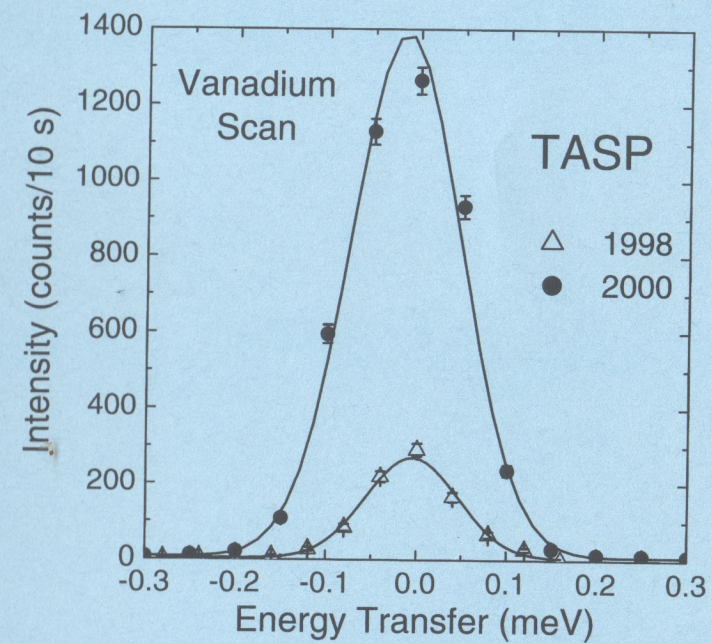


SWISS NEUTRON NEWS



Schweizerische Gesellschaft für Neutronenstreuung
Société Suisse pour la Diffusion des Neutrons

Cover illustration:

Within the last two years the neutron flux at TASP has increased rather dramatically. The main reasons are: Installation of the lead target, replacement of target E, increase in proton current, and modifications at the analyser.

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La page du président de la SSDN

Dear members,

The awareness for neutron science is high but does not always reflect a correct image of this discipline. For quite a few scientists and persons carrying science responsibilities it is considered merely as a technique, and neutron sciences at various institutions. Both attitudes are harmful for our society.

- ### Inhaltsverzeichnis
- | | Seite |
|------------------------------------------------------------------------------------------|-------|
| ● La page du président de la SSDN
<i>K. Yvon</i> | 3 |
| ● 8 th Summer School on Neutron Scattering in Zuzoz | 4 |
| ● Annual Meeting 2000 of the SGK/SSCr
and SGN/SSDN at PSI | 5 |
| ● Personelles | 8 |
| ● Advertisements in Swiss Neutron News | 8 |
| ● Neue Mitglieder
<i>P. Böni</i> | 10 |
| ● Important Dates | 11 |
| ● Mitgliederbeiträge, Membership Fees | 12 |
| ● Wissenschaftlicher Beitrag:
The Barocaloric Effect
<i>Thierry Stässle</i> | 13 |
| ● Anmeldeformular für Beitritt zur Schweizerischen
Gesellschaft für Neutronenstreuung | 19 |
| ● Proposal Form SINQ | 21 |
| ● Job vacancy at ILL | 23 |

November 2000

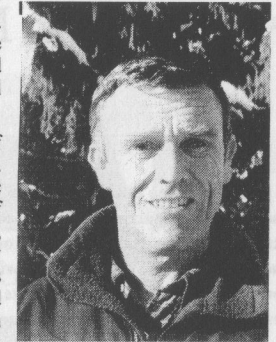
Klaus Yvon

La page du président de la SSDN

Dear members,

The awareness for neutron scattering in Switzerland is generally high but does not always reflect a correct image of this discipline. For quite a few scientists and persons carrying science responsibilities it is considered merely as a technique, and neutron sources as service institutions. Both attitudes are harmful for our scientific future and should be revised.

Neutron scattering addresses an extremely vast inventory of fundamental questions relating to the solid state of matter. Consequently, it caters to a large and diversified scientific community that consists not only of physicists, but also of chemists, biologists, crystallographers, materials scientists, engineers, etc. It needs big installations that have to be constantly upgraded in order to meet new scientific demands such as investigating more complex systems and subtle structural and dynamical features. On the other hand, the advances in methodology in this field often drive new science (for example: polarization analysis for magnetism). In view of the fact that neutron scattering is so intimately related with solving questions of fundamental interest it can hardly be considered as a technique. As a corollary, advances in this discipline cannot be achieved as a service but only on the basis of a close collaboration between scientists from within and outside the neutron scattering centers.



