

LLB 2003-2004

Contents

Foreword	1
Scientific Highlights	
1. Structures and Phase Transitions	3
2. Magnetism and Superconductivity	35
3. Materials Science	63
4. Physical Chemistry and Soft Matter	87
5. Life Science	111
6. Modelling	131
7. Technical and Instrumental Developments	149
Experimental Programme and User Activities	167
Presentation of LLB	183
Publications	189

1 - STRUCTURES AND PHASE TRANSITIONS

1. Crystallographic Structures of austenitic and martensitic hydrides of $\text{Ti}_{0.64}\text{Zr}_{0.36}\text{Ni}$ intermetallic compound **14**
F. Cuevas, M. Latroche, A. Percheron-Guégan.
2. Giant H/D isotopic effect in $\text{YFe}_2(\text{H}_y\text{D}_{1-y})_{4.2}$ compounds **15**
V. Paul-Boncour, M. Guillot, G. André, F. Bourée, G. Wiesinger, A. Percheron-Guégan
3. Silicon doped hydroxyapatites **16**
D. Arcos, J. Rodríguez-Carvajal, M. Vallet-Regí
4. Simulated annealing on neutron and synchrotron powder diffraction DATA **18**
A. Carretero-Genevri, F. Damay, A. Cousson, W. Van Beek, J. Rodríguez-Carvajal
5. Magnetic structures of transition metal (Mn, Co, Ni, Cu) Hydroxysulfates **20**
S. Vilminot, G. André, M. Richard-Plouet, M. Kurmoo, F. Bourée-Vigneron, M. Ben Salah
6. Crystal and magnetic structures of the Mn^{3+} orbital ordered manganite $\text{Y}_2\text{Ba}_2\text{Mn}_4\text{O}_{11}$ **22**
L. Pinsard-Gaudart, C. Perca, A. Daoud-Aladine, M. T. Fernández-Díaz, J. Rodríguez-Carvajal
7. Spin Speierls ground state in $(\text{TMTTF})_2\text{PF}_6$ **24**
P. Foury-Leylekian, D. Le Bolloc'h, B. Hennion, S. Ravy, A. Moradpour, J.-P. Pouget
8. Neutral-to-ionic phase transition under pressure: towards the quantum limit **26**
M.H. Lemée-Cailleau, M. Buron, E. Collet, H. Cailleau, T. Luty, B. Ouladdiaf, F. Moussa, T. Hasegawa
9. Interactions in self-Assembled molecular crystals **28**
L. Bourgeois, B. Toudic, C. Ecolivet, P. Bourges, T. Breczewski
10. Phonon anomalies in high T_c superconductors related to charge stripe order **30**
D. Reznik, L. Pintschovius, M. Sato, M. Itoh, S. Iikubo, S. Yamada
11. Magnetic order in high-pressure oxygen **32**
I. Goncharenko, O. Makarova, L. Ulivi

2 - MAGNETISM AND SUPERCONDUCTIVITY

1. Two-dimensional geometry of spin excitations in the high-transition-temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{6.85}$ **44**
V. Hinkov, S. Pailhès, P. Bourges, Y. Sidis, A. Ivanov, A. Kulakov, C. T. Lin, D. P. Chen, C. Bernhard, B. Keimer
2. Small Angle Neutron Scattering from the flux lines lattice: new developments **46**
A. Pautrat, Ch. Simon, G. Poullain, C. Goupil, J. Scola, P. Mathieu, A. Brûlet
3. Lattice distortions related to charge ordering in $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$ **48**
M. Braden, J. Etrillard, A. Gukasov, U. Ammerahl, A. Revcolevschi
4. $\text{La}_{-5}(\text{Sr,Ca})_9\text{Cu}_{24}\text{O}_{41}$: a 1D Toy model for hole doped cuprates **50**
R. Klingeler, A. Gukasov, T. Kroll, J. Geck, M. Hücker, U. Ammerahl, A. Revcolevschi, B. Büchner
5. Confined spin waves reveal an assembly of nanosize domains in $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ ($x=0.17, 0.2$) **52**
M. Hennion, F. Moussa, P. Kober-Lehouelleur, F. Wang, A. Ivanov, L. P. Regnault, J. Kulda
6. Magnetic filaments in resistive manganites **54**
M. Viret, F. Ott, J.P. Renard, H. Glättli, L. Pinsard-Gaudart, A. Revcolevschi
7. Magnetic ground state in the frustrated $S=1/2$ square lattice of V^{4+} in $\text{Li}_2\text{VO}_2\text{SiO}_4$ **56**
A. Bombardi, J. Rodríguez-Carvajal, S. Di Matteo, F. de Bergevin, L. Paolasini, P. Carretta, P. Millet, R. Caciuffo
8. Temperature renormalization of the spin correlations in the dimer spin-Liquid TlCuCl_3 **58**
Ch. Rüegg, Ch. Niedermayer, A. Furrer, J. Mesot, M. Matsumoto, B. Normand, M. Sigrist, T.M. Rice, K.W. Krämer, H.-U. Güdel, H. Mutka, P. Bourges, Y. Sidis
9. Domain structures in $\text{Fe}/\text{Fe}_2\text{N}$ multilayers **60**
W. Szuszkiewicz, K. Fronc, B. Hennion, and M. Aleszkiewicz

