( \text{La}_{1.48}\text{Nd}_{0.4}\text{Sr}_{0.12}\text{CuO}_4 \) (LNSCO) \(^3\)–\(^5\) where the effect is concomitant to a structural phase transition from a high-\( T \) orthorhombic (HTO) to a low-\( T \) tetragonal (LTT) phase. \(^6\) A similar anomaly was found in the LSCO system at \( x \approx 0.115 \) \(^7\) however without a structural HTO-LTT transition and without a complete suppression of SC. A stripe model with spatial modulations of spin and charge densities has been suggested to account for the incomensurate magnetic and simultaneous charge order observed in neutron diffraction experiments on \( \text{La}_{1.48}\text{Nd}_{0.4}\text{Sr}_{0.12}\text{CuO}_4 \) (LNSCO). \(^3\)–\(^5\) In this model dynamic stripe correlations of spins and holes are stabilized for \( x \approx 1/8 \) in the LTT phase and suppress SC.

Starting from \( \text{La}_{1.88}\text{Sr}_{0.12}\text{CuO}_4 \), there are several routes to reach the 1/8 state. One way is simply to substitute Sr with Ba or La with Nd. An alternative is to introduce pinning centers into the CuO\(_2\)-planes. \( \mu \)SR results on Zn doped \( \text{La}_{2-x}\text{Sr}_x\text{Cu}_{1-y}\text{Zn}_y\text{O}_4 \) show an enhancement of magnetism in the vicinity of 1/8 doping, \(^9\) suggesting that small amounts of nonmagnetic impurities act as pinning centers for dynamical stripe correlations. The observation of similar magnetic anomalies in Zn substituted Bi-2212 and YBa\(_2\text{Cu}_3\text{O}_6+x \) seems to indicate that the 1/8-anomaly is not just a specific feature of the La-based compounds, but a general property of HTSC. \(^10\),\(^11\)

The subtle balance between the competing orders may also be changed by external perturbations such as magnetic fields \(^12\),\(^13\) or pressure. \(^14\) For example, it was demonstrated that the static IC magnetic neutron response for LSCO with doping close to 1/8 is enhanced by the application of a magnetic field perpendicular to the CuO\(_2\)-planes \(^12\),\(^13\). The microscopic mechanisms behind the 1/8-anomaly, as well as the primary cause of the field effect remain however poorly understood.

We have therefore performed a systematic study of the competition between the AF and SC order parameters in the vicinity of 1/8 doping. By combining \( \mu \)SR and neutron diffraction results obtained on the same single crystals we show that for samples in the 1/8 doping state the AF order is already fully developed in zero field (ZF) and can therefore not be enhanced by the application of an external magnetic field. A field induced enhancement of the staggered moment is only observed in samples with a reduced ZF magnetic response.

**II. METHODS**

High quality LSCO with \( x = 0.105 \), \( x = 0.12 \), and \( x = 0.145 \) and LNSCO single crystals were grown by the travelling solvent floating zone method. \(^15\) The Sr content was reassessed by measuring the structural transition from a high-\( T \) tetragonal (HTT) to a low-\( T \) orthorhombic (LTO) phase, which vary strongly with hole doping. \(^16\),\(^17\) The magnetic onset temperature was determined for all samples with both \( \mu \)SR \( (T^\muSR_i) \) and neutron scattering \( (T^\gamma_i) \). The difference among \( T^\muSR_i \) and \( T^\gamma_i \) is due to the different observation time scales of the two experimental techniques. Table 1 summarizes the properties of the single crystals used in this study.
The zero field (ZF) μSR experiments were performed at the πM3 beamline of the Paul Scherrer Institute (PSI), which provides 100% spin-polarized positive muons. They are implanted into the sample and come to rest at interstitial lattice sites without losing their initial polarization. The spin of the muon then acts as a very sensitive local magnetic probe through its precession in the internal field $B(r)$. In cuprate materials the muon stopping site is close to an apical oxygen and $B(r)$ arises from dipolar fields created by the surrounding Cu$^{2+}$ moments.

The neutron scattering experiments were carried out on the cold neutron spectrometers RITA II at PSI, FLEX at the Hahn-Meitner Institute and IN14 at Institut Laue-Langevin. The experiments were performed with a fixed incoming and final wavevector $(k_f = k_i = 1.5$ or $1.9\text{Å}^{-1})$. A Be- or PG-filter was installed before the analyzer in order to eliminate higher order contamination. The samples were mounted in vertical 15 Tesla cryomagnets such that $(Q_h, Q_k, 0)$ were accessible. All measurements in an external magnetic field $\mu_0 H$ were performed after field cooling.

### III. RESULTS AND DISCUSSION

Incommensurate AF order is observed at $Q_{IC} = (0.5, 0.5 \pm \delta, 0), (0.5 \pm \delta, 0.5, 0)$ in tetragonal units of $2\pi/a = 1.65 \text{Å}^{-1}$. The incommensurability $\delta$ depends on the Sr content as in Ref. 23. Fig. (1) summarizes the results of our elastic neutron diffraction experiments. The panels in Fig. (1a-d) are presented with increasing elastic response in ZF. For $x = 0.145$ [Fig. (1a)], no elastic response is observed in ZF. However, application of $\mu_0 H = 13$ T induces an elastic response at $\delta = 0.13$, confirming a previous report. For $x = 0.105$ and $x = 0.12$ an elastic response exists already in ZF and an applied magnetic field enhances the magnetic response for $T < T_{IC}$ [Fig 1b,c]. LNSCO shows the strongest ZF response and the absence of a field effect at all T.