The situation is similar to, although somewhat different from that in particle physics where new (and very expensive) accelerators are built and instruments developed to answer specific questions of fundamental interest for a relatively small scientific community. No one would consider these experiments purely as techniques and the CERN as a service institution.

Fortunately, the current image of our national neutron source SINQ does not cause major concern because most responsible scientists recognize it both as a service institution and a place of genuine research and important developments. However, as time goes on and SINQ reaches maturity this could easily change in the sense that this source is considered exclusively under the angle of a service institution. Indications exist that this starts to happen with other sources in Europe such as ILL. If this sort of attitude prevails it would be detrimental for our scientific life and that of our society. Clearly, sources such as ILL and SINQ should never be, or considered to be, or presented as service institutions only, but as scientific partners that do also their own research, in particular in the field of advanced methodology from which we will ultimately all benefit.

I encourage all those who share these views to constantly recall them at appropriate occasions to fellow scientists, in particular those not belonging to the neutron scattering community, and to persons carrying science responsibilities. It would also seem to be appropriate to mention neutron scattering experiments explicitly in funding requests. This would reinforce the image of neutron scattering as a discipline that is in constant development and meets the expectations of many physicists, chemists, biologists, crystallographers, materials scientists, engineers, etc. Of course, much of what is said above also applies to some aspects of X-ray scattering and could be the subject of discussions at our forthcoming common meeting with the Swiss Crystallographic Society.

Best wishes to all of you

Brisbane, 25 May 2000

Klaus Yvon



NEUTRON SCATTERING IN NOVEL MATERIALS

8th PSI Summer School on Neutron Scattering
5-11 August 2000, Lyceum Alpinum, Zuz, Switzerland

The purpose of the Summer School is to give participants an introduction to the basic principles of neutron scattering and its application to the study of novel materials. The lectures will cover both theoretical and experimental aspects, with particular emphasis on the utilisation of the instrumentation set up at the spallation neutron source SINQ at PSI. No previous knowledge of the subject is required, but an honours degree in natural sciences (equivalent to the diploma) is essential. The programme of the School will include exercises to deepen the accumulated knowledge as well as poster and discussion sessions in which the participants can present their own results in the field of neutron scattering from novel materials.

Organisation of the School:

W.E. Fischer (School Chairman), A. Furrer (Programme Chairman), R. Bercher (Secretary)

Programme Committee:

P. Allenspach^a, G. Bauer^a, A. Bill^a, P. Böni^a,
H.B. Braun^a, D. Clemens^a, B. Delley^a, B. Dorner^c,
P. Fischer^b, W.E. Fischer^a, A. Furrer^b, S. Janssen^a,
J. Mesot^a, R. Morf^a, J. Schefer^a, W. Wagner^a
(^a Villigen, ^b Zurich & Villigen, ^c Grenoble)

List of topics and invited lecturers:

Introduction to Neutron Scattering:
J. Schefer (Villigen)

Materials Science:
M. Grosse (Villigen), A.W. Hewat (Grenoble),
E. Lehmann (Villigen), R. Rupp (Vienna),
B. Schillinger (Munich), B. Schönfeld (Zürich)

Biology and Soft Condensed Matter:
A. Arbe (San Sebastian), D. Middendorf (Oxford),
M. Monkenbusch (Jülich),
W. Pyckhout-Hintzen (Jülich),
O. Zimmer (Mainz)

Surfaces and Interfaces:
D. Clemens (Villigen), W. Wagner (Villigen)

Rare-Earth Compounds:
L. Keller (Villigen), A. Mirmelstein (Ekaterinburg),
R. Radwanski (Cracow)

Magnetic Excitations:
N. Cavadini (Villigen), B. Roessli (Villigen)

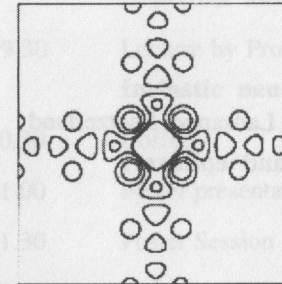
Superconductivity and Superfluidity:
M. Adams (Villigen), Ph. Bourges (Saclay),
S. Lee (St Andrews), J. Mesot (Villigen)

Residential accommodation will be available at the Lyceum Alpinum in Zuz (costs: 600 Swiss Francs, including full board, banquet, and Proceedings). The number of participants will be limited to 100. The language of the School is English. Closing date for applying is 30 June 2000. For further information and application forms, contact Renate Bercher, Paul Scherrer Institut, CH-5232 Villigen PSI, Tel.: +41-56-310 34 02, Fax: +41-56-310 31 31, E-mail: renate.bercher@psi.ch.

