PHYSICAL REVIEW B

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

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

THIRD SERIES, VOLUME 72, NUMBER 14 *CONTENTS* **OCTOBER 2005-1(II)**

RAPID COMMUNICATIONS

Structure, structural phase transitions, mechanical properties, defects

Rare-earth adsorption at intergranular interfaces in silicon nitride ceramics: Subnanometer observations and theory *(4 pages)* . . . . . 140101(R)
N. Shibata, G. S. Painter, R. L. Satet, M. J. Hoffmann, S. J. Pennycook, and P. F. Becher

Atomistic treatment of depolarizing energy and field in ferroelectric nanostructures *(4 pages)* . . . . . 140102(R)
I. Ponomareva, I. I. Naumov, I. Kornev, Huaxiang Fu, and L. Bellaiche

Inhomogeneous, disordered, and partially ordered systems

Topological *k*-space refinement of the configurational energy of alloys *(4 pages)* . . . . . 140201(R)
O. Shchyglo, V. N. Bugaev, R. Drautz, A. Udyansky, H. Reichert, and H. Dosch

Dynamics, dynamical systems, lattice effects, quantum solids

Nuclear resonant scattering from the subnanosecond lifetime excited state of ^{201}Hg *(4 pages)* . . . . . 140301(R)
D. Ishikawa, A. Q. R. Baron, and T. Ishikawa

Magnetism

One-magnon Raman scattering in La_2CuO_4: The origin of the field-induced mode *(4 pages)* . . . . . 140401(R)
M. B. Silva Neto and L. Benfatto

Thermal conductivity of a classical one-dimensional Heisenberg spin model *(4 pages)* . . . . . 140402(R)
A. V. Savin, G. P. Tsironis, and X. Zotos

Current induced pressure on a tilted magnetic domain wall *(4 pages)* . . . . . 140403(R)
M. Viret, A. Vanhaverbeke, F. Ott, and J.-F. Jacquinot

Effect of interface states on spin-dependent tunneling in Fe/MgO/Fe tunnel junctions *(4 pages)* . . . . . 140404(R)
K. D. Belashchenko, J. Velev, and E. Y. Tsymbal

Intrinsic volume scaling of thermoinduced magnetization in antiferromagnetic nanoparticles *(4 pages)* . . . . . 140405(R)
G. Brown, A. Janotti, M. Eisenbach, and G. M. Stocks

Magnetic short-range order above the Curie temperature of Fe and Ni *(4 pages)* . . . . . 140406(R)
Vladimir Antropov

Suppressed magnetization in $La_{0.7}Ca_{0.3}MnO_3/YBa_2Cu_3O_{7-\delta}$ superlattices *(4 pages)* . . . . . 140407(R)
A. Hoffmann, S. G. E. te Velthuis, Z. Sefrioui, J. Santamaría, M. R. Fitzsimmons, S. Park, and M. Varela

Copyright 2005 by The American Physical Society

1098-0121(20051001)72:14;1-6

(Continued)

PHYSICAL REVIEW B THIRD SERIES, VOLUME 72, NUMBER 14 OCTOBER 2005-1(II)

Scaling of entanglement entropy in the random singlet phase *(4 pages)* . . . . . 140408(R)
Nicolas Laflorencie

Superfluidity and superconductivity

Superconducting proximity effect through a magnetic domain wall *(4 pages)* . . . . . 140501(R)
Alexander Konstandin, Juha Kopu, and Matthias Eschrig

Ballistic effects in a proximity induced superconducting diffusive metal *(4 pages)* . . . . . 140502(R)
W. Escoffier, C. Chapelier, and F. Lefloch

Anomalous features of the proximity effect in triplet superconductors *(4 pages)* . . . . . 140503(R)
Y. Tanaka, Y. Asano, A. A. Golubov, and S. Kashiwaya

Fiske steps studied by flux-flow resistance oscillation in a narrow stack of $Bi_2Sr_2CaCu_2O_{8+\delta}$ junctions *(4 pages)* . . . . . 140504(R)
S. M. Kim, H. B. Wang, T. Hatano, S. Urayama, S. Kawakami, M. Nagao, Y. Takano, T. Yamashita, and K. Lee

BRIEF REPORTS

Magnetism

Spin and orbital ordering in $La_{2-2x}Sr_{1+2x}Mn_2O_7$ compounds *(4 pages)* 142401
Qinfang Zhang, Weiyi Zhang, and Zhengsheng Jiang

ARTICLES

Structure, structural phase transitions, mechanical properties, defects

First-principles study of epitaxial strain in perovskites *(9 pages)* 144101
Oswaldo Diéguez, Karin M. Rabe, and David Vanderbilt

Relativistic effects in atomic inner-shell ionization by a focused electron probe *(8 pages)* 144102
Christian Dwyer

Second-harmonic-generation microscopic observations of polar state in Li-doped $KTaO_3$ under an electric field *(6 pages)* 144103
Hiroko Yokota, Taeko Oyama, and Yoshiaki Uesu