Next, we plot in Fig. (1e) the T-dependence of the intensity $I$ at $Q_{IC}$. The $T$-axis and $I$-axis are normalized to $T_{IC}$ and $I(2K)$ [for LNSCO we used $I(5K)$ to stay above the Nd ordering temperature]. Due to the absence of a field effect in LNSCO we plot, for simplicity, only the ZF data in this figure. The ZF elastic response of LNSCO exhibits an order parameter like $T$-dependence whereas the ZF response for $x = 0.105$ and $x = 0.12$ is significantly different and close to a linear $T$-dependence as indicated by the dashed lines. It is remarkable that the application of an external magnetic field changes the $T$-dependence in such a way, that the normalized data now also fall on the same order parameter like curve.

The superconducting transition temperature is strongly suppressed in LNSCO [$T_c \approx 7$ K] and we therefore consider this compound to closest mimic the physics of the so-called 1/8-state. The time evolution of the muon spin polarization $A(t)$ exhibits a strongly damped oscillatory behavior that is well described by a Bessel function with a frequency $\nu = 3.5$ MHz [see Fig. 2]. This observation is consistent with the existence of an IC SDW state. We stress that similar results are obtained for La$_{15/8}$Ba$_{1/8}$CuO$_4$ and for the AF-ordered volume fraction in superoxigenated La$_{2-x}$Sr$_x$CuO$_{4+y}$. The latter com-
pound was shown to phase separate into optimally doped SC regions and an AF-ordered phase closely related to the 1/8-state. The characteristic features of the 1/8-state are therefore (i) a strongly suppressed $T_c$, (ii) the observation of a Bessel like relaxation with $\nu \approx 3.5$ MHz in the $\mu$SR time spectra and (iii) incommensurate SDW order with $\delta \approx 0.125$ and the absence of a field effect. The 1/8-state consist, most likely, of static stripes with an associated SDW order, which in turn suppresses the SC order parameter. The 1/8-anomaly is limited to a very narrow doping range and slight variations of the doping level lead to very noticeable changes in the physical properties.

Due to its dipolar character, $B(r)$ is directly proportional to the ordered Cu$^{2+}$ moment. For LNSCO the internal field at $T = 5$ K is found to be 27 mT which is about 2/3 of the value observed in the undoped compound La$_2$CuO$_4$.$^{28,29}$ Assuming a value of 0.6 $\mu_B$ for the Cu$^{2+}$ moment in La$_2$CuO$_4$, the internal field corresponds to a local ordered moment $\mu_{lo} = 0.36 \mu_B$. The average ordered moment estimated from the neutron diffraction experiments suggest $\mu_{av} = 0.07 \mu_B$, consistent with a previous report.$^4$ Note, that for a sinusoidal SDW there is a factor of two between $\mu_{lo}$ and $\mu_{av}$.$^{19}$ However, there is still a discrepancy between $\mu_{lo}$ estimated by $\mu$SR and $\mu_{av}$ determined by neutron diffraction (see also Ref. 30). A full knowledge of the microscopic spin topology might be necessary to solve this issue.

When moving away from 1/8 doping the ordered moment at ZF decreases systematically with decreasing doping. For $x = 0.12$, $A(t)$ still exhibits the characteristic Bessel type oscillation, albeit with a reduced frequency and an increased damping [see Fig. 2]. Note that we observe the full muon asymmetry, i.e. all muons experience $B(r) \neq 0$. This implies that the magnetic order persists throughout the entire volume of the sample, which is a remarkable result for a superconductor with a $T_c$ as high as 27 K. We emphasize that the magnetic ground state may still be inhomogeneous but the characteristic length scale for this inhomogeneity has to be smaller than $\sim$ 10−20 Å, which is the typical range for dipolar fields that originate from AF ordered moments. In fact, a nanoscale inhomogeneous state consisting of SC droplets and patches of AF correlated regions is a likely candidate for the ground state in a region of the phase diagram where the antiferromagnetic and superconducting phases are very close in energy.$^{31,32}$

The neutron scattering results confirm the existence of IC magnetic order in ZF and in addition reveal a significant enhancement of the elastic intensity by an applied magnetic field [see Fig. 1b].$^{12}$ Combining the ZF $\mu$SR data with the neutron results, we are able to display the field dependence for the different samples in a common plot (see Fig. 3). It can be inferred from this figure that for $x = 0.12$ the applied field tends to restore the magnetism characteristic for 1/8 doping. This suggests that the effect of the field is to drive the system towards the 1/8 ground state.

