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 67, NUMBER 1 *CONTENTS* JANUARY 2003-1(I)

Announcement: Color Online Only for Physical Review iii
Physical Review B Editorial Policies and Practices v
Physical Review B Information for Contributors ix
Subject Matter Categories for Physical Review B xii

BRIEF REPORTS

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

Pressure-induced photoluminescence in Mn^{2+}-doped BaF_2 and SrF_2 fluorites *(4 pages)* 012101
Ignacio Hernández and Fernando Rodríguez
Optical hysteresis in a spin-crossover complex *(3 pages)* 012102
X. J. Liu, Y. Moritomo, T. Kawamoto, A. Nakamoto, and N. Kojima
Lattice dielectric response of $CdCu_3Ti_4O_{12}$ and $CaCu_3Ti_4O_{12}$ from first principles *(4 pages)* 012103
Lixin He, J. B. Neaton, David Vanderbilt, and Morrel H. Cohen

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

Band narrowing in semiclassical nonadiabatic electron transfer *(4 pages)* 012301
Tianjian Lu and David H. Dunlap
Raman study of $Ba_xSr_{1-x}TiO_3$ films: Evidence for the existence of polar nanoregions *(4 pages)* 012302
D. A. Tenne, A. Soukiassian, M. H. Zhu, A. M. Clark, X. X. Xi, H. Choosuwan, Qi He, R. Guo, and A. S. Bhalla

Magnetism

Magnetic surface phase of thin helimagnetic films *(4 pages)* 012401
V. D. Mello, C. V. Chianca, Ana L. Dantas, and A. S. Carriço
Surface magnetic canting in a ferromagnet *(4 pages)* 012402
P. Betti, M. G. Pini, and A. Rettori
Microscopic phase separation and ferromagnetic microdomains in Cr-doped $Nd_{0.5}Ca_{0.5}MnO_3$ *(3 pages)* 012403
S. Mori, R. Shoji, N. Yamamoto, T. Asaka, Y. Matsui, A. Machida, Y. Moritomo, and T. Katsufuji
Transmission-electron-microscopy study of charge-stripe order in $La_{1.725}Sr_{0.275}NiO_4$ *(4 pages)* 012404
Jianqi Li, Yimei Zhu, J. M. Tranquada, K. Yamada, and D. J. Buttrey
Elastic anomaly in Tb under uniaxial tension: Evidence of the change in the Fermi surface topology responsible for the magnetic ordering type *(4 pages)* 012405
A. Vl. Andrianov and O. A. Savel'eva
High-field magneto-optic measurements of amorphous Gd-Si alloys *(4 pages)* 012406
F. Hellman, W. Geerts, and B. Donehew

Copyright 2003 by The American Physical Society

0556-2813(200301)67:1;1-Q

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 67, NUMBER 1** **JANUARY 2003-1(I)**

Ab initio electron theory for magnetism in Fe: Pressure dependence of spin-wave energies, exchange parameters, and Curie temperature *(4 pages)* 012407
S. Morán, C. Ederer, and M. Fähnle
Nonexponential relaxation and quantum tunnel splitting in the molecular magnet Fe_8 *(4 pages)* 012408
Zhi-De Chen and Shun-Qing Shen
Size-dependent spin reorientation transition in nanoplatelets *(4 pages)* 012409
E. Y. Vedmedenko, H. P. Oepen, and J. Kirschner
Direct measurement of spin accumulation in a metallic mesoscopic structure *(4 pages)* 012410
J.-M. George, A. Fert, and G. Faini
Magnetic moment formation at dilute Cd impurities in $R\mathrm{Ni}_2$ and $R\mathrm{Co}_2$ intermetallic compounds *(4 pages)* . . . 012411
A. L. de Oliveira, N. A. de Oliveira, and A. Troper

