PHYSICAL REVIEW B

For editorial and subscription correspondence,
please see inside front cover
(ISSN: 1098-0121)

PERIODICALS
Postmaster send address changes to:
APS Subscription Services
Suite 1NO1
2 Huntington Quadrangle
Melville, NY 11747-4502

THIRD SERIES, VOLUME 75, NUMBER 9 *CONTENTS* **MARCH 2007-1(I)**

BRIEF REPORTS

Structure, structural phase transitions, mechanical properties, defects

Phase stability in α- and β-rhombohedral boron *(4 pages)* 092101
Shunli Shang, Yi Wang, Raymundo Arroyave, and Zi-Kui Liu

Dominance of shear elastic energy far from a point defect in a solid *(4 pages)* 092102
Jeppe C. Dyre

Silver molybdate nanoparticles, nanowires, and nanorods embedded in glass nanocomposites *(4 pages)* 092103
S. Bhattacharya and A. Ghosh

Inhomogeneous, disordered, and partially ordered systems

Hopping transport in granular superconductors *(4 pages)* 092201
A. V. Lopatin and V. M. Vinokur

Residual entropy of ordinary ice from multicanonical simulations *(4 pages)* 092202
Bernd A. Berg, Chizuru Muguruma, and Yuko Okamoto

Dynamics, dynamical systems, lattice effects, quantum solids

Lattice dynamics of RuO_2: Theory and experiment *(4 pages)* 092301
K.-P. Bohnen, R. Heid, O. de la Peña Seaman, B. Renker, P. Adelmann, and H. Schober

Inelastic x-ray scattering from phonons under multibeam conditions *(4 pages)* 092302
Alexey Bosak and Michael Krisch

Magnetism

Spin-polarized standing waves at an electronically matched interface detected by Fermi-surface photoemission *(4 pages)* 092401
J. Schäfer, M. Hoinkis, Eli Rotenberg, P. Blaha, and R. Claessen

Enhanced magnetic entropy in $GdNi_2$ *(4 pages)* 092402
N. V. Baranov, A. V. Proshkin, E. G. Gerasimov, A. Podlesnyak, and J. Mesot

Anomalous thermoelectric power in $SrFeO_{3-\delta}$ from charge ordering and phase separation *(4 pages)* 092403
E. K. Hemery, G. V. M. Williams, and H. J. Trodahl

Effect of strain and electric field on the electronic soft matter in manganite thin films *(4 pages)* 092404
Tara Dhakal, Jacob Tosado, and Amlan Biswas

Copyright 2007 by The American Physical Society

1098-0121(20070301)75:9;1-C

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 75, NUMBER 9** **MARCH 2007-1(I)**

Resistance noise in spin valves *(4 pages)* 092405
Jørn Foros, Arne Brataas, Gerrit E. W. Bauer, and Yaroslav Tserkovnyak

Thermodynamic properties of the coupled dimer system $Cu_2(C_5H_{12}N_2)_2Cl_4$ *(3 pages)* 092406
S. Capponi and D. Poilblanc

Doping of Mn_2VAl and Mn_2VSi Heusler alloys as a route to half-metallic antiferromagnetism *(4 pages)* 092407
I. Galanakis, K. Özdoğan, E. Şaşıoğlu, and B. Aktaş

Superfluidity and superconductivity

Pressure-induced ferromagnetic solid ^{3}He layer on ^{4}He preplated graphite *(3 pages)* 092501
Akira Yamaguchi, Takamichi Watanuki, Ryuichi Masutomi, and Hidehiko Ishimoto

Contribution of disorder to the Hall effect in $Bi_2Sr_2CuO_{6+\delta}$ *(4 pages)* 092502
L. Fruchter, H. Raffy, F. Bouquet, and Z. Z. Li

Theory of coexistence of superconductivity and ferroelectricity *(4 pages)* 092503
Y. Krivolapov, A. Mann, and Joseph L. Birman

ARTICLES

Structure, structural phase transitions, mechanical properties, defects

Atomistic simulations of correlations between volumetric change and shear softening in amorphous metals *(5 pages)* 094101
Qi-Kai Li and Mo Li