For $x = 0.105$, $A(t)$ does no longer show the features of a Bessel function, but is now well described by a single exponential decay [see Fig. 2]. The static nature of $B(r)$ was verified by longitudinal field experiments. We deduce a static field distribution $\Delta \approx$10 mT
TABLE I: Compilation of μSR and neutron scattering results on La-based compounds. μlo and μav denote the local and average Cu moment as determined by μSR and neutron scattering, respectively. T_{f_{μSR}} and T_{f_{Neu.}} are the corresponding, time scale dependent freezing temperatures. δ is the incommensurability. The values in the last column indicate the structural transition temperatures.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Nominal doping</th>
<th>T_{c} onset</th>
<th>μlo/μ_{lo}(1/8)</th>
<th>μav/μ_{av}(1/8)</th>
<th>T_{f_{μSR}}</th>
<th>T_{f_{Neu.}}</th>
<th>δ</th>
<th>T_{LTO-HTO}</th>
</tr>
</thead>
<tbody>
<tr>
<td>La_{2−x}Nd_{x}Sr_{y}CuO_{4}</td>
<td>x = 0.12, y = 0.4</td>
<td>7 K</td>
<td>0.35(2) μB</td>
<td>0.071(4) μB</td>
<td>50 K</td>
<td>65 K</td>
<td>0.122(4)</td>
<td>70 K</td>
</tr>
<tr>
<td>La_{2−x}Ba_{x}CuO_{4}</td>
<td>x = 0.125</td>
<td>5 K^{18}</td>
<td>0.35 μB</td>
<td>–</td>
<td>40 K^{20}</td>
<td>50 K^{18}</td>
<td>0.118^{18}</td>
<td>55 K^{18}</td>
</tr>
<tr>
<td>La_{2−x}Sr_{x}CuO_{4+y}</td>
<td>x = 0.09, y = 0.03</td>
<td>40 K^{21}</td>
<td>0.36 μB^{21}</td>
<td>–</td>
<td>40 K^{21}</td>
<td>40 K</td>
<td>0.12321</td>
<td>–</td>
</tr>
</tbody>
</table>

FIG. 1: (a-d) Q-scans around Q_{IC} performed on x = 0.145, x = 0.105, x = 0.12, and LNSCO respectively. Solid lines are gaussian fits to the data. Note the different x-axis scale for the left and right panel. The magnetic correlation length is derived from the FWHM of the magnetic peaks. Data in c and d are resolution limited. (e) T-dependence of the intensity at Q_{IC} for x = 0.105, x = 0.12, and LNSCO. Open symbols indicate data taken in ZF while filled symbols represent data taken in a magnetic field. Lines are guides to the eye.

FIG. 2: μSR time spectra obtained in ZF and low temperatures. The solid lines are fits with a Bessel function for LNSCO and x = 0.12, a simple exponential decay (x = 0.105) and a Kubo-Toyabe function (x = 0.145).
which is significantly reduced from the 27 mT observed in the 1/8-compounds. Application of $\mu_0 H = 12$ T doubles the amplitude of the elastic signal [see Fig. 1b]. The value characteristic for static stripe order, however, can not be fully restored in this system.

For the $x = 0.145$ compound, $A(t)$ does not exhibit any relaxation due to electronic moments. The slow decay of $A(t)$ is well fitted by a static Kubo-Toyabe function [see Fig. 2], which describes the field distribution $P(B)$ arising from nuclear moments alone. The width of $P(B)$ defines an upper limit for the electronic moments $\mu_0 < 0.005 \mu_B$. Neutron diffraction studies on this sample show field-induced static AF-order resembling that of underdoped compounds for $\mu_0 H > \mu_0 H_c$ with $\mu_0 H_c \approx 7$ T [see Fig. 4]. A previous report found $\mu_0 H_c \approx 3$ T, which might indicate that the doping level of that sample is slightly lower.

We have also performed a systematic study of the vortex lattice (VL) in $x = 0.105, x = 0.12,$ and $x = 0.145$ by small angle neutron scattering. For $x = 0.145$, we observe a VL resembling that at optimum doping but only for $\mu_0 H < 7$ T. No VL could be detected in $x = 0.12$ where the largest elastic field effect is observed. Although vortices might exist in disordered structures, we find it difficult to correlate the elastic field effect with vortex matter physics. Instead, we interpret our data in terms of competing order parameters. Recently, we reported the observation of a single d-wave gap in the ARPES spectra of the $x = 0.145$ sample. The most likely ZF ground state of $x = 0.145$ is therefore pure d-wave SC similar to that observed at optimum doping. Application of a magnetic field tunes the system into a different ground state where
static IC AF coexists with SC. This ground state resembles that of more strongly underdoped LSCO (x < 0.13) where static AF and SC orders compete even in ZF. For x \approx 0.12, the ordered Cu moment at H = 15 T is close to that the 1/8 ground state [see Fig. 3]. Therefore we argue, that the effect of the applied field is to drive the system towards the 1/8 ground state.

IV. CONCLUSIONS

To summarize our combined μSR and neutron diffraction experiments we present in Fig. 4 a schematic H – x phase diagram, in which the ordered Cu moment is depicted by a false color scheme. The 1/8 state and the pure d-wave SC ground state is pictured by the dark red and the blue regions, respectively. Colors in between represent a state where AF and SC coexist. With the application of a magnetic field one can tune the pure SC state into the mixed state of AF and SC. At the specific doping x = 0.12, we found that the field drives the system towards the 1/8 state. The different ground states are therefore very close in energy. Our results clearly support the notion of competing SC and static AF order parameters. The systematics of our data shows that the existence of AF is intrinsic and not due to defects or chemical inhomogeneities. Any suppression of superconductivity by either a change of chemistry or by an external perturbation goes along with a concurrent and systematic enhancement of static magnetism.

V. ACKNOWLEDGEMENTS

This work was supported by the Swiss NSF (through NCCR, MaNEP, and grant Nr 200020-105151, PBEZP2-122855) and the Ministry of Education and Science of Japan. A major part of this work was performed at the Swiss spallation source SINQ and the Swiss Muon Source, Paul Scherrer Institut, Villigen, Switzerland.