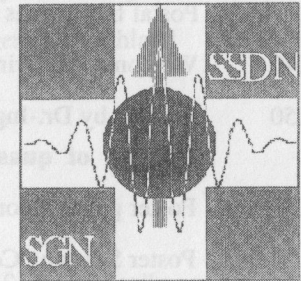
Free neutron beam time at SINQ
will be awarded to
the best young scientists' presentations!

P-880-05-04-5232-0491

Swiss Crystallographic Society Swiss Society for Neutron Scattering



joint



Annual Meeting

Thursday and Friday, October 5 /6, 2000

at Paul Scherrer Institute, CH-5232 Villigen PSI

General Theme

Materials and their Investigation
with Neutrons and Synchrotron Radiation

Programme Of the Annual Meeting 2000

Thursday, October 5

- 9.27 Postal bus arrives from Brugg
- 9.40 Welcome (H. Grimmer)
- 9.50 Lecture by Dr.-Ing. H.J. Scheel, EPFL, Lausanne, Switzerland
Growth of quasi-perfect crystals and epilayers
- 10.50 Poster presentations SGK/SSCr
- 11.20 Poster Session / Coffee
- 12.00 *Annual Meeting of SGN/SSDN, the Swiss Neutron Scattering Society*
- 12.45 Lunch
- 14.00 Visit of the Spallation Neutron Source SINQ
- 15.00 Coffee
- 15.30 Lecture by Dr. C.C. Wilson, ISIS, Oxford, UK
Importance of crystal quality and size for neutron and x-ray diffraction studies
- 16.30 Lecture by Dr. Cusack, EMBL, Grenoble, France
Exploiting third generation synchrotron sources for crystallographic studies of protein RNA complexes
- 17.30 Break
- 17.45 *User Meeting SNBL*
- 18.30 Apéro Oase
- 19.00 Dinner Oase
- 20.44 Postal bus leaves for Brugg

Friday, October 6

- 8.15 Postal bus arrives from Brugg
- 8.30 Lecture by Dr. C. Vettier, ILL, Grenoble, France
Neutrons and synchrotron x-rays for magnetism
- 9.30 Lecture by Prof. G. Eckold, Göttingen, Deutschland
Inelastic neutron scattering
- 10.30 Coffee
- 11.00 Poster presentations SGN / SSDN
- 11.30 Poster Session
- 12.00 *Annual Meeting of SKG / SSCr, the Swiss Crystallographic Society*
- 12.45 Lunch
- 14.00 Visit of the Swiss Light Source SLS
- 15.00 Coffee
- 15.30 Lecture by Dr. P. Radaelli, ISIS, Oxford, UK
Neutron and x-ray synchrotron powder diffraction: the way ahead
- 16.30 Lecture by Prof. Kostorz, ETHZ, Zurich, Switzerland
Local order and decomposition in alloys – r-ray and neutron scattering studies
- 17.30 Closing remarks (K. Yvon)
- 17.51 Postal bus leaves for Brugg