Superfluidity and superconductivity

Lattice stability of Sr_2RuO_4 under pressure *(4 pages)* 012501
S. V. Halilov and D. J. Singh
Disorder-induced phase transition of vortex matter in MgB_2 *(4 pages)* 012502
M. Angst, R. Puzniak, A. Wisniewski, J. Jun, S. M. Kazakov, and J. Karpinski
Modification of vortex liquid structure and dynamics of a $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystal induced by excessive-oxygen doping *(4 pages)* 012503
D. Darminto, A. A. Menovsky, and M. O. Tjia
Observation of two-dimensional spin fluctuations in the bilayer ruthenate $Sr_3Ru_2O_7$ by inelastic neutron scattering *(4 pages)* 012504
L. Capogna, E. M. Forgan, S. M. Hayden, A. Wildes, J. A. Duffy, A. P. Mackenzie, R. S. Perry, S. Ikeda, Y. Maeno, and S. P. Brown
Superconducting transition and phase diagram of single-crystal MgB_2 *(4 pages)* 012505
U. Welp, A. Rydh, G. Karapetrov, W. K. Kwok, G. W. Crabtree, Ch. Marcenat, L. Paulius, T. Klein, J. Marcus, K. H. P. Kim, C. U. Jung, H.-S. Lee, B. Kang, and S.-I. Lee
Evidence for nonlocality and the crossover from nonlocal to local behavior near the critical temperature in superconducting metals *(4 pages)* 012506
Ismardo Bonalde, Brian D. Yanoff, Myron B. Salamon, and Elbert E. M. Chia

ARTICLES

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

Short hydrogen-hydrogen separation in $R\mathrm{NiInH}_{1.333}$ ($R=$La, Ce, Nd) *(11 pages)* 014101
P. Vajeeston, P. Ravindran, R. Vidya, A. Kjekshus, H. Fjellvåg, and V. A. Yartys
Critical droplets and phase transitions in two dimensions *(5 pages)* 014102
Santo Fortunato
No role for phonon entropy in the fcc→fcc volume collapse transition in $Ce_{0.9}Th_{0.1}$ at ambient pressure *(5 pages)* 014103
M. E. Manley, R. J. McQueeney, B. Fultz, T. Swan-Wood, O. Delaire, E. A. Goremychkin, J. C. Cooley, W. L. Hults, J. C. Lashley, R. Osborn, and J. L. Smith
Order-disorder mechanism of the I-II phase transition in $CsZnPO_4$ *(6 pages)* 014104
Isao Yamashita, Hitoshi Kawaji, Tooru Atake, Yoshihiro Kuroiwa, and Akikatsu Sawada
Theory of the quantum paraelectric-ferroelectric transition *(9 pages)* 014105
R. Roussev and A. J. Millis
Molecular dynamics investigation of structural properties of a zeolite ZSM-5 based amorphous material *(11 pages)* 014106
A. B. Mukhopadhyay, C. Oligschleger, and M. Dolg

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 67, NUMBER 1** **JANUARY 2003-1(I)**

Orbital-ordering-induced phase transition in $LaVO_3$ and $CeVO_3$ *(6 pages)* 014107
Y. Ren, A. A. Nugroho, A. A. Menovsky, J. Strempfer, U. Rütt, F. Iga, T. Takabatake, and C. W. Kimball

Ab initio study of phase transformations in boron nitride *(9 pages)* 014108
W. J. Yu, W. M. Lau, S. P. Chan, Z. F. Liu, and Q. Q. Zheng

Raman and infrared study of the quasi-one-dimensional betaine arsenate-phosphate mixed-crystal system *(8 pages)* 014109
S. Lanceros-Méndez, H. Ebert, G. Schaack, and A. Klöperpieper

Self-organizing stripe patterns in two-dimensional frustrated systems with competing interactions *(6 pages)* 014110
Yan Mu and Yu-qiang Ma

Inhomogeneous, disordered, and partially ordered systems

Evaluation of diffusion mechanisms in NiAl by embedded-atom and first-principles calculations *(9 pages)* 014201
Y. Mishin, A. Y. Lozovoi, and A. Alavi

Atomic positional disorder in fcc metal nanocrystalline grain boundaries *(8 pages)* 014202
P. M. Derlet and H. Van Swygenhoven