3 - MATERIALS SCIENCE

1. Residual stress redistribution in a wheel/axle assembly due to cyclic loading **72**
A. Yameogo', A. Carrado, C. Prioul, A. Lodini
2. Residual stresses in welded aluminium joints for aerospace applications **74**
V. Stelmukh, S. Ganguly, L. Edwards and M. E. Fitzpatrick
3. Investigation of the α and β texture evolution of hot forged titanium alloy products **76**
J. Delfosse, C. Rey, M.H. Mathon
4. Impurities effects on the mechanisms of recrystallization of wire-drawn copper **78**
S. Jakani, T. Baudin, M. Benyoucef, Ph. Gerber, C.H. de Novion, M.H. Mathon
5. Nanocluster formation in electron irradiated lithium oxide **80**
G. Krexner, M. Prem, F. Beuneu, P. Vajda
6. Combined X-ray & neutron powder diffraction study of a dimorphic C_{60} solvate: $C_{60} \cdot CH_2Cl_2$ **82**
R.J. Papoular, R. Céolin, H. Allouchi, P. Espeau, A. Kurbakov', J.-LL. Tamarit
7. Local order around Nd^{3+} ions in an organic solution as determined by neutron scattering experiment **84**
B. Belhorma, M.-C. Bellissent-Funel, M.-C. Charbonnel, J.-P. Dognon

1. Bottle brush shape polymacromonomers : conformation and dynamics in solutions and melts **94**
S. Desvergne, F. Boué, A. Brûlet, V. Héroguez, Y. Gnanou
2. Aqueous supramolecular polymer formed by an amphiphilic perylene derivative **96**
Alix Arnaud, Joël Belleney, François Boué, Laurent Bouteiller, Géraldine Carrot, Véronique Wintgens
3. Swelling and collapse of a weak polyelectrolyte as a function of pH **98**
P. Topham, c. J. Crook, J. R. Howse, A. J. Ryan, A. J. Parnell, L. Ruiz-Pérez, R. A. L. Jones, M. Geoghegan, A. Menelle
4. Polymer-polymer adhesion of uncrosslinked elastomers studied by neutron reflectivity **100**
R. Schach, C. Creton, Y. Tran
5. Atom transfer radical polymerization from silica nanoparticles : following chemical synthesis using S.A.N.S. **102**
A. El Harrak, G. Carrot, J. Oberdisse, J. Jestin, F. Boué
6. Highly stretched polymer brushes with a low swelling capacity **104**
C. Devaux, F. Cousin, J-P. Chapel
7. New structural model for Nafion® membranes **106**
Laurent Rubatat, Olivier Diat, Gérard Gebel
8. Local dynamics of bulk and nanoparticle filled poly(vinyl acetate) observed by quasielastic neutron scattering **108**
Chuhong Zhang, Valeria Arrighi

1. Experimental evidence of a liquid-liquid transition at 0 K in interfacial water 118
J.-M. Zanotti, M.-C. Bellissent-Funel, S.-H. Chen
2. Hydration water dynamics of hydrophobic oligopeptide 120
D. Russo, P. Baglioni, E. Peroni, J. Teixeira
3. Hydration of ds-DNA and ss-DNA 122
M. Bastos, V. Castro, G. Mrevlishvili, J. Teixeira
4. Diffusion of water in halophilic archaea 124
K. Wood, S. Longeville, B. Franzetti, M.-C. Bellissent-Funel, D. Oesterhelt, G. Zaccai, B.-Z. Ginzburg
5. Structure of proteins-polyelectrolyte complexes 126
F. Cousin, J. Gummel, I. Schmidt, C. Huchon, F. Boué, M. Axelos

6 - MODELLING

1. The weakly coupled Rotor-Morse oscillator system: A toy model for selective chemical dissociation. **140**
S. Aubry and A. Memboeuf
2. Spin dynamics of the electron-doped high T_c superconducting cuprates **143**
F. Onufrieva and P. Pfeuty
3. Faults, a new program for refinement of powder diffraction patterns from layered structures **144**
M. Casas-Cabanas, J. Rodríguez-Carvajal, M.R. Palacín
4. Dynamics of lysozyme under pressure seen by molecular simulation and neutron scattering **146**
G.R. Kneller, K. Hinsén, V. Hamon, M.-C. Bellissent-Funel

7 - TECHNICAL AND INSTRUMENTAL DEVELOPMENTS

- 1 Papyrus : a dedicated tool to study surfaces at the nanoscale **155**
G. Chaboussant, F. Cousin, S. Gautrot, H. Glatli, J. Jestin, F. Ott, M. Viret
2. Very small angle neutron scattering spectrometer (TPA) **158**
J. Oberdisse, R. Kahn, V. Thévenot, A. Gabriel, P. Permingeat, D. Lairez, B. Hannighofer, S. Désert, A. Brûlet
3. Technical developmentS dedicated to “in situ” temperature analysis of crystallographic textures by neutron diffraction **160**
Ph. Gerber, J.P. Ambroise, M.H. Mathon
4. Neutron holographic study of palladium hydride **162**
L. Cser, G. Krexner, M. Prem, I. Sharkov, Gy. Török
5. Replacement of first elements of Guides 1 to 6 **164**
A. Menelle
6. Report on a first neutron test of a new D position-sensitive detector of thermal neutrons **165**
A. Kuklin, G.Eckold , V.Gordeliy, S.Kutuzov, A.Islamov, A.Smirnov, P.Utrobin, A.Bogdzal, N.Alekseev, V.Comparat, A.Pelissier, J. Ballon, J. Teixeira , G.Koskas, A.Gabriel