Personelles

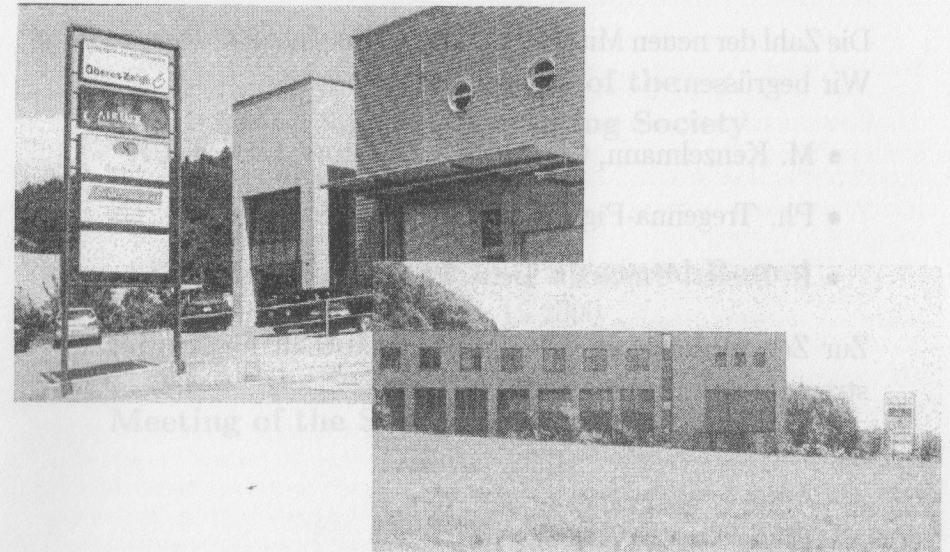
P. Böni

Wie Sie vielleicht wissen, habe ich am 31. Mai 2000 meine Arbeit am Labor für Neutronenstreuung ETH & PSI beendet und am 1. Juni 2000 eine Stelle am Physik-Department an der Technischen Universität München in Garching angetreten. Aus diesem Grund wird das Swiss Neutron News Nr. 17 die letzte Ausgabe sein, die ich editieren durfte. Ich hoffe, das Sie viel Spass an den bisherigen Ausgaben des Swiss Neutron News hatten und wünsche meinem Nachfolger viel Vergnügen und Erfolg an dieser Arbeit.

Advertisements in Swiss Neutron News

We should like to remind you that since the beginning of the publishing activities of the Swiss Neutron Scattering Association there is the possibility to advertise products in Swiss Neutron News. The price per page (in black and white) is only CHF 200.-.

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www.swissneutronics.ch

Neue Mitglieder

P. Böni

Die Zahl der neuen Mitglieder hat jetzt die Zahl 200 überschritten.
Wir begrüßen:

- M. Kenzelmann, Clarendon Laboratory, Oxford, UK
- Ph. Tregenna-Piggott, Universität Bern, Bern
- R. Basler, Universität Bern, Bern

Zur Zeit zählt die schweizerische Gesellschaft für Neutronenstreuung 201 Mitglieder.

The SGN is on the Web!

our address:

<http://www.psi.ch/sgn>

Important Dates in 2000/01

**General Assembly of the
Swiss Neutron Scattering Society**

October 5 2000

Deadline for Next SINQ Proposal Round

November 15 2000

Meeting of the Scientific Committee for SINQ

January 2001

Mitgliederbeitrag 2000

Wir bitten alle Mitglieder der Schweizerischen Gesellschaft für Neutronenstreuung (ausgenommen die Ehrenmitglieder), den Jahresbeitrag 2000 mit anliegendem Einzahlungsschein auf unser Postcheckkonto einzuzahlen. Der Beitrag beträgt immer noch nur die Wenigkeit von CHF 10.–.

Wir bitten unsere ausländischen Kollegen, Ihren Beitrag bei Gelegenheit in bar zu bezahlen (z.B. während einer Konferenz), da die Gebühren für Überweisungen oft höher sind als der Mitgliederbeitrag selbst.

Membership Fees 2000

We ask our foreign colleagues to pay the membership fee for 2000 in cash at a reasonable occasion (for example during a conference) because the fees for forwarding the money to our account is usually higher than our modest fee of CHF 10.–.

The Barocaloric Effect

Thierry Strässle

Laboratory for Neutron Scattering ETH and PSI
CH-5232 Villigen PSI

1 Introduction

Ever since Warburg (1881) first observed the heat evolution in iron upon the application of a magnetic field, the so-called magnetocaloric effect (MCE) attracted science. The effect is a consequence of the variation of the material's total entropy by the magnetic field. It was first Debye (1926) and Giauque (1927) who proposed the principle of adiabatic cooling, i.e. cooling by the MCE. In a first stage, a magnetic field is applied isothermally (the system is in contact with a heat sink), thus reducing the system's magnetic entropy. In a second stage, the magnetic field is removed adiabatically (the system is isolated from the heat sink). In order to keep its entropy unchanged the system is forced to lower its temperature.

Progress in the theoretical as well as the experimental characterization of the magnetothermal properties of materials has renewed the interest in the investigation of the MCE for two reasons: first, the MCE can yield information on magnetic phase transitions not obtainable by other techniques, second, its potential for the implementation of magnetic cooling machines (magnetic refrigerators) [1]. These days, magnetic refrigeration proved to be one of the most efficient cooling techniques in a wide range of temperatures. For the time before the rise of ^3He dilution cryostats, the MCE represented the only technique allowing temperatures below 4.2 K down to the milli Kelvin range (Giauque(1927)). Nowadays, cooling at room temperature and even higher has been demonstrated for a wide class of rare-earth compounds [2, 3]. Up to now, all magnetic refrigerators suffer the drawback of needing large magnetic fields of a few Tesla in order to achieve cooling effects in the Kelvin range.