Coarse-grained molecular dynamics: Nonlinear finite elements and finite temperature *(32 pages)* 144104
Robert E. Rudd and Jeremy Q. Broughton

Analytic bond-order potential for predicting structural trends across the *sp*-valent elements *(14 pages)* 144105
Ralf Drautz, Dewey A. Murdick, Duc Nguyen-Manh, Xiaowang Zhou, Haydn N. G. Wadley, and David G. Pettifor

Cmcm phase of GeS at high pressure *(4 pages)* 144106
Murat Durandurdu

Low-temperature polymorphs of ZrO_2 and HfO_2: A density-functional theory study *(9 pages)* 144107
John E. Jaffe, Rafał A. Bachorz, and Maciej Gutowski

High-pressure Raman study of the ferroelastic rutile-to-$CaCl_2$ phase transition in ZnF_2 *(6 pages)* 144108
Aristides Perakis, Dimitrios Lampakis, Yannis C. Boulmetis, and Constantine Raptis

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 72, NUMBER 14** **OCTOBER 2005-1(II)**

Structure, energetics, and mechanical stability of Fe-Cu bcc alloys from first-principles calculations *(16 pages)* 144109
Jefferson Z. Liu, A. van de Walle, G. Ghosh, and M. Asta

Inhomogeneous, disordered, and partially ordered systems

X-ray intensity fluctuation spectroscopy studies of ordering kinetics in a Cu-Pd alloy *(9 pages)* 144201
K. Ludwig, F. Livet, F. Bley, J.-P. Simon, R. Caudron, D. Le Bolloc'h, and A. Moussaid

Five-dimensional model of the $S1$-superstructure phase in Al-Ni-Co quasicrystals *(7 pages)* 144202
Akiji Yamamoto, Hiroyuki Takakura, and Eiji Abe

Dynamics, dynamical systems, lattice effects, quantum solids

NMR spin-lattice relaxation and ionic conductivity in lithium thioborogermanate fast-ion-conducting glasses *(13 pages)* 144301
Benjamin Meyer, Ferdinando Borsa, David M. Martin, and Steve W. Martin

Classical waves on nonlinear lattices *(9 pages)* 144302
G. D. Mahan

Magnetism

Multipole ordering in f-electron systems on the basis of a j-j coupling scheme *(12 pages)* 144401
Katsunori Kubo and Takashi Hotta

Multicritical point relations in three dual pairs of hierarchical-lattice Ising spin glasses *(6 pages)* 144402
Michael Hinczewski and A. Nihat Berker

Magnetic, transport, and thermoelectric properties of the delafossite oxides $CuCr_{1-x}Mg_xO_2$ $(0 \leqslant x \leqslant 0.04)$ *(5 pages)* 144403
T. Okuda, N. Jufuku, S. Hidaka, and N. Terada

Thickness dependence and magnetocrystalline anisotropy of the x-ray transverse magneto-optical Kerr effect at the Co $2p$ edges of ultrathin Co films on W(110) *(10 pages)* 144404
A. Kleibert, V. Senz, J. Bansmann, and P. M. Oppeneer

Effect of second-rank random anisotropy on critical phenomena of a random-field O(N) spin model in the large N limit *(18 pages)* 144405
Yoshinori Sakamoto, Hisamitsu Mukaida, and Chigak Itoi

Detection of electromagnetic multipoles by x-ray spectroscopies *(6 pages)* 144406
S. Di Matteo, Y. Joly, and C. R. Natoli

Spinel-type gallium oxynitrides attainable at high pressure and high temperature *(4 pages)* 144407
Peter Kroll

Effect of chemical bonding on the magnetic stability and magnetic moment in Mn-based binary compounds *(7 pages)* 144408
Hyun-Min Hong, Yong-Ju Kang, Joongoo Kang, E.-C. Lee, Y.-H. Kim, and K. J. Chang

Evolution of the magnetic phase transition in MnO confined to channel type matrices: Neutron diffraction study *(5 pages)* 144409
I. V. Golosovsky, I. Mirebeau, V. P. Sakhnenko, D. A. Kurdyukov, and Y. A. Kumzerov

ESR studies of MnO embedded into silica nanoporous matrices with different topology *(6 pages)* 144410
I. V. Golosovsky, D. Arčon, Z. Jagličič, P. Cevc, V. P. Sakhnenko, D. A. Kurdyukov, and Y. A. Kumzerov

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 72, NUMBER 14** **OCTOBER 2005-1(II)**

Magnetic properties of $Fe_3Si/GaAs(001)$ hybrid structures *(5 pages)* 144411
K. Lenz, E. Kosubek, K. Baberschke, H. Wende, J. Herfort, H.-P. Schönherr, and K. H. Ploog

Characterization and magnetic properties of $Fe_{1-x}Ni_x$ nanowire arrays *(6 pages)* 144412
Qingfang Liu, Jianbo Wang, Zhongjie Yan, and Desheng Xue