Short- and medium-range order in $(Zr_{70}Cu_{20}Ni_{10})_{90-x}Ta_xAl_{10}$ bulk amorphous alloys *(8 pages)* 014203
T. C. Hufnagel and S. Brennan

Tile Hamiltonian for decagonal AlCoCu derived from first principles *(10 pages)* 014204
Ibrahim Al-Lehyani and Mike Widom

Piezoresistivity and conductance anisotropy of tunneling-percolating systems *(6 pages)* 014205
C. Grimaldi, T. Maeder, P. Ryser, and S. Strässler

Kinetics of phase separation in the driven lattice gas: Self-similar pattern growth under anisotropic nonequilibrium conditions *(12 pages)* 014206
P. I. Hurtado, J. Marro, P. L. Garrido, and E. V. Albano

Giant electron-driven anomaly in the ion dynamics of a saturated solution of lithium in deuterated ammonia *(7 pages)* 014207
F. Sacchetti, E. Guarini, C. Petrillo, L. E. Bove, B. Dorner, F. Demmel, and F. Barocchi

Phenomenological model of anisotropic microstructures in a-As_2S_3 chalcogenide glass *(6 pages)* 014208
K. E. Asatryan, B. Paquet, T. V. Galstian, and R. Vallée

Avoiding crossing of dielectric resonances in three-component composites *(5 pages)* 014209
Ying Gu and Qihuang Gong

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

Numerical study of the $E\otimes e$ Jahn-Teller polaron and bipolaron *(8 pages)* 014301
S. El Shawish, J. Bonča, Li-Chung Ku, and S. A. Trugman

Effects of dispersion, correction term, and isotopes on the thermal conductivity of LiF crystal *(11 pages)* 014302
B. K. Singh, M. K. Roy, V. J. Menon, and K. C. Sood

Muon location and muon dynamics in $DyNi_5$ *(10 pages)* 014303
A. M. Mulders, C. T. Kaiser, S. J. Harker, P. C. M. Gubbens, A. Amato, F. N. Gygax, A. Schenck, P. Dalmas de Réotier, A. Yaouanc, K. H. J. Buschow, and A. A. Menovsky

Binding of carriers by an external potential in the presence of electron-phonon coupling *(4 pages)* 014304
E. Ya. Sherman

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 67, NUMBER 1** **JANUARY 2003-1(I)**