Despite the fact that adiabatic cooling has to be associated by no means with an entropy change induced by an external magnetic field, its implementation by variation of a different external *thermodynamic field* has hardly been investigated. Müller and Furrer proposed to implement adiabatic cooling by the application of pressure in the vicinity of a pressure induced structural phase transition in a rare-earth compound [4]. A pressure induced structural phase transition will change the point symmetry of the rare-earth ion. In general this will result in a different splitting of its $2J + 1$ -fold degenerate ground-state J-multiplet by the crystalline electric field (CEF). In rare-earth compounds the CEF splitting of typically a few Kelvin governs the system's thermodynamic properties, and thus also its magnetic entropy

$$S_{mag} = -R \sum_i n_i \ln n_i, \quad \text{with } n_i = \frac{1}{Z} e^{-E_i/k_B T} \quad (1)$$

where the E_i 's are for the CEF energy levels, Z the partition function and k_B and R the Boltzmann and the molar gas constant, respectively. Thus external pressure p may

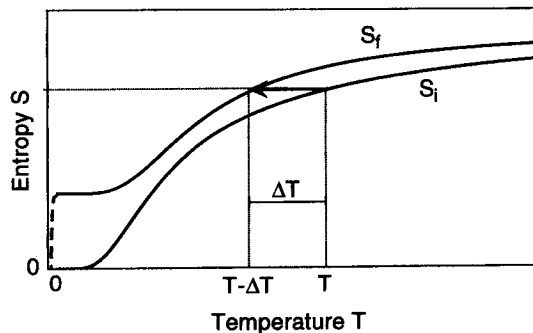


Figure 1: Principle of adiabatic cooling: due to an external influence the system's entropy gets changed ($S_i \rightarrow S_f$).

well serve to change the system's magnetic entropy in the very same way as an external magnetic field does in the MCE. In analogy to the magnetocaloric effect, the associated effect has been given the name *barocaloric effect* (BCE).

Let us give an example for the principle of adiabatic cooling in general and more specific for the BCE (Figure 1). We assume a system being initially in a state i of large CEF splitting and low degeneracy of its lowest CEF levels ($p = 0$ or $p > 0$). Therefore its magnetic entropy will increase only slowly with temperature, Eq. (1). The application or removal of external pressure can bring the system via a pressure-induced structural phase transition into a state f of small CEF splitting and high degeneracy of its CEF energy levels ($p > 0$ or $p = 0$). In state f the system happens to have a higher entropy than in state i at the same temperature ($S_f(T) > S_i(T)$). Thus if the transition $i \rightarrow f$ is performed adiabatically the system must cool down by ΔT in order to fulfill

$$S_f(T - \Delta T) = S_i(T) \quad (2)$$

Even though no magnetic ordering in this system is present, ΔT is solely a consequence of the variation in the *magnetic* entropy! Note however, that in Eq. (2) the total entropy of the system ($S = S_e + S_{latt} + S_{mag}$) has to be considered [5].

Significant changes in the magnetic entropy can also be realized by a pressure-induced magnetic phase transition [5]. Many rare-earth compounds show pronounced pressure-dependencies in their ordering temperatures and thus may be suitable candidates for the BCE. In the ordered state a splitting of the CEF levels due to the internal magnetic field occurs (Zeeman effect). Thus cooling can be realized by a transition from the ordered state i (which shows low entropy) into the disordered state f in the very same way as in the structurally driven case ¹.

Whether the BCE is driven structurally or magnetically, detailed knowledge about the microscopic properties of the material is indispensable for the explanation of the BCE and in the search for best-suited BCE materials. Elastic and inelastic neutron scattering

¹In this sense the magnetically driven BCE can also be considered as an *internal MCE* using the system's molecular field instead of an external magnetic field.