*Electronic address: christof.niedermayer@psi.ch
S. Katano, M. Sato, K. Yamada, T. Suzuki, and T. Fukase, Phys. Rev. B 62, R14677 (2000), note that the field effect reported here is stronger than the one reported by Katano et al., but given the significantly lower $T_c = 12$ K of their $x = 0.12$ sample the different magnitude of the field enhancement can easily be understood.


A similar phase diagram was reported by J. M. Tranquada, see Handbook of High Temperature Superconductivity, Springer 2007.
The Lyceum Alpinum in Zuoz hosted August 17–21, 2008 the 7th edition of the PSI Condensed Matter Research Summer School entitled ‘Probing the Nanometer Scale with Neutrons, Photons, and Muons’. The lectures by 22 speakers (that can be found at http://num.web.psi.ch/zuoz2008/) demonstrated that nanoscience is of relevance to, on the one hand, fundamental physics, material science, and food science and, on the other hand, key technologies for medicine, transportation, information, and sustainable economic growth.

Nanoscience is a multidisciplinary effort to probe matter in a window of wavelengths ranging from the ultraviolet (the size of a protein say) to the X-rays (the size of an atom say) for which large facilities such as PSI play a central role (Helmut Dosch). There are three complementary probes that can be used to explore the static and dynamic properties of matter at the nanometer scale; photons, neutrons, and muons, as was illustrated in the introductory courses to neutrons and photons reflectometry (Jens Als-Nielsen), polarized low-energy muons (Elvezio Morenzoni), small angle scattering and photocorrelation spectroscopy (Joachim Kohlbrecher), powder neutron diffraction (Denis Sheptyakov), bulk muon spectroscopy (Alex Amato), and inelastic neutron scattering (Kim Lefmann).

Like a wall made of bricks, heterostructures are man-made materials obtained by layering nanometer thick crystals that can differ by their structures, as well as by their electronic, and magnetic properties. Heterostructures can display bulk and interface properties distinct from their constituents. Novel quantum states can arise from competing orders (Christian Bernhard), while the physics in the bulk can be qualitatively different from the physics at the interface (Philip Willmott). Superconducting interfaces between insulating layers are possible (Jean-Marc Triscone), while exotic one-atom thick crystals such as graphene can be stabilized at
The School participants in front of the beautiful lecture building of the Lyceum Alpinum in Zuoz.

the surfaces (Christopher Mudry). Probing magnetism in heterostructures at the nanometer scale, i.e., with X-rays (Laura Jane Heyderman) or with neutrons (Steve Lee) might improve performances of recording media and might be useful to the new frontier of quantum computing (Andreas Wallraff).

Nanoscience is not limited to the crystalline state of matter. On the one hand, the ductility-to-brittle transition in metallic glasses can be studied with synchrotron X-rays, microtomography, and small angle neutron scattering (Jörg Löffler). On the other hand, these observations can be compared to computational models (Helena Van Swygenhoven and Peter Derlet). Nanoscience is also the study with neutrons and photons of emerging multiple time and length scales induced by interacting classical objects of nanoscale sizes – colloids (Anna Stradner) – that make up, for example, food at the macroscopic scale (Peter Fischer).

Imaging of an object by shining on it a wave requires the measurement of both the scattered intensity and scattering phase shift (Franz Pfeiffer and Marco Stampanoni). However, the scattering phase shifts of current photons and neutrons probing the nanoscale
are partially lost. Coherent X-ray imaging at future X-ray free electron laser sources have been proposed to remedy the phase problem (Franz Pfeiffer). These new generations of photon sources offer a promising future to nanoscience (Helmut Dosch).

A scientific excursion to the world of ferroelectrics and multiferroic materials was given by Michel Kenzelmann who introduced the audience to phase transitions in the three-dimensional thermodynamic limit.

The school brought together 101 participants with 26 different nationalities: 1 master student, 61 Ph.D. students, 9 Postdocs and 30 senior scientists with affiliations to Swiss (58%), Russian (7%), Danish (6%), German (6%), Italian (3%), Indian (3%), Polish (3%) and other (14%) institutions.

We thank the school secretary Mrs Renate Bercher for the perfect organization and support before, during, and after the school. Financial support by the EU I3 Integrated Infrastructure Initiative IA-SFS/Networking is gratefully acknowledged.

The title of the 2009 PSI summer school will be ‘Functional Materials’. The school will be held again in Zuoz from August 1–7, 2009. For the first time it will be accomplished by a practical session at the PSI user facilities. For further information and registration please visit: http://school.web.psi.ch.

“River rafting” has already become a traditional social activity during the Zuoz schools!
Software does matter. Adequate, fast and user friendly software for data acquisition, data reduction and data analysis increases the scientific output of a facility and makes it attractive to users in an increasingly competitive scientific market. Sadly, software for neutron and x-ray scattering is frequently in a sorry state. Thus more than 80 software professionals from neutron and synchrotron facilities around the world met from November 3–5, 2008 in Cronulla, Sydney, Australia in order to discuss how to collaborate on improving this.

Scientific software construction does not only need resources but also a qualified management. The participants identified the following guidelines as crucial for a successful software project:

- Users need to be involved in the software construction process at all stages
- An iterative process with frequent releases and feedback loops
- The project team should ideally consist of scientists and software engineers
- The software has to be designed in an extendable and modular way
- Software is not complete without adequate user and developer documentation.