Characteristics and signatures of dipole vortices in ferroelectric nanodots: First-principles-based simulations and analytical expressions *(9 pages)* 094102
S. Prosandeev and L. Bellaiche

Influence of oxygen vacancies on the dielectric properties of hafnia: First-principles calculations *(8 pages)* 094103
Eric Cockayne

Vacancy migration in hexagonal boron nitride *(7 pages)* 094104
A. Zobelli, C. P. Ewels, A. Gloter, and G. Seifert

First-principles calculations of second- and third-order elastic constants for single crystals of arbitrary symmetry *(7 pages)* 094105
Jijun Zhao, J. M. Winey, and Y. M. Gupta

Octahedral tilt-suppression of ferroelectric domain wall dynamics and the associated piezoelectric activity in $Pb(Zr,Ti)O_3$ *(8 pages)* 094106
R. Eitel and C. A. Randall

Vacancies on the Ti sublattice in titanium monoxide TiO_y studied using positron annihilation techniques *(6 pages)* 094107
A. A. Valeeva, A. A. Rempel, W. Sprengel, and H.-E. Schaefer

Point defects and their interaction in TiNi from first-principles calculations *(7 pages)* 094108
J. M. Lu, Q. M. Hu, L. Wang, Y. J. Li, D. S. Xu, and R. Yang

Behavior of vacancies near edge dislocations in Ni and α-Fe: Positron annihilation experiments and rate theory calculations *(11 pages)* 094109
Koichi Sato, Toshimasa Yoshiie, Toshitaka Ishizaki, and Qiu Xu

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 75, NUMBER 9** **MARCH 2007-1(I)**

Pressure on charged domain walls and additional imprint mechanism in ferroelectrics *(6 pages)* 094110
P. Mokrý, A. K. Tagantsev, and J. Fousek

Vibrational spectra of $CsHSO_4$ at high pressure and high temperature *(5 pages)* 094111
Hiroshi Yamawaki, Hiroshi Fujihisa, Mami Sakashita, and Kazumasa Honda

Elastic interaction among transition metals in one-dimensional spin-crossover solids *(10 pages)* 094112
K. Boukheddaden, S. Miyashita, and M. Nishino

Multistate modified embedded atom method *(16 pages)* 094113
M. I. Baskes, S. G. Srinivasan, S. M. Valone, and R. G. Hoagland

Inhomogeneous, disordered, and partially ordered systems

Entropy of solid ^{4}He: The possible role of a dislocation-induced glass *(5 pages)* 094201
A. V. Balatsky, M. J. Graf, Z. Nussinov, and S. A. Trugman

ac and dc percolative conductivity of magnetite-cellulose acetate composites *(13 pages)* 094202
C. Chiteme, D. S. McLachlan, and G. Sauti

Atomic-scale understanding of structural relaxation in simple and complex borosilicate glasses *(7 pages)* 094203
S. Sen, T. Topping, P. Yu, and R. E. Youngman

Boundary multifractality in critical one-dimensional systems with long-range hopping *(7 pages)* 094204
A. Mildenberger, A. R. Subramaniam, R. Narayanan, F. Evers, I. A. Gruzberg, and A. D. Mirlin

Dynamics, dynamical systems, lattice effects, quantum solids

Thermal conductivity of porous structures *(10 pages)* 094301
L. Braginsky, V. Shklover, G. Witz, and H.-P. Bossmann

Scanning tunneling microscope observation of plasmid DNA under electron irradiation at 8–40 eV *(5 pages)* 094302
K. Mochiji, H. Hashimoto, Y. Tanaka, N. Ninomiya, and M. Takeo

Theoretical study of atomic transport via interstitials in dilute Fe-P alloys *(8 pages)* 094303
E. Meslin, Chu-Chun Fu, A. Barbu, F. Gao, and F. Willaime

Prediction of Bragg-scattering-induced band gaps in phononic quasicrystals *(11 pages)* 094304
Daniel Sutter-Widmer, Sofia Deloudi, and Walter Steurer

Magnetism

Curie temperature of Kondo lattice films with finite itinerant charge carrier density *(9 pages)* 094401
J. Kienert and W. Nolting

