PHYSICAL REVIEW B

For editorial and subscription correspondence,
please see inside front cover
(ISSN: 0163-1829)

PERIODICALS
Postmaster send address changes to:
American Institute of Physics
Suite 1NO1
2 Huntington Quadrangle
Melville, NY 11747-4502

THIRD SERIES, VOLUME 68, NUMBER 18 *CONTENTS* **NOVEMBER 2003-1(II)**

RAPID COMMUNICATIONS

Structure, structural phase transitions, mechanical properties, defects, etc.

Long-term correlations distinguish coarsening mechanisms in alloys *(4 pages)* . . . . . 180101(R)
Lorenz-M. Stadler, Bogdan Sepiol, Richard Weinkamer, Markus Hartmann, Peter Fratzl, Jan W. Kantelhardt, Federico Zontone, Gerhard Grübel, and Gero Vogl

Dislocation cross slip and formation of terraces around nanoindentations in Au(001) *(4 pages)* . . . . . 180102(R)
E. Carrasco, O. Rodríguez de la Fuente, M. A. González, and J. M. Rojo

Magnetism

Dynamic frustrated magnetism in $Tb_2Ti_2O_7$ at 50 mK *(4 pages)* . . . . . 180401(R)
J. S. Gardner, A. Keren, G. Ehlers, C. Stock, Eva Segal, J. M. Roper, B. Fåk, M. B. Stone, P. R. Hammar, D. H. Reich, and B. D. Gaulin

Size dependence of the internal energy in Ising and vector spin glasses *(4 pages)* . . . . . 180402(R)
Helmut G. Katzgraber and I. A. Campbell

Microscopic model for the magnetization plateaus in NH_4CuCl_3 *(4 pages)* . . . . . 180403(R)
Masashige Matsumoto

Curling spin density and orbital structures in a magnetic vortex core of an Fe quantum dot *(4 pages)* . . . . . 180404(R)
Kohji Nakamura, Tomonori Ito, and A. J. Freeman

^{57}Fe-NMR determination of the local magnetic structure of the molecular nanomagnet Fe8 *(4 pages)* . . . . . 180405(R)
Y. Furukawa, S. Kawakami, K. Kumagai, S-H. Baek, and F. Borsa

Magnetism in Mn clusters: Role of correlation effects *(4 pages)* . . . . . 180406(R)
Florentino López-Urías and Alejandro Díaz-Ortiz

Photoinduced spin dynamics in $La_{0.6}Sr_{0.4}MnO_3$ observed by time-resolved magneto-optical Kerr spectroscopy *(4 pages)* . . . . . 180407(R)
T. Ogasawara, M. Matsubara, Y. Tomioka, M. Kuwata-Gonokami, H. Okamoto, and Y. Tokura

Superfluidity and superconductivity

Superfluid density in cuprate high-T_c superconductors: A new paradigm *(4 pages)* . . . . . 180501(R)
J. L. Tallon, J. W. Loram, J. R. Cooper, C. Panagopoulos, and C. Bernhard

Evidence for unconventional superconductivity in the nonoxide perovskite $MgCNi_3$ from penetration depth measurements *(4 pages)* . . . . . 180502(R)
R. Prozorov, A. Snezhko, T. He, and R. J. Cava

Optimal inhomogeneity for superconductivity *(4 pages)* . . . . . 180503(R)
E. Arrigoni and S. A. Kivelson

Tunneling spectroscopy of $Bi_2Sr_2CaCu_2O_{8+\delta}$: Eliashberg analysis of the spectral dip feature *(4 pages)* . . . . . 180504(R)
J. F. Zasadzinski, L. Coffey, P. Romano, and Z. Yusof

Copyright 2003 by The American Physical Society

0163-1829(20031101)68:18;1-U

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 68, NUMBER 18** **NOVEMBER 2003-1(II)**

Synthesis and high-pressure behavior of $Na_{0.3}CoO_2 \cdot 1.3H_2O$ and related phases *(4 pages)* . . . . . 180505(R)
Sangmoon Park, Yongjae Lee, Arnie Moodenbaugh, and Thomas Vogt
Theory of quasiparticle interference patterns in the pseudogap phase of the cuprate superconductors *(4 pages)* . . . . . 180506(R)
T. Pereg-Barnea and M. Franz

ARTICLES

Structure, structural phase transitions, mechanical properties, defects, etc.