Magnetism

Multiple magnetic phases of $La_2CoMnO_{6-\delta}$ ($0 \leqslant \delta \leqslant 0.05$) *(9 pages)* 014401
R. I. Dass and J. B. Goodenough
Magnetization reversal of ferromagnetic nanowires studied by magnetic force microscopy *(8 pages)* 014402
T. G. Sorop, C. Untiedt, F. Luis, M. Kröll, M. Raşa, and L. J. de Jongh
Staggered flux and stripes in doped antiferromagnets *(19 pages)* 014403
Martin Andersson and Stellan Östlund
Specific heat of URu_2Si_2 in fields up to 42 T: Clues to the hidden order *(7 pages)* 014404
J. S. Kim, D. Hall, P. Kumar, and G. R. Stewart
Intra-atomic noncollinear magnetism and the magnetic structures of antiferromagnetic FeMn *(4 pages)* 014405
Kohji Nakamura, Tomonori Ito, A. J. Freeman, Lieping Zhong, and Juan Fernandez-de-Castro
Observation of antiferromagnetic resonance affected by hyperfine interaction in GdBi *(4 pages)* 014406
Takahiro Tomimatsu, Keiichi Koyama, Makoto Yoshida, Dexin Li, and Mitsuhiro Motokawa
Structural and magnetic properties of the alternating Heisenberg spin-chain compound dichloro(2,5-dithiahexane)copper(II) *(9 pages)* 014407
E. Herrling, G. Fischer, S. Matejcek, B. Pilawa, H. Henke, I. Odenwald, and W. Wendl
General formula for the thermoelectric transport phenomena based on Fermi liquid theory: Thermoelectric power, Nernst coefficient, and thermal conductivity *(16 pages)* 014408
Hiroshi Kontani
Magnetic and orbital ordering in electron-doped manganites *(5 pages)* 014409
S. M. Dunaevsky and V. V. Deriglazov
Percolative transitions with first-order characteristics in the context of colossal magnetoresistance manganites *(6 pages)* 014410
J. Burgy, E. Dagotto, and M. Mayr
Magnetic relaxation in finite two-dimensional nanoparticle ensembles *(9 pages)* 014411
S. I. Denisov, T. V. Lyutyy, and K. N. Trohidou
Nonlocal coherent potential approximation for the paramagnetic state of the degenerate double-exchange model *(13 pages)* 014412
I. V. Solovyev
Ground-state numerical study of the three-dimensional random-field Ising model *(6 pages)* 014413
I. Dukovski and J. Machta
Optical probe of charge-spin-lattice dynamics in half-doped $La_{1.5}Sr_{0.5}NiO_4$ *(6 pages)* 014414
K. Yamamoto, K. Ishizaka, E. Saitoh, S. Shinomori, T. Tanabe, T. Katsufuji, and Y. Tokura
Enhancement of anisotropy in $Nd_2Fe_{14}B$ driven by Eu substitution *(4 pages)* 014415
Jesús Chaboy, Neculai Plugaru, Juan Bartolomé, and Gloria Subías
High-temperature expansions for the J_1-J_2 Heisenberg models: Applications to *ab initio* calculated models for Li_2VOSiO_4 and Li_2VOGeO_4 *(9 pages)* 014416
H. Rosner, R. R. P. Singh, W. H. Zheng, J. Oitmaa, and W. E. Pickett
Spin reorientation and crystal-field interaction in $TbFe_{12-x}Ti_x$ single crystals *(8 pages)* 014417
J. L. Wang, B. García-Landa, C. Marquina, M. R. Ibarra, F. M. Yang, and G. H. Wu
Magnetoelectric effects in ferrite-lead zirconate titanate layered composites: The influence of zinc substitution in ferrites *(10 pages)* 014418
G. Srinivasan, E. T. Rasmussen, and R. Hayes
Observation of low-field peaks and the temperature evolution of four kinds of magnetization processes in $Pr_{0.8}Nd_{0.2}Fe_{11}Ti$ *(7 pages)* 014419
T. Zhao, Z. D. Zhang, W. Liu, X. K. Sun, and R. Grössinger
Enhancement of magnetocrystalline anisotropy in ferromagnetic Fe films by intra-atomic noncollinear magnetism *(6 pages)* 014420
Kohji Nakamura, Tomonori Ito, A. J. Freeman, Lieping Zhong, and Juan Fernandez-de-Castro

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 67, NUMBER 1** **JANUARY 2003-1(I)**

Spin-drift transport and its applications *(5 pages)* 014421
Ivar Martin
Electronic properties of 4-nm FePt particles *(12 pages)* 014422
B. Stahl, J. Ellrich, R. Theissmann, M. Ghafari, S. Bhattacharya, H. Hahn, N. S. Gajbhiye, D. Kramer, R. N. Viswanath, J. Weissmüller, and H. Gleiter
Jahn-Teller effects in the mixed vanadate/phosphate crystals $TbV_{1-x}P_xO_4$ ($0 \leqslant x \leqslant 0.32$) *(7 pages)* 014423
Y. Hirano, N. Wakabayashi, C.-K. Loong, and L. A. Boatner
Exchange interaction in the $YbCrBr_9{}^{3-}$ mixed dimer: The origin of a strong Yb^{3+}-Cr^{3+} exchange anisotropy *(28 pages)* 014424
V. S. Mironov, L. F. Chibotaru, and A. Ceulemans
Relaxation processes in a multilevel spin system investigated by linewidth analysis of the multifrequency high-frequency EPR spectra *(11 pages)* 014425
M. Martinelli, C. A. Massa, L. A. Pardi, V. Bercu, and F. F. Popescu