There is little collaboration on data acquisition software. This is due to the fact that some 50% of the value of any data acquisition system is concentrated in the hardware driver layer. And of course anyone has different hardware. However, there are some patterns, which emerge: All successful systems have a scripting system built in. Instrument control varies from day to day and from experiment to experiment. A strong, reliable and documented scripting component goes a long way to help with this. In the synchrotron community a common architecture is widespread: TANGO or EPICS are used for device access. On top of this there is some scripting server, which executes scripts on behalf of the user or graphical user interfaces. The preferred scripting language is python. Neutron sources should consider to apply this proven pattern for new or upgraded facilities. One particular
contribution (P. Lewis) showed that closed source software and operating systems are not suitable for data acquisition as they lack in interoperability, security, stability, multi user capabilities and transparency. In neutron scattering, there is a trend towards event mode data acquisition. This enables some new science and more flexible experimental techniques.

For data analysis there is a trend towards component-based frameworks with the components glued together through scripting in python. Two such projects, DANSE and mantid, were presented. The challenge is to get the granularity of the components and the data exchange between components right. Opportunities for collaboration in data analysis and data reduction usually come in method specific clusters.

There is a strong trend in the community to give users access to data, training materials, computational resources and even instruments through the WWW or grid technologies. While the Grid is primarily geared towards the storage and processing of large data sets, both the synchrotron and neutron community can benefit from the virtual organization and authentication infrastructure developed for the Grid to allow users access to facility resources in a secure way.

NOBUGS 2008 was unique in that way that the conference was briefly interrupted to watch the Melbourne Cup. This is a horse race, which is so important that the whole of Australia grinds to a halt on that day. The race was won by a horse called ‘Viewed’, ridden by Blake Shinn, just by a thou.

All in all the quality of the presentations and material presented was very good. Some interesting insights were provided by members of the Australian astronomy community who have different but related concerns. Nick Hauser and his team at ANSTO did a great job organizing this conference.
Gumtree Swiss Edition: A New User Interface To SINQ Instrumentation

M. Könnecke
Solid State Research with Neutrons and Muons, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

SINQ neutron instruments are controlled through the SICS instrument control software. SICS is a client server system with a server doing all the hard work and clients implementing the user interface. Up to now SICS was mainly controlled via the command line or through hand written batch files. Some graphical applications exist, which allow to monitor the status of the measurement. Up to now users had to learn Tcl and the SICS command language in order to perform experiments at SINQ. These days may soon be over as a new graphical user interface to SINQ instruments has been developed, which is...

Figure 1: GTSE in Parameter and command editor mode.
called Gumtree Swiss Edition or, GTSE. GTSE has been developed in collaboration with ANSTO, the organization in Australia, which hosts the OPAL research reactor. GTSE is a Java application based on the Eclipse Rich Client Platform. GTSE is organized into perspectives. Perspective allow to swap the layout of the user interface in order to match the task at hand. GTSE currently contains perspectives for:

- A parameter and command editor
- A batch file editor
- An online graphics display
- A terminal window
- The SINQ status
- A quickview of important instrument parameters

One of the traits of the system is that more perspectives can be added when the application evolves. To get an idea how this looks like, see Figure 1, a screen shot of GTSE in the parameter and command editor perspective.

The top row of the interface shows a row of buttons which allows to switch between the various perspectives. To the left we have a tree of instrument parameters. Expand nodes to access more detail as needed. Double clicking on one of the nodes opens an editor in the top right corner of the user interface. In such editors parameter values or command parameters may be changed. In the screen shot, a default editor is shown. But it is possible to integrate custom node specific

![GTSE Interface Screenshot](null)

Figure 2: GTSE batch editor
editors into GTSE in the future. Once the desired changes have been made, they can be forwarded to SICS for execution. The bottom right window shows SICS response to your input.

Figure 2 shows the GTSE batch editor. You choose commands and parameter changes to add to your batch file from the tree at the left, edit them in the middle and commit them to the batch queue displayed on the right. Editing nodes already in the queue is possible, as well as multiplying entries through drag and drop or cut and paste. The row of buttons at the bottom allows to load and save batch files to SICS and execute them.

Figure 3 shows the GTSE graphics display. To the left is a list of all the graphics views the instrument has to offer. On the right is a tab pane where the selected graphics can be viewed, together with some controls to modify the view. Data is automatically updated by SICS during a measurement.

GTSE is now available at 8 SINQ instruments. The development is ongoing and we strive to make GTSE available for all SINQ instrument eventually. GTSE is destined to replace all other SICS client applications in the long run. Please try it out and let SINQ staff know what you like and what you don’t, such that we can improve GTSE to match your needs.

Figure 3: GTSE graphics display for FOCUS
On May 13, 1988, the contract was signed, making Switzerland an official member country of the Institut Laue-Langevin ‘ILL’ in Grenoble, France. Since then a very fruitful partnership with manyfold collaborations has been established.

On the occasion of the 20th anniversary of the Swiss ILL membership the ‘Swiss State Secretariat for Education and Research’ together with the Paul Scherrer Institut (PSI) invited for a dedicated symposium, which was held at PSI on November 28, 2008.

In his welcome address Paul E. Zinsli, from the Swiss State Secretariat, not only mentioned the successful history of the partnership, but also announced that the contract for the next five years has just been signed, continuing access to the ILL for the Swiss user community.

The new director of PSI – Joël F. Mesot – reminded of the many collaborations between Swiss users and the ILL: in particular he mentioned the use of polarised neutrons (Cryopad/ILL and Mupad/SINQ), the fruitful collaborations on hybrid time-of-flight spectrometers (IN4/IN6 concept influenced FOCUS/SINQ) and the PSI development of supermirrors (e.g. SINQ neutron guides), which are now used at ILL routinely, as well.