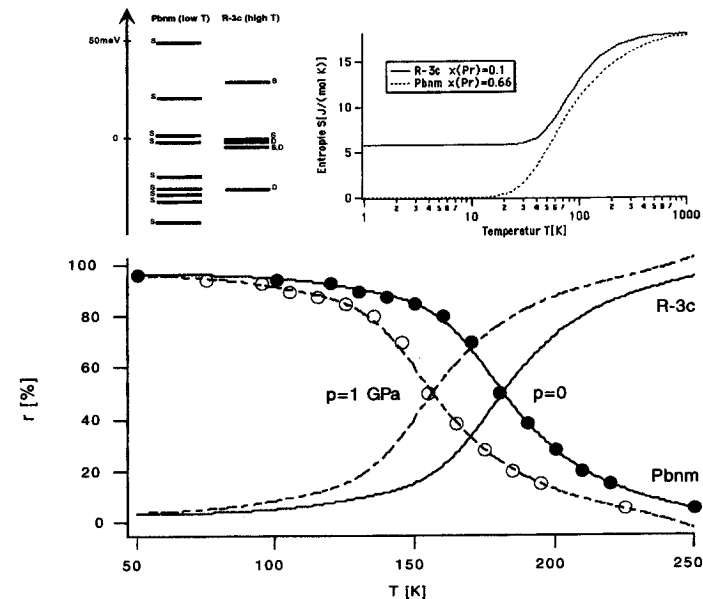


Figure 2: *upper left*: CEF scheme of the two phases in $\text{Pr}_x\text{La}_{1-x}\text{NiO}_3$ (S: singlet, D: doublet). *upper right*: magnetic entropies of the two phases. *lower part*: volume fractions of $\text{Pr}_{0.5}\text{La}_{0.5}\text{NiO}_3$ at $p = 0$ and $p = 1$ GPa [4].

together with macroscopic measurements of the specific heat and the magnetization proved to be the experimental techniques of choice in order to study the BCE.

2 Examples for Materials showing a BCE

Below two examples are given demonstrating the structurally and the magnetically driven BCE.

The perovskite $\text{Pr}_x\text{La}_{1-x}\text{NiO}_3$ crystallizes in an orthorhombic low temperature phase (Pbnm) with a singlet CEF ground state and a rhombohedral high temperature phase ($R\bar{3}c$) with a doublet CEF ground state, respectively. The phase transition temperature T_{SPT} depends on both the Pr concentration and the external hydrostatic pressure ($dT_{SPT}/dp \approx -50\text{K/GPa}$). The lower part of Figure 2 shows the volume fractions of $\text{Pr}_{0.5}\text{La}_{0.5}\text{NiO}_3$ as a function of temperature for $p = 0$ and $p = 1$ GPa determined by neutron diffraction [6]. The phase transition is very broad (about 80K). The upper part of Figure 2 shows the CEF energy levels and the entropy curves for the two pure phases. At temperatures close to T_{SPT} a pressure-induced structural phase transition can be realized from the low temperature phase i (Pbnm) to the high temperature phase f ($R\bar{3}c$). If done adiabatically cooling occurs as the high temperature phase shows a larger entropy ($S_f(T) > S_i(T)$). Cooling rates of -0.1 K per 0.5 GPa could be observed for $x = 0.66$ at a temperature of $T \approx 350$ K [4]. The effect is expected to be more pronounced at lower temperatures, where the phononic contribution to the entropy is smaller. Unfortunately only polycrystalline samples of $\text{Pr}_x\text{La}_{1-x}\text{NiO}_3$ are available. At low temperatures the

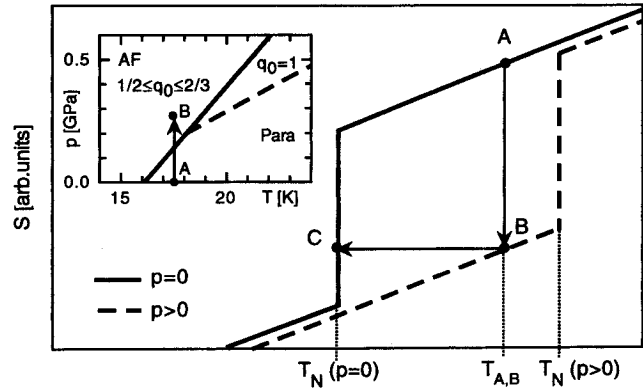


Figure 3: Schematic plot of the temperature and pressure dependence of the entropy in CeSb. Inset: schematic magnetic phase diagram of CeSb (after [7]).

friction effect between single grains becomes very large and overcompensates the cooling by the BCE. Thus at low temperatures applying uniaxial pressure on single crystal samples has shown to be more promising than hydrostatic pressure on polycrystalline samples.