Superfluidity and superconductivity

Relaxation and coarsening dynamics in superconducting arrays *(8 pages)* 014501
Gun Sang Jeon, Sung Jong Lee, and M. Y. Choi
Soft x-ray absorption spectroscopy studies of doped Pr-containing cuprates *(6 pages)* 014502
J. M. Chen, S. J. Liu, C. F. Chang, J.-Y. Lin, Y. S. Gou, and H. D. Yang
Influence of twin boundaries and randomly oriented correlated disorder on the liquid vortex plasticity of $YBa_2Cu_3O_7$ *(8 pages)* 014503
Jordi Figueras, Teresa Puig, and Xavier Obradors
Low-temperature electronic properties of Sr_2RuO_4. I. Microscopic model and normal-state properties *(12 pages)* 014504
Ralph Werner and V. J. Emery
Low-temperature electronic properties of Sr_2RuO_4. II. Superconductivity *(19 pages)* 014505
Ralph Werner
Low-temperature electronic properties of Sr_2RuO_4. III. Magnetic fields *(8 pages)* 014506
Ralph Werner
Low-field vortex matter in $YBa_2Cu_3O_{7-\delta}$: An atomic beam magnetic-resonance study *(13 pages)* 014507
Harald Hauglin, Nathan G. Woodard, Samuel Dapore-Schwartz, and Gregory P. Lafyatis
Crossing lattices in thin films of isotropic superconductors *(4 pages)* 014508
M. G. Blamire, C. H. Marrows, N. A. Stelmashenko, and J. E. Evetts
Statistical correlation for a three-terminal normal-metal–superconductor–superconductor hybrid system *(7 pages)* 014509
Baigeng Wang and Jian Wang
Field switching of superconductor-insulator bistability in artificially tuned organics *(5 pages)* 014510
H. Taniguchi, K. Kanoda, and A. Kawamoto
Spontaneous rearrangement of the checkerboard charge order to stripe order in $La_{1.5}Sr_{0.5}NiO_4$ *(5 pages)* 014511
R. Kajimoto, K. Ishizaka, H. Yoshizawa, and Y. Tokura
Coherence peak in the spin susceptibility from nesting in spin-triplet superconductors: A probe for line nodes in Sr_2RuO_4 *(7 pages)* 014512
Mayumi Yakiyama and Yasumasa Hasegawa
Conduction anisotropy, Hall effect, and magnetoresistance of $(TMTSF)_2ReO_4$ at high temperatures *(8 pages)* 014513
Bojana Korin-Hamzić, Emil Tafra, Mario Basletić, Amir Hamzić, Gabriele Untereiner, and Martin Dressel
Magnetic and superconducting phase diagram of electron-doped $Pr_{1-x}LaCe_xCuO_4$ *(5 pages)* 014514
M. Fujita, T. Kubo, S. Kuroshima, T. Uefuji, K. Kawashima, K. Yamada, I. Watanabe, and K. Nagamine

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 67, NUMBER 1** **JANUARY 2003-1(I)**

SO(5) as a critical dynamical symmetry in the SU(4) model of high-temperature superconductivity *(11 pages)* 014515
Lian-Ao Wu, Mike Guidry, Yang Sun, and Cheng-Li Wu

Refinement of the pressure-temperature phase diagram of the organic superconductor with asymmetric anions $(TMTSF)_2FSO_3$ *(7 pages)* 014516
Y. J. Jo, E. S. Choi, Haeyong Kang, W. Kang, I. S. Seo, and O. H. Chung

In-plane anisotropy and temperature dependence of oxygen phonon modes in $YBa_2Cu_3O_{6.95}$ *(9 pages)* 014517
J.-H. Chung, T. Egami, R. J. McQueeney, M. Yethiraj, M. Arai, T. Yokoo, Y. Petrov, H. A. Mook, Y. Endoh, S. Tajima, C. Frost, and F. Dogan

Phase diagram of Josephson junction arrays with capacitive disorder *(7 pages)* 014518
F. P. Mancini, P. Sodano, and A. Trombettoni