ILL general director Richard Wagner pointed out that between 1988 and 2007 a total of 939 Swiss proposals were submitted with a success rate of approximately 80%. 682 publications resulted from Swiss experiments at ILL, which makes an average of 45 per year. He also took the opportunity to thank P.E. Zinsli for the strong Swiss support in the ILL steering committee, especially during the difficult shutdown period from 1990–1994.

Albert Furrer – from 1984 to 2004 head of the Laboratory for Neutron Scattering at PSI&ETH Zürich – took the audience on a tour through the early days of Swiss ILL use. With several humorous anecdotes he recalled the phase of preparing and contracting the Swiss membership at the ILL. The ‘projects & tech-
niques division’ director of the ILL Jose-Luiz Martínez Peña also described the existing collaborations between Swiss users and the ILL, but also presented the latest news from the Millennium Programme and the future plans of the ILL. Finally, on behalf of the ILL steering committee, ISIS director Andrew Taylor congratulated both ILL and the Swiss neutron community on their fruitful collaboration over the past 20 years.

Then it was time to let users speak about their science. In five highly interesting presentations, examples from different scientific fields were given: Roger Cowley (University of Oxford, UK) on ‘Relaxor Ferroelectrics’, Peter Schurtenberger (University of Fribourg,
Switzerland) on ‘Soft Matter and Neutrons’, Christian Rüegg (London Centre for Nanotechnology, UK) on ‘Quantum Phase Transitions’, Bertrand Roessli (PSI) on ‘Neutron Polarimetry’ and Klaus Kirch (PSI) about ‘Ultracold Neutrons’; all presented results using instruments at SINQ and at the ILL, and clearly demonstrated the complementarity between both neutron facilities.

The event was completed by a tour of the SINQ facilities followed by a banquet in the PSI restaurant, during which ILL Science Division’s director Andrew Harrison gave a brilliant ‘Afterdinner speech’ that demonstrated the British sense of humour.

Kurt N. Clausen – the organizer of the symposium (left) – with Roger Cowley, University of Oxford.

Thomas Brückel (IFF, Forschungszentrum Jülich), Andrew Taylor (director of ISIS) and Andrew Harrison (ILL associate director), from left.

Albert Furrer (PSI&ETH Zürich), Winfried Petry and Peter Böni (both TU Munich), Peter Allenspach (PSI), from left.

Peter Schurtenberger (University of Fribourg and Adolphe Merkle Institut) during his presentation on ‘Soft Matter and Neutrons’.

Fotos: Markus Fischer, PSI
The Paul Scherrer Institut celebrates its 20th birthday

S. Janssen
Solid State Research with Neutrons and Muons, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

In 1988 the two formerly separate institutions EIR (Eidgenössisches Institut für Reaktorforschung) und SIN (Schweizerisches Institut für Nuklearforschung) merged into the Paul Scherrer Institut, PSI. Since then the institute has undergone major changes. Nowadays the institute’s main task is to develop, build and operate major and complex research facilities like SLS, SINQ or SμS and to provide those to the international user communities. The main focus of in-house research is on solid state physics and materials sciences, particle physics, biology and medical sciences as well as energy and environmental research. PSI has 1300 members of staff and is the largest national research institute in Switzerland.

On the occasion of its 20th anniversary several events were organized during the course of 2008.

INAUGURATION OF ‘ILAB’:

On April 4, 2008 the new experimental laboratory for school children ‘iLab’ (http://ilab.web.psi.ch) was inaugurated. The facility is unique in Switzerland and is dedicated mainly to pupils in the age of 14–15 years. The idea of iLab is to fascinate the school children for natural sciences in general and

![PSI experimental laboratory ‘iLab’](image-url)
physics in particular. Hence ‘iLab’ offers the possibility to actively perform experiments well adjusted to the state of education. At present the experiments cover the physics of waves like propagation in different media, reflection, diffraction or interference. That field was carefully chosen to relate the laboratory experiments in ‘iLab’ to those performed at the large user facilities of PSI.

Doing experiments at ‘iLab’ is accomplished by a tour of the PSI facilities, where the pupils have the chance to get into contact with PSI researchers.

The first months of running ‘iLab’ have already been very promising and the manyfold positive reactions of the visitors confirm the concept very well.

‘CLIMATE SUNDAY’:
Ten days later PSI opened its doors to the public in the framework of the ‘KLIMAsonntag (Climate Sunday)’ on April 14, 2008. 1300 people used the opportunity to get informed about the actual problem of climate change and its consequences. PSI scientists gave various public talks on hot topics related to global warming or CO$_2$ emissions. Lifely discussions and many questions from the audience demonstrated the broad public interest in that matter. The visitors also used the opportunity to visit ‘iLab’ and the ‘psi forum’.

Even the PSI restaurant offered ecologically beneficial food: The guests were informed how much CO$_2$ is used to prepare the various dishes, which were offered. Nevertheless the ‘low emission’ vegetarian food (0.3 kg CO$_2$) was clearly less demanded than the legendary ‘Züri Geschnetzeltes’ (3 kg CO$_2$) …

PSI ROADSHOW ‘AM PULS DER FORSCHUNG’:
2008 was the first ever year that PSI went ‘on tour’. The idea was to give a series of talks on science undertaken at the institute for the general audience in nearby towns: Three towns, three weeks, three talks each evening was the motto. Each evening – from Wednesday to Sunday a special topic out of the PSI research portfolio was chosen such as ‘people and health’, ‘small particles for novel applications’, ‘Swiss Light Source SLS’, ‘climate, energy and environment’ and ‘visions of cutting edge science’.