Spin excitations in the antiferromagnet $NaNiO_2$ *(10 pages)* 094402
S. de Brion, C. Darie, M. Holzapfel, D. Talbayev, L. Mihály, F. Simon, A. Jánossy, and G. Chouteau

Degenerate perturbation theory of quantum fluctuations in a pyrochlore antiferromagnet *(31 pages)* 094403
Doron L. Bergman, Ryuichi Shindou, Gregory A. Fiete, and Leon Balents

Muon-spin relaxation measurements on the dimerized spin-1/2 chains $NaTiSi_2O_6$ and TiOCl *(5 pages)* 094404
P. J. Baker, S. J. Blundell, F. L. Pratt, T. Lancaster, M. L. Brooks, W. Hayes, M. Isobe, Y. Ueda, M. Hoinkis, M. Sing, M. Klemm, S. Horn, and R. Claessen

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 75, NUMBER 9** **MARCH 2007-1(I)**

Numerical study of Thouless-Anderson-Palmer metastable states in three-body Ising spin glasses *(6 pages)* 094405
Yukinori Tonosaki, Koujin Takeda, and Yoshiyuki Kabashima

Devil's staircases, quantum dimer models, and stripe formation in strong coupling models of quantum frustration *(20 pages)* 094406
Stefanos Papanikolaou, Kumar S. Raman, and Eduardo Fradkin

Electronic structure and magnetism in the frustrated antiferromagnet $LiCrO_2$: First-principles calculations *(5 pages)* 094407
I. I. Mazin

Neutron scattering study on the field-induced O_{xy}-type antiferroquadrupolar ordering of the heavy-fermion superconductor $PrOs_4Sb_{12}$ *(7 pages)* 094408
K. Kaneko, N. Metoki, R. Shiina, T. D. Matsuda, M. Kohgi, K. Kuwahara, and N. Bernhoeft

Towards a microscopic understanding of the phonon bottleneck *(13 pages)* 094409
D. A. Garanin

Energy gap formation in the valence fluctuating compound CeIrSb probed by Sb NMR and NQR *(5 pages)* 094410
Y. Kawasaki, M. Izumi, Y. Kishimoto, T. Ohno, H. Tou, Y. Inaoka, M. Sera, K. Shigetoh, and T. Takabatake

High-dimensional fractionalization and spinon deconfinement in pyrochlore antiferromagnets *(23 pages)* 094411
Z. Nussinov, C. D. Batista, B. Normand, and S. A. Trugman

Electronic structure and magnetic properties of $Fe_{0.125}Sn_{0.875}O_2$ *(7 pages)* 094412
Shu-jun Hu, Shi-shen Yan, Xin-xin Yao, Yan-xue Chen, Guo-lei Liu, and Liang-mo Mei

Orbital-dependent metamagnetic response in $Sr_4Ru_3O_{10}$ *(5 pages)* 094413
Y. J. Jo, L. Balicas, N. Kikugawa, E. S. Choi, K. Storr, M. Zhou, and Z. Q. Mao

Edge singularities in high-energy spectra of gapped one-dimensional magnets in strong magnetic fields *(7 pages)* 094414
A. Friedrich, A. K. Kolezhuk, I. P. McCulloch, and U. Schollwöck

Quantum simulation of spin ordering with nuclear spins in a solid-state lattice *(10 pages)* 094415
Georgios Roumpos, Cyrus P. Master, and Yoshihisa Yamamoto

Magnetization damping in a local-density approximation *(10 pages)* 094416
Hans Joakim Skadsem, Yaroslav Tserkovnyak, Arne Brataas, and Gerrit E. W. Bauer

Andreev reflection measurements of spin polarization *(16 pages)* 094417
P. Chalsani, S. K. Upadhyay, O. Ozatay, and R. A. Buhrman

Oxygen vacancies and induced changes in the electronic and magnetic structures of $La_{0.66}Sr_{0.33}MnO_3$: A combined *ab initio* and photoemission study *(11 pages)* 094418
S. Picozzi, C. Ma, Z. Yang, R. Bertacco, M. Cantoni, A. Cattoni, D. Petti, S. Brivio, and F. Ciccacci