Ab initio study of the ideal tensile strength and mechanical stability of transition-metal disilicides *(10 pages)* 184101
M. Friák, M. Šob, and V. Vitek
Ab initio determination of the ground-state properties of $Ca_2MgSi_2O_7$ åkermanite *(7 pages)* 184102
Razvan Caracas and Xavier Gonze
Ab initio study on divacancy binding energies in aluminum and magnesium *(5 pages)* 184103
Tokuteru Uesugi, Masanori Kohyama, and Kenji Higashi
Molecular dynamics study of damage accumulation in GaN during ion beam irradiation *(7 pages)* 184104
J. Nord, K. Nordlund, and J. Keinonen
Effect of pressure on nucleation and growth in the $Zr_{46.75}Ti_{8.25}Cu_{7.5}Ni_{10}Be_{27.5}$ bulk glass-forming alloy investigated using *in situ* x-ray diffraction *(6 pages)* 184105
W. H. Wang, T. Okada, P. Wen, X.-L. Wang, M. X. Pan, D. Q. Zhao, and W. Utsumi
Effect of stress on the energy levels of the vacancy-oxygen-hydrogen complex in Si *(11 pages)* 184106
J. Coutinho, O. Andersen, L. Dobaczewski, K. Bonde Nielsen, A. R. Peaker, R. Jones, S. Öberg, and P. R. Briddon
Ultraviolet-excited radiative decay channels of defect states in high-density sixfold-coordinated SiO_2 *(4 pages)* 184107
A. Paleari, N. Chiodini, D. Di Martino, F. Meinardi, and P. Fumagalli
Cubic Hf_3N_4 and Zr_3N_4: A class of hard materials *(5 pages)* 184108
M. Mattesini, R. Ahuja, and B. Johansson
Ferroquadrupole ordering and Γ_5 rattling motion in the clathrate compound $Ce_3Pd_{20}Ge_6$ *(10 pages)* 184109
Yuichi Nemoto, Takashi Yamaguchi, Takenobu Horino, Mitsuhiro Akatsu, Tatsuya Yanagisawa, Terutaka Goto, Osamu Suzuki, Andreas Dönni, and Takemi Komatsubara
Direct structural measurements of relaxation processes during transformations in amorphous ice *(5 pages)* 184110
Malcolm Guthrie, Jacob Urquidi, Chris A. Tulk, Chris J. Benmore, Dennis D. Klug, and Jeorg Neuefeind
Structural and dielectric properties of Sr_2TiO_4 from first principles *(9 pages)* 184111
Craig J. Fennie and Karin M. Rabe
First-principles calculations of boron-related defects in SiO_2 *(8 pages)* 184112
Minoru Otani, Kenji Shiraishi, and Atsushi Oshiyama
Point defects in NiAl: The effect of lattice vibrations *(10 pages)* 184113
A. Y. Lozovoi and Y. Mishin

Inhomogeneous, disordered, and partially ordered systems

Resistivity of the liquid gallium-lead miscibility gap system *(9 pages)* 184201
A. Ben Abdellah, J. G. Gasser, A. Makradi, B. Grosdidier, and J. Hugel
Signature of small rings in the Raman spectra of normal and compressed amorphous silica: A combined classical and *ab initio* study *(12 pages)* 184202
Abdelali Rahmani, Magali Benoit, and Claude Benoit

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 68, NUMBER 18** **NOVEMBER 2003-1(II)**

Contribution of local atomic arrangements and electronic structure to high electrical resistivity in the $Al_{82.6-x}Re_{17.4}Si_x$ ($7 \leqslant x \leqslant 12$) 1/1-1/1-1/1 approximant *(10 pages)* 184203
T. Takeuchi, T. Onogi, T. Otagiri, U. Mizutani, H. Sato, K. Kato, and T. Kamiyama

History-dependent relaxation and the energy scale of correlation in the electron glass *(7 pages)* 184204
Z. Ovadyahu and M. Pollak

Long-time relaxation of interacting electrons in the regime of hopping conduction *(10 pages)* 184205
D. N. Tsigankov, E. Pazy, B. D. Laikhtman, and A. L. Efros

Multifractality of Hamiltonians with power-law transfer terms *(5 pages)* 184206
E. Cuevas

Dynamics, dynamical systems, lattice effects, quantum solids, etc.

Complex lithium ion dynamics in simulated $LiPO_3$ glass studied by means of multitime correlation functions *(11 pages)* 184301
Michael Vogel

Electrons on hexagonal lattices and applications to nanotubes *(9 pages)* 184302
Betti Hartmann and Wojtek J. Zakrzewski

Absorption intensities of the multipole-field-induced double transitions involving a homonuclear-heteronuclear pair of hydrogen molecules in condensed phase *(8 pages)* 184303
Adya P. Mishra and Robert W. Field

Spectral function of electron-phonon models by cluster perturbation theory *(10 pages)* 184304
Martin Hohenadler, Markus Aichhorn, and Wolfgang von der Linden