Emergence of multiple Fermi surface maps in angle-resolved photoemission from $Bi_2Sr_2CaCu_2O_{8+\delta}$ *(7 pages)* 014519
M. C. Asensio, J. Avila, L. Roca, A. Tejeda, G. D. Gu, M. Lindroos, R. S. Markiewicz, and A. Bansil

Optical sum rule violation and the kinetic energy change at the phase coherence transition in superconductors with pseudogap *(5 pages)* 014520
T. K. Kopeć

Vortex viscosity in the moderately clean limit of layered superconductors *(11 pages)* 014521
M. A. Skvortsov, D. A. Ivanov, and G. Blatter

Current-injection in a ballistic multiterminal superconductor/two-dimensional electron gas Josephson junction *(10 pages)* 014522
Th. Schäpers, V. A. Guzenko, R. P. Müller, A. A. Golubov, A. Brinkman, G. Crecelius, A. Kaluza, and H. Lüth

Thermodynamic properties of ferromagnet/superconductor/ferromagnet nanostructures *(9 pages)* 014523
I. Baladié and A. Buzdin

Parity effect in a tiny SQUID *(4 pages)* 014524
Masahiko Hayashi and Hiromichi Ebisawa

Numerical study of duality and universality in a frozen superconductor *(16 pages)* 014525
T. Neuhaus, A. Rajantie, and K. Rummukainen

Phonon-mediated anisotropic superconductivity in the Y and Lu nickel borocarbides *(5 pages)* 014526
P. Martínez-Samper, H. Suderow, S. Vieira, J. P. Brison, N. Luchier, P. Lejay, and P. C. Canfield

Nonlocality and strong coupling in the heavy fermion superconductor $CeCoIn_5$: A penetration depth study *(4 pages)* 014527
Elbert E. M. Chia, D. J. Van Harlingen, M. B. Salamon, Brian D. Yanoff, I. Bonalde, and J. L. Sarrao

Superconductivity in carbon nanotube ropes *(12 pages)* 014528
J. González

Quantum melting of incommensurate domain walls in two dimensions *(10 pages)* 014529
Tsutomu Momoi

Universality of delocalization in unconventional dirty superconducting wires with broken spin-rotation symmetry *(5 pages)* 014530
P. W. Brouwer, A. Furusaki, and C. Mudry

Flux transitions in a superconducting ring *(7 pages)* 014531
Jorge Berger

Vortex lattice in the presence of a tunable periodic pinning potential *(7 pages)* 014532
W. V. Pogosov, A. L. Rakhmanov, and V. V. Moshchalkov

Periodic density-of-states modulations in superconducting $Bi_2Sr_2CaCu_2O_{8+\delta}$ *(10 pages)* 014533
C. Howald, H. Eisaki, N. Kaneko, M. Greven, and A. Kapitulnik

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 67, NUMBER 1** **JANUARY 2003-1(I)**

Zn-induced one-dimensional electronic modulation in $YBa_2Cu_3O_{7-\delta}$ *(4 pages)* 014534
Makoto Maki, Terukazu Nishizaki, and Norio Kobayashi

COMMENTS

Comment on ''Fe magnon dispersion curve calculated with the frozen spin-wave method'' *(4 pages)* 016401
D. M. C. Nicholson and R. H. Brown
Reply to ''Comment on 'Fe magnon dispersion curve calculated with the frozen spin-wave method' '' *(1 page)* 016402
Leonard Kleinman and Qian Niu

ERRATA

Erratum: Critical size and anomalous lattice expansion in nanocrystalline $BaTiO_3$ particles [Phys. Rev. B **62**, 3065 (2000)] *(1 page)* . . . . . 019901(E)
S. Tsunekawa, S. Ito, T. Mori, K. Ishikawa, Z.-Q. Li, and Y. Kawazoe
Erratum: First-principles electronic thermal pressure of metal Au and Pt [Phys. Rev. B **66**, 094115 (2002)] *(1 page)* . . . . . 019902(E)
Taku Tsuchiya and Katsuyuki Kawamura

Cumulative Author Index xiii