T. Strässle during his presentation ‘im Zelt’.


For every topic three different popularized talks were given by PSI scientists. After each talk a lot of time was available for questions and discussions, which was intensively used by the audience. SINQ and science with neutrons was well represented in the program. The second evening of the series was completely dedicated to the physics of accelerators, neutron imaging and neutron scattering.

The towns visited were Baden, followed by Aarau and Waldshut (Germany). A total of 45 public talks were given. Additionally the audience could watch a film on PSI’s 20 years history and on its future project, the PSI-XFEL.

Approximately 3000 people came to listen to the talks, confirming again that science can be transported very attractively to the public.

OFFICIAL CEREMONIAL ACT:
More than 200 invited guests participated in the official ceremonial act on the occasion of the 20th anniversary on August 25. Representatives from science, industry and politics came to congratulate, among them Jasmin Staiblin (ABB), Paul Herrling (Novartis, vice chairman of ETH-board), Dieter Imboden (Swiss National Science Foundation) and Massimo Altarelli (DESY). The guest of honour was Pascal Couchepin, the acting Swiss Federal President.

In his talk Massimo Altarelli covered the new big future project of PSI: the X-Ray Free Electron Laser ‘PSI-XFEL’. He pointed out that PSI-XFEL will enable experiments, which are far from being feasible at the moment and might lead to novel important applications e.g. in the fields of medical and environmental sciences or electronics.

Martin Jermann and his successor as director of PSI, Joël Mesot, reminded on the foundation and the first years of PSI but they also made clear that PSI looks into a bright future: ‘PSI is a good example, how a research facility keeps up-to-date and ensures its future by the ability to adapt and to change’.

PSI VISITOR DAYS:
The biggest event was still to come: On October 25 and 26 PSI opened its doors completely and organized two public visitor days. More than 500 PSI staff members were involved in the organization and the various presentations. The feedback was extraordinary: Totally 12,000 visitors took the opportunity to get informed about the activities of the Paul Scherrer Institut and made the event a huge success.

At 20 different stations all over the campus the visitors received information and could discuss with the PSI scientists, engineers and technicians about manyfold topics such as future energy resources, pollution, cancer
treatment with protons, accelerator facilities, neutrons and X-rays, protein structures, solar technologies, detectors, precision welding, vacuum technology etc. Even the PSI apprentices presented their work and the various options for job education at PSI. One highlight was the electronic ‘iLukas’, where the ‘strong men’ could compete with each other.

Six out of those 20 stations were presented as large multimedia shows, where every 30 minutes a popular talk was given making use of trailers, movies, live experiments and other demonstrations. Within the SINQ halls two of those show stations were located: The first one explained the options and applications of neutron imaging and tomography for works of art and the second one the research on novel materials like GMR hard disks or high capacity batteries with neutron scattering techniques.

A comedy physics stage show ‘Die Physikanten’ and the various delicious catering options offered by the team of the PSI restaurant completed these two successful days. The positive feedback also encourages the organizers to continue such kind of events since they give the unique opportunity to inform many people in a popular way about the research activities and to receive understanding, what use PSI makes of the public funding it receives.

10 YEARS OF PSI FORUM
On November 11, 1998 the PSI visitor centre ‘psi forum’ (http://www.psiforum.ch) was inaugurated. Each year several thousand visitors come to PSI and they usually all start their visit in the ‘forum’ before they go on a dedicated tour through parts of the institute and the large facilities. The anniversary of both PSI and the ‘forum’ was used to completely renovate and renew the exhibitions of the visitor centre.

Visitors are now guided through various themes like energy and environment, which have a direct relation to the PSI research topics. One highlight of the new exhibition is the ‘future globe’, which informs the visitors interactively about the hot topic of climate change.

In total almost 17,000 people participated in the various events during the jubilee year of PSI. Further 12,000 people visit PSI each year during the regular – non-scientific – visits (school classes, students, clubs etc). Another 1,000 school children visited the ‘iLab’ since its start in April such that in total approximately 30,000 laypersons were attracted to the Paul Scherrer Institut in 2008, which demonstrates impressively the impact and the need for public activities of this kind.
Announcements

SGN/SSDN Members
Presently the SGN has 197 members. Online registration for new members of our society is available from the SGN website: http://sgn.web.psi.ch

SGN/SSDN Annual Member Fee
The SGN/SSDN members are kindly asked to pay their annual member fees. The fee is still CHF 10.– and can be paid either by bank transfer or in cash during your next visit at PSI. The bank account of the society is accessible for both Swiss national and international bank transfers. The coordinates are as follows: Postfinance: 50-70723-6 (BIC: POFICHBE), IBAN: CH39 0900 0000 5007 0723 6.

Joint Users’ Meeting at PSI: JUM@P ‘09
On October 12-13, 2009 the first joint users’ meeting of the PSI user facilities will be organized. Please note the date within your agendas already now! The idea is to arrange topical workshops, which will bring together users from all three (X, n, μ) communities of the PSI facilities. For that purpose PSI will publish an online questionnaire, where the users can select their preference for workshop topics. The user communities will be informed electronically about the questionnaire as soon as it is online.