Magnetism and heat capacity of $Dy_5Si_2Ge_2$ *(8 pages)* 094419
R. Nirmala, A. V. Morozkin, and S. K. Malik

Origin of the second coherent peak in the dynamical structure factor of an asymmetric spin-ladder *(5 pages)* 094420
P. N. Bibikov and M. I. Vyazovsky

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 75, NUMBER 9** **MARCH 2007-1(I)**

Magnetic order in the $S=1/2$ two-dimensional molecular antiferromagnet copper pyrazine perchlorate $Cu(Pz)_2(ClO_4)_2$ *(7 pages)* 094421
T. Lancaster, S. J. Blundell, M. L. Brooks, P. J. Baker, F. L. Pratt, J. L. Manson, M. M. Conner, F. Xiao, C. P. Landee, F. A. Chaves, S. Soriano, M. A. Novak, T. P. Papageorgiou, A. D. Bianchi, T. Herrmannsdörfer, J. Wosnitza, and J. A. Schlueter

Pinning of magnetic domain walls to structural defects in thin layers within a Heisenberg-type model *(5 pages)* 094422
Thomas Jourdan, Frédéric Lançon, and Alain Marty

Magnetoresistance and efficiency measurements of Alq_3-based OLEDs *(5 pages)* 094423
Pratik Desai, P. Shakya, T. Kreouzis, W. P. Gillin, N. A. Morley, and M. R. J. Gibbs

Neutron diffraction studies of nuclear and magnetic structures in the $S=1/2$ square Heisenberg antiferromagnets $(d_6\text{-}5CAP)_2CuX_4$ (X=Br and Cl) *(11 pages)* 094424
F. C. Coomer, V. Bondah-Jagalu, K. J. Grant, A. Harrison, G. J. McIntyre, H. M. Rønnow, R. Feyerherm, T. Wand, M. Meißner, D. Visser, and D. F. McMorrow

Spin-flop transition in uniaxial antiferromagnets: Magnetic phases, reorientation effects, and multidomain states *(13 pages)* 094425
A. N. Bogdanov, A. V. Zhuravlev, and U. K. Rößler

Separation of energy scales in the kagome antiferromagnet TmAgGe: A magnetic-field-orientation study up to 55 T *(5 pages)* 094426
P. A. Goddard, J. Singleton, A. L. Lima Sharma, E. Morosan, S. J. Blundell, S. L. Bud'ko, and P. C. Canfield

Magnetism of Gd_5Ge_4 from first principles *(6 pages)* 094427
Durga Paudyal, V. K. Pecharsky, K. A. Gschneidner, Jr., and B. N. Harmon

Electronic structure and x-ray magnetic circular dichroism of gadolinium beyond the local spin density approximation *(11 pages)* 094428
Samir Abdelouahed, N. Baadji, and M. Alouani

Phase diagram of the electronic states of trilayered ruthenate $Sr_4Ru_3O_{10}$ *(5 pages)* 094429
D. Fobes, M. H. Yu, M. Zhou, J. Hooper, C. J. O'Connor, M. Rosario, and Z. Q. Mao

Three-dimensional micromagnetic domain structure of MnAs films on GaAs(001): Experimental imaging and simulations *(10 pages)* 094430
R. Engel-Herbert, T. Hesjedal, and D. M. Schaadt

Magnetic structure of free cobalt clusters studied with Stern-Gerlach deflection experiments *(10 pages)* 094431
F. W. Payne, Wei Jiang, J. W. Emmert, Jun Deng, and L. A. Bloomfield

Magnetic phases in the Kagomé staircase compound $Co_3V_2O_8$ studied using powder neutron diffraction *(6 pages)* 094432
N. R. Wilson, O. A. Petrenko, and L. C. Chapon

Magnetic-field tuning of the low-temperature state of $YbNiSi_3$ *(5 pages)* 094433
Sergey L. Bud'ko, Paul C. Canfield, Marcos A. Avila, and Toshiro Takabatake

Effect of random interactions in spin baths on decoherence *(12 pages)* 094434
S. Camalet and R. Chitra