Magnetism

Low-temperature magnetic order and spin dynamics in $YbRh_2Si_2$ *(14 pages)* 184401
K. Ishida, D. E. MacLaughlin, Ben-Li Young, K. Okamoto, Y. Kawasaki, Y. Kitaoka, G. J. Nieuwenhuys, R. H. Heffner, O. O. Bernal, W. Higemoto, A. Koda, R. Kadono, O. Trovarelli, C. Geibel, and F. Steglich

Theory for spin and orbital orderings in high-temperature phases in YVO_3 *(7 pages)* 184402
Theja. N. De Silva, Anuvrat Joshi, Michael Ma, and Fu Chun Zhang

Magnetic ground state of electron-doped $La_{1-x}Ce_xCoO_3$ compounds *(5 pages)* 184403
Qinfang Zhang and Weiyi Zhang

Magnetic origin of enhanced top exchange biasing in Py/IrMn/Py multilayers *(8 pages)* 184404
G. Malinowski, M. Hehn, S. Robert, O. Lenoble, A. Schuhl, and P. Panissod

Magnetic and thermal properties of $4f$-$3d$ ladder-type molecular compounds *(14 pages)* 184405
M. Evangelisti, M. L. Kahn, J. Bartolomé, L. J. de Jongh, C. Meyers, J. Leandri, Y. Leroyer, and C. Mathonière

Polarization of Fe(001) covered by MgO analyzed by spin-resolved x-ray photoemission spectroscopy *(9 pages)* 184406
M. Sicot, S. Andrieu, P. Turban, Y. Fagot-Revurat, H. Cercellier, A. Tagliaferri, C. De Nadai, N. B. Brookes, F. Bertran, and F. Fortuna

Magnetic behavior in the $Er(Mn,Al)_2$ system: Neutron diffraction study *(5 pages)* 184407
I. V. Golosovsky, A. I. Kurbakov, I. Mirebeau, A. S. Markosyan, and I. Yu. Gaidukova

Characterization of the $S=9$ excited state in Fe_8Br_8 by electron paramagnetic resonance *(6 pages)* 184408
D. Zipse, J. M. North, N. S. Dalal, S. Hill, and R. S. Edwards

Brillouin light scattering investigation of dynamic spin modes confined in cylindrical Permalloy dots *(7 pages)* 184409
G. Gubbiotti, G. Carlotti, T. Okuno, T. Shinjo, F. Nizzoli, and R. Zivieri

Dipolar field and energy anisotropy in magnetic thin films *(9 pages)* 184410
E. Estevez-Rams, J. Martinez-Garcia, J. Martinez-Garcia, J. Hiram-Espina, and H. Fuess

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 68, NUMBER 18** **NOVEMBER 2003-1(II)**

Vortex-vacancy interactions in two-dimensional easy-plane magnets *(11 pages)* 184411
G. M. Wysin
Observation of polarization-dependent x-ray absorption spectra arising from Cu $3d$-F $2p$ hybridization in the two-dimensional ferromagnets A_2CuF_4 ($A=$K, Cs) *(4 pages)* 184412
H. Manaka, T. Koide, T. Shidara, and I. Yamada
Quantum dynamics of tunneling between ferromagnets *(7 pages)* 184413
Yu-Li Lee and Yu-Wen Lee
Hysteretic behavior of the dynamic permeability on a Ni-Fe thin film *(4 pages)* 184414
O. Acher, S. Queste, M. Ledieu, K.-U. Barholz, and R. Mattheis
Magnetic critical behavior in the $[Cu(1\text{-hydroxybenzotriazolate})_2(MeOH)]_n$ molecule-based random-field magnet *(9 pages)* 184415
M. Fardis, C. Christides, G. Diamantopoulos, V. Psycharis, C. Raptopoulou, V. Tangoulis, and G. Papavassiliou
Thermodynamic properties of the two-dimensional $S=\frac{1}{2}$ Heisenberg antiferromagnet coupled to bond phonons *(9 pages)* 184416
Carsten H. Aits and Ute Löw
Itinerant-electron metamagnetism and giant magnetocaloric effect *(7 pages)* 184417
H. Yamada and T. Goto
Induced fourfold anisotropy and bias in compensated NiFe/FeMn double layers *(7 pages)* 184418
T. Mewes, B. Hillebrands, and R. L. Stamps
Thermal expansion and magnetovolume effects in the heavy-fermion system Ce_2RhIn_8 *(12 pages)* 184419
A. Malinowski, M. F. Hundley, N. O. Moreno, P. G. Pagliuso, J. L. Sarrao, and J. D. Thompson
Scaling behavior of the dipole-coupling energy in two-dimensional disordered magnetic nanostructures *(5 pages)* 184420
P. J. Jensen and G. M. Pastor
Magnetization of ultrathin (Ga,Mn)As layers *(5 pages)* 184421
R. Mathieu, B. S. Sørensen, J. Sadowski, U. Södervall, J. Kanski, P. Svedlindh, P. E. Lindelof, D. Hrabovsky, and E. Vanelle
Jahn-Teller dynamics of the organic ferromagnet-tetrakis(dimethylamine) ethylene-C_{60} *(8 pages)* 184422
P. Jeglič, R. Blinc, T. Apih, A. Omerzu, and D. Arčon
Electrical transport in manganite granular systems *(5 pages)* 184423
S. L. Yuan, Z. C. Xia, L. Liu, W. Chen, L. F. Zhao, J. Tang, G. H. Zhang, L. J. Zhang, H. Cao, W. Feng, Y. Tian, L. Y. Niu, and S. Liu
Quantum Monte Carlo simulation for the conductance of one-dimensional quantum spin systems *(7 pages)* . . . 184424
Kim Louis and Claudius Gros