The magnetically driven BCE could be demonstrated in the rare-earth monopnictide CeSb at temperatures of about 20 K. CeSb crystallizes in the NaCl structure. It shows antiferromagnetic order below 16.1 K in various phases ($1/2 \leq q_0 \leq 2/3$). The sixfold degenerate ground state J-multiplet is CEF split into a ground state doublet and an excited quartet at ≈ 40 K. In the ordered state the ground state doublet is Zeeman split by the molecular field into two singlets resulting in a decreased entropy. Uniaxial pressure along the [100] axis increases the Néel temperature by $dT_N/dp \approx 8$ K/GPa [7]. Therefore at temperatures close above $T_N(p=0)$ uniaxial pressure can drive the system from the paramagnetic state into the ordered state. If this is done isothermally the system is giving heat to the heat sink while lowering its entropy (Figure 3, A \rightarrow B). Subsequent fast release of the pressure will bring the system back into the paramagnetic state, while this step is done adiabatically (i.e. fast) the system is forced to lower its temperature (Figure 3, B \rightarrow C).

The BCE has been measured on a cubic single crystal of 3 mm side length [8, 9]. The temperature was tracked by a thermocouple glued on the crystal's surface, while uniaxial pressure was changed *in situ* by a dedicated uniaxial pressure device mounted in a standard cryostat. Figure 4 shows the BCE as a function of temperature for $p = 0.26$ GPa. A maximal cooling of -2 K for a pressure release of 0.5 GPa could be observed. The triangular shape of the $BCE(T)$ curve nicely reflects the $p-T$ phase diagram of CeSb. The BCE can be modelled for CeSb on the basis of a CEF calculation in the molecular field approximation

$$\hat{H} = B_4^0(\hat{O}_4^0 + 5\hat{O}_4^4) - J_0\bar{J}_z\hat{J}_z - K_0\bar{O}_2^0\hat{O}_2^0 \quad (3)$$

where the first two terms denote the CEF part and the last two terms the dipolar and quadrupolar field parts of the Hamiltonian, respectively.

Figure 5 shows the calculated entropies for $p = 0$ and $p > 0$ together with the expected BCE. Qualitatively the calculations describe the observed BCE fairly well. However the

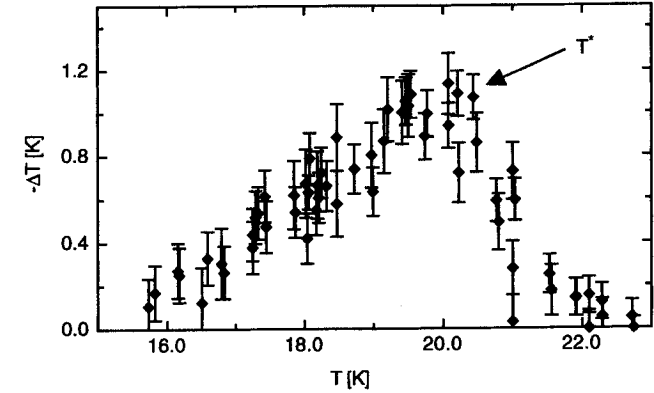


Figure 4: Temperature dependence of the measured BCE upon the release of $p = 0.26$ GPa.

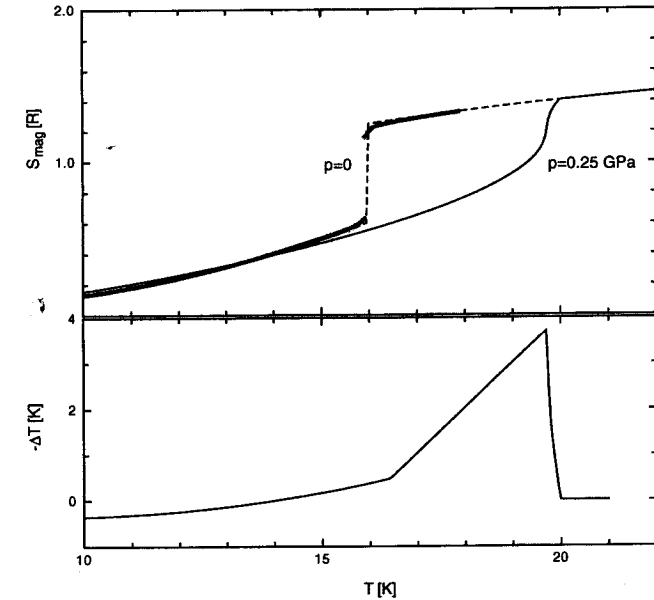


Figure 5: BCE based on a molecular field calculation. upper part: experimental entropy for $p = 0$ (from c_p) [gray] and calculated entropies for $p = 0$ [dashed black] and $p = 0.25$ GPa [solid black] lower part: expected cooling $-\Delta T$.

observed BCE happens to be almost two times smaller than expected, which can be ascribed to heat leakage through the sample support and to the inertia of the thermocouple. Both effects are likely to be better suppressed in future experiments.