Magnetic properties and structural implications for nanocrystalline Fe-Ti-N thin films *(11 pages)* 094435
Jaydip Das, Sangita S. Kalarickal, Kyoung-Suk Kim, and Carl E. Patton

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 75, NUMBER 9** **MARCH 2007-1(I)**

Magnetic thermal hysteresis in $Fe_m/Dy_n/Fe_m$ and $Gd_m/Dy_n/Gd_m$ trilayers *(6 pages)* 094436
Ana L. Dantas, R. E. Camley, and A. S. Carriço

Superfluidity and superconductivity

Supersolidity and phase diagram of soft-core bosons on a triangular lattice *(5 pages)* 094501
Jing-Yu Gan, Yu-Chuan Wen, and Yue Yu

Disentangling the effective single-particle gap in electron-doped cuprates: Electronic Raman absorption *(6 pages)* 094502
Hong-Yan Lu and Qiang-Hua Wang

Origin of the magnetization peak effect in the Nb_3Sn superconductor *(6 pages)* 094503
R. Lortz, N. Musolino, Y. Wang, A. Junod, and N. Toyota

Tunable pinning of a superconducting vortex by a magnetic vortex *(10 pages)* 094504
Gilson Carneiro

Spin rotationally symmetric domain flux phases in underdoped cuprate superconductors *(6 pages)* 094505
Marcin Raczkowski, Didier Poilblanc, Raymond Frésard, and Andrzej M. Oleś

Fluctuations, dissipation, and nonuniversal superfluid jumps in two-dimensional superconductors *(9 pages)* 094506
R. W. Crane, N. P. Armitage, A. Johansson, G. Sambandamurthy, D. Shahar, and G. Grüner

Nonequilibrium characteristics in all-superconducting tunnel structures *(7 pages)* 094507
M. A. Laakso, P. Virtanen, F. Giazotto, and T. T. Heikkilä

Electronic Raman scattering in a multiband model for cuprate superconductors *(18 pages)* 094508
Ivan Kupčić and Slaven Barišić

In-plane and transverse superconducting fluctuation diamagnetism in the presence of charge-density waves in $2H$-$NbSe_2$ single crystals *(6 pages)* 094509
F. Soto, H. Berger, L. Cabo, C. Carballeira, J. Mosqueira, D. Pavuna, and F. Vidal

Pair correlations and the survival of superconductivity in and around a superconducting impurity *(6 pages)* 094510
Yonatan Dubi

Itinerant in-plane magnetic fluctuations and many-body correlations in Na_xCoO_2 *(9 pages)* 094511
M. M. Korshunov, I. Eremin, A. Shorikov, V. I. Anisimov, M. Renner, and W. Brenig

Interplane and intraplane heat transport in quasi-two-dimensional nodal superconductors *(13 pages)* 094512
I. Vekhter and A. Vorontsov

Electron energy down-conversion in thin superconducting films *(12 pages)* 094513
A. G. Kozorezov, J. K. Wigmore, D. Martin, P. Verhoeve, and A. Peacock

Theory of the Josephson effect in unconventional superconducting junctions with diffusive barriers *(10 pages)* 094514
T. Yokoyama, Y. Tanaka, and A. A. Golubov

Pulse and hold strategy for switching current measurements *(10 pages)* 094515
Jochen Walter, Erik Tholén, David B. Haviland, and Joachim Sjöstrand

Functional renormalization-group calculation of the Fermi surface of a spin ladder *(7 pages)* 094516
G. Abramovici and M. Héritier

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 75, NUMBER 9** **MARCH 2007-1(I)**

ERRATA

Erratum: Topological constraints on the charge distributions for the Thomson problem [Phys. Rev. B **74**, 052102 (2006)] *(1 page)* . . . . . 099901(E)
Alfredo Iorio and Siddhartha Sen

Erratum: Antiferromagnetic superconductors with effective-mass anisotropy in magnetic fields [Phys. Rev. B **74**, 024518 (2006)] *(1 page)* . . . . . 099902(E)
Yuuichi Suginishi and Hiroshi Shimahara