Superfluidity and superconductivity

Kinetic energy driven superconductivity in doped cuprates *(7 pages)* 184501
Shiping Feng
Charge expulsion and electric field in superconductors *(9 pages)* 184502
J. E. Hirsch
Calculation of $\kappa_2(T)$ for s-wave type-II superconductors *(13 pages)* 184503
Takafumi Kita
Carrier-density-dependent momentum shift of the coherent peak and the LO phonon mode in p-type high-T_c superconductors *(19 pages)* 184504
S. Sugai, H. Suzuki, Y. Takayanagi, T. Hosokawa, and N. Hayamizu
Generalized BCS ansatz for pairing correlations in superconducting grains *(4 pages)* 184505
M. A. Fernández and J. L. Egido
A theoretical study of tunneling conductance in $PrOs_4Sb_{12}$ superconducting junctions *(8 pages)* 184506
Yasuhiro Asano, Yukio Tanaka, Yuji Matsuda, and Satoshi Kashiwaya

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 68, NUMBER 18** **NOVEMBER 2003-1(II)**

Quantum size effects on the superconducting parameters of zero-dimensional Pb nanoparticles *(6 pages)* 184507
W.-H. Li, C. C. Yang, F. C. Tsao, and K. C. Lee
Domain-wall superconductivity in hybrid superconductor-ferromagnet structures *(7 pages)* 184508
A. Yu. Aladyshkin, A. I. Buzdin, A. A. Fraerman, A. S. Mel'nikov, D. A. Ryzhov, and A. V. Sokolov
Potential and current distribution in strongly anisotropic $Bi_2Sr_2CaCu_2O_8$ single crystals at current breakdown *(9 pages)* 184509
I. Pethes, A. Pomar, B. Sas, G. Kriza, K. Vad, Á. Pallinger, F. Portier, and F. I. B. Williams
Effects of Pauli paramagnetism on the superconducting vortex phase diagram in strong fields *(17 pages)* 184510
Hiroto Adachi and Ryusuke Ikeda
Vortex lines nearly parallel to the surface of a single-crystal superconductor disk in a perpendicular field *(10 pages)* 184511
Katsuhiro Kawashima and Oliver B. Wright
Three-dimensional resonating-valence-bond liquids and their excitations *(8 pages)* 184512
R. Moessner and S. L. Sondhi
Signature of stripe pinning in optical conductivity *(5 pages)* 184513
L. Benfatto and C. Morais Smith
Anisotropic electrodynamics of MgB_2 detected by optical reflectance *(8 pages)* 184514
Y. Fudamoto and S. Lee
Transformation of in-plane $\rho(T)$ in $YBa_2Cu_3O_{7-\delta}$ at fixed oxygen content *(9 pages)* 184515
M. M. Abdelhadi and J. A. Jung
Order parameter and current-phase relation in Josephson junctions composed of $g+s$-wave superconductors *(7 pages)* 184516
Zengxu Wang, Weiyi Zhang, and Zidan Wang
Phonon thermal conductivity in doped La_2CuO_4: Relevant scattering mechanisms *(7 pages)* 184517
C. Hess, B. Büchner, U. Ammerahl, and A. Revcolevschi

COMMENTS

Comment on "Evidence for the immobile bipolaron formation in the paramagnetic state of the magnetoresistive manganites" *(5 pages)* 186401
Aritra Banerjee, S. Bhattacharya, S. Mollah, H. Sakata, H. D. Yang, and B. K. Chaudhuri

ERRATA

Publisher's Note: Zero-frequency transport properties of one-dimensional spin-$\frac{1}{2}$ systems [Phys. Rev. B **68**, 134436 (2003)] *(1 page)* ..... 189901(E)
F. Heidrich-Meisner, A. Honecker, D. C. Cabra, and W. Brenig

Cumulative Author Index i