3 Summary and Outlook

A novel cooling technique has been introduced based on a pressure-induced variation of the magnetic entropy in rare-earth compounds. The barocaloric effect is an adiabatic cooling technique similar to the well-known magnetocaloric effect, however without the need of large magnetic fields. The BCE can be induced by a structural or magnetic phase transition. The above mentioned two example compounds rather serve as a demonstration of this new effect. Mechanisms combining both the structurally and magnetically driven BCE, the BCE in localized+itinerant magnetic compounds and systems with quantum critical points are promising candidates for the BCE to be further investigated. It is very likely that other suitable compounds can be found, showing a BCE effect of similar or even larger size than the MCE materials do these days.

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Email: SINQ@psi.ch, Web: www.psi.ch/sinq**EXPERIMENT REQUEST***Proposal number* Short term proposal (next allocation period) Long term proposal (2 years)**Proposer** (to whom correspondence will be addressed)Name and first name:
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Email:**Co-proposer:**
Name:

Address: (if different from above)

Phone/Fax/Email:

Sample description

Substance and formula:

Mass:

Size:

 Polycrystalline Single crystal Multilayer Liquid Gas

Sample Container: Space group: Unit cell: a= b= c=

Hazard

Is there any danger associated with the sample or sample environment?

 No Yes Uncertain If yes or uncertain, please give details of the risks associated:**Experimental details**

Instrument	Days	Sample cond.: Temp., Pressure, Magn. field	Exp. cond.: E, ΔE , λ , $\Delta\lambda$, Q, ΔQ

Requested dates:**Unacceptable dates:**

Title of Experiment:

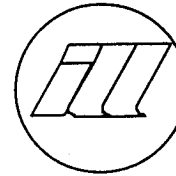
Research funded by:

Scientific background/Aim of experiment: *(Please restrict to the space given within this box!)*

I certify that the above details are complete and correct.

Date:

Signature of proposer:



VACANCY

RESEARCH SCIENTIST

The Institut Laue-Langevin (ILL) is an international research institute funded by France, Germany and the United Kingdom. Agreements on scientific collaboration have also been signed with Austria, Italy, Spain, Switzerland, the Czech Republic and Russia. The Institute operates the most powerful source of neutrons in the world, a 58 MW reactor, which was completely refurbished in 1995. The reactor forms the basis for a programme of research covering a wide variety of fields, supplying neutrons to a broad range of instruments which are available to scientists from the member countries.

The post, which is offered on a fixed-term basis, represents an excellent opportunity for a young postdoctoral scientist to develop his expertise, broaden his experience and interact with leading scientists from around the world. More experienced scientists on detachment may also be considered.

The successful candidate will be a highly motivated scientist having a PhD. He/she will be expected to carry out his/her own research programme, assist ILL users in conducting their experiments and participate in the operation and development of the relevant instrument.

The vacancy exists in the Nuclear and Particle Physics Group : at the Lohengrin spectrometer (PN1), a program was started to investigate very neutron rich nuclei produced in nuclear fission. Dedicated measurements comprise gamma ray spectroscopy of isotopes far from stability with the aim to determine ground state lifetimes, search for microsecond isomers and investigation of gamma and conversion electron transitions following beta decay. The successful candidate will share responsibility for the instrument PN1. He/she will participate in spectroscopic work on this instrument and collaborate in the project for measurements with the European MINIBALL set up. He/she will also join a project to design and build a dedicated germanium cluster array on the spectrometer.

The successful candidate will be offered a fixed-term contract, the duration of which will under no circumstances exceed five (5) years. In addition to a competitive salary, certain benefits (reimbursement of removal expenses, adaptation allowance, etc.) may be offered.

Further information can be obtained by contacting the head of the Nuclear and Particle Physics group : Dr. H. Börner ; tel: (33) 4.76.20.73 94; e-mail: borner@ill.fr or via the World Wide Web (<http://www.ill.fr/nfp/>).

An application with curriculum vitae, a list of publications and the names of two academic referees should be sent, quoting reference 00/17, no later than **31st July 2000** to:

Dr. H. Börner, Head of NPP Group
INSTITUT LAUE LANGEVIN
B.P. 156 - 38042 Grenoble Cedex 9 - France