SINQ Call for Proposals
The next deadline for the submission of beam time requests for the Swiss spallation neutron source ‘SINQ’ (http://sinq.web.psi.ch) will be:

May 15, 2009

SINQ long term proposals
First for a test period of two cycles (I/09 and II/09) the submission of new long term proposals will be disabled. Instead we ask our users to submit short term proposals followed by continuation requests.

Registration of publications
Please remember to register all publications either based on data taken at SINQ, SLS, SμS or having a PSI co-author to the Digital User Office: https://duo.psi.ch. Please follow the link ‘Publications’ from your DUO main menu.

Open Positions at ILL
To check the open positions at ILL please have a look at the following ILL-Webpage: http://www.ill.eu/careers
The 2009 Walter Hälg Prize
of the
European Neutron Scattering Association

The Walter Hälg Prize
The prize was made available to the European Neutron Scattering Association (ENSA) by a donation from Professor Walter Hälg who is the founder of neutron scattering in Switzerland. The Prize is awarded biennially to a European scientist for outstanding, coherent work in neutron scattering with long-term impact on scientific and/or technical neutron scattering applications. The previous Prize winners were F. Mezei (1999), J. Brown (2001), R. Cowley (2003), A. Furrer and H.U. Güdel (2005), J. Penfold (2007). The sixth award of the Prize (10’000 CHF) is to be made at a special ceremony and session at the International Conference on Neutron Scattering (ICNS 2009), 3-7 May 2009, Knoxville, USA. Information on previous laureates is available on the ENSA web-site (http://neutron.neutron-eu.net/n-ensa).

Selection Committee
Nominations for the prize will be considered by a Selection Committee, which consists of authorities representing the major scientific disciplines. It includes acknowledged experts both in neutron scattering and from outside the neutron scattering community. Membership in the Selection Committee is obtained by invitation extended by the ENSA Committee.

Call for Nominations
Nominations for the 2009 Walter Hälg Prize of the European Neutron Scattering Association (ENSA) may be submitted by European scientists as individuals or on behalf of a Division, Section or Group. To establish a high standard it is necessary that the Committee receive proposals, which represent the breadth and strength of European neutron scattering. Nominations should include the motivation for the award, a brief curriculum vitae of the nominee and a short list of major publications. Letters of support from authorities in the field, which outline the importance of the work would also be helpful. Nominations for the Prize will be treated in confidence and although they will be acknowledged there will be no further communication. Previous nominations have to be up-dated and resubmitted.

Deadline
Nominations should be sent before February 28, 2009 to the Chairman of the Selection Committee, preferably by electronic mail in pdf format:

Dr. Peter Allenspach
ENSA Chairman
Paul Scherrer Institute
CH-5232 Villigen PSI, Switzerland
Phone: +41 56 310 2527
Fax: +41 56 310 2939
E-mail: peter.allenspach@psi.ch
Conferences and Workshops 2009

January

3rd MaNEP Winter School: Exploring New Phases of Electronic Matter
January 11–16, 2009, Saas Fee, Switzerland

USPAS: The US Particle Accelerator School
January 12–23, 2009, Nashville, Tennessee, USA

High Spatial Resolution Neutron Reflection Methods for the Study of Gold Supported Biomembranes

SOLEIL Users’ Meeting 2009
January 21–22, 2009, Gif-sur-Yvette, France

From Micro to Macro: Microstructural and texture analysis from diffraction data
January 26–30, 2009, Milano, Italy

3rd European XFEL Users’ Meeting
January 28–29, 2009, Hamburg, Germany

TMS Symposium on Emerging Applications of Neutron Scattering in Materials Science and Engineering
February 15–19, 2009, San Francisco, USA

Neutrons and X-rays meet biology
February 25–27, 2009, Berlin, Germany

March

NMI3 General Meeting 2009
March 30–31, 2009, Paul Scherrer Institut, Villigen, Switzerland

May

ICNS 2009: International Conference on Neutron Scattering
May 3–7, 2009, Knoxville, USA

ICCS 2009: Ninth International Conference on Computational Science
May 25–27, 2009, Baton Rouge, USA
June

ICC 14: XIV International Clay Conference
*June 14–20, 2009, Castellaneta, Italy*

ICNX 2009: International Conference on Neutron and X-Ray Scattering
*June 29 – July 1, 2009, Kuala Lumpur, Malaysia*

July

ICM 2009: 18th International Conference on Magnetism
*July 26–31, 2009, Karlsruhe, Germany*

International Conference on ‘Energy materials research using neutron and synchrotron radiation’
*July 27–30, 2009, Berlin, Germany*

August

8th PSI Summer School on Condensed Matter Research: Functional Materials
*August 1–7, 2009, Zuoz, Switzerland*

Polarized Neutrons and Synchrotron X-rays for Magnetism 2009
*August 3–5, 2009, Bonn, Germany*

ECM 25: 25th European Crystallographic Meeting
*August 16–21, 2009, Istanbul, Turkey*

Diffusion Fundamentals III
*August 23–26, 2009, Athens, Greece*

September

SAS-2009: XIV International Conference on Small-Angle Scattering
*September 13–18, 2009, Rutherford Appleton Laboratory, Oxford, United Kingdom*

October

SKIN2009: Studying Kinetics with neutrons (SANS and Reflectometry)
*October 5–7, 2009, Grenoble, France*

JUM@P 09: Joint Users’ Meeting at PSI
*October 12–13, 2009, Paul Scherrer Institut, Villigen, Switzerland*

(an updated list with online links can be found here: http://sinq.web.psi.ch/sinq/links.html)