Phase separation in Fe-Si and Co-Si sputtered ferromagnetic alloys and the origin of their magnetic anisotropy *(15 pages)* 144413
J. Díaz, R. Morales, S. M. Valvidares, and J. M. Alameda

Electronic properties of Fe, Co, and Mn ultrathin films at the interface with MgO(001) *(8 pages)* 144414
M. Sicot, S. Andrieu, F. Bertran, and F. Fortuna

Theoretical study of the spin and orbital ordered states of $LaBaMn_2O_{5.5}$ *(7 pages)* 144415
Qinfang Zhang, Weiyi Zhang, and Zhengsheng Jiang

Monte Carlo simulations of the phase transition of the three-dimensional isotropic Heisenberg spin glass *(20 pages)* 144416
Koji Hukushima and Hikaru Kawamura

Nature of phase transitions in the striped phase of a triangular-lattice Ising antiferromagnet *(10 pages)* 144417
S. E. Korshunov

Theory of transverse spin dynamics in a polarized Fermi liquid and an itinerant ferromagnet *(9 pages)* 144418
V. P. Mineev

Size effect on the ordering of $L1_0$ FePt nanoparticles *(5 pages)* 144419
T. Miyazaki, O. Kitakami, S. Okamoto, Y. Shimada, Z. Akase, Y. Murakami, D. Shindo, Y. K. Takahashi, and K. Hono

Ab initio investigation of the magnetism of tetragonal Mn: Bulk, surface, ultrathin films, and multilayers *(19 pages)* 144420
J. Hafner and D. Spišák

Effect of pressure on single-chain magnets with repeating units of the Mn^{III}-Ni^{II}-Mn^{III} trimer *(9 pages)* 144421
Masaki Mito, Hiroyuki Deguchi, Takayuki Tajiri, Seishi Takagi, Masahiro Yamashita, and Hitoshi Miyasaka

Magnetodielectric response of the spin-ice $Dy_2Ti_2O_7$ *(5 pages)* 144422
Masafumi Saito, Ryuji Higashinaka, and Yoshiteru Maeno

Nonequilibrium magnetic properties of single-crystalline $La_{0.7}Ca_{0.3}CoO_3$ *(6 pages)* 144423
Asish K. Kundu, P. Nordblad, and C. N. R. Rao

Frustrated magnetism in the two-dimensional triangular lattice of Li_xCoO_2 *(9 pages)* 144424
J. Sugiyama, H. Nozaki, J. H. Brewer, E. J. Ansaldo, G. D. Morris, and C. Delmas

First-principles study of thin magnetic transition-metal silicide films on Si(001) *(12 pages)* 144425
Hua Wu, Peter Kratzer, and Matthias Scheffler

Deconfined quantum criticality in the two-dimensional Kondo lattice model *(6 pages)* 144426
Ki-Seok Kim

Magnetic properties of selected Mn-based transition metal compounds with β-Mn structure: Experiments and theory *(11 pages)* 144427
T. Eriksson, L. Bergqvist, Y. Andersson, P. Nordblad, and O. Eriksson

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 72, NUMBER 14** **OCTOBER 2005-1(II)**

Local measurements of magnetization in Mn_{12} crystals *(6 pages)* 144428
Nurit Avraham, Ady Stern, Yoko Suzuki, K. M. Mertes, M. P. Sarachik, E. Zeldov, Y. Myasoedov, H. Shtrikman, E. M. Rumberger, D. N. Hendrickson, N. E. Chakov, and G. Christou

Magnetodielectric consequences of phase separation in the colossal magnetoresistance manganite $Pr_{0.7}Ca_{0.3}MnO_3$ *(6 pages)* 144429
R. S. Freitas, J. F. Mitchell, and P. Schiffer

Superfluidity and superconductivity

Persistent photo-excitation in $GdBa_2Cu_3O_{6.5}$ in a simultaneous Raman and electrical-transport experiment *(6 pages)* 144501
S. Bahrs, J. Guimpel, A. R. Goñi, B. Maiorov, A. Fainstein, G. Nieva, and C. Thomsen

Theory of disordered flux-line liquids *(25 pages)* 144502
A. M. Ettouhami

Temperature-modulation analysis of superconductivity-induced transfer of in-plane spectral weight in $Bi_2Sr_2CaCu_2O_8$ *(9 pages)* 144503
A. B. Kuzmenko, H. J. A. Molegraaf, F. Carbone, and D. van der Marel

Superconductivity and physical properties of $Ba_{24}Si_{100}$ determined from electric transport, specific-heat capacity, and magnetic susceptibility measurements *(6 pages)* 144504
Takeshi Rachi, Harukazu Yoshino, Ryotaro Kumashiro, Masaki Kitajima, Kensuke Kobayashi, Keiichi Yokogawa, Keizo Murata, Noriaki Kimura, Haruyoshi Aoki, Hiroshi Fukuoka, Syoji Yamanaka, Hidekazu Shimotani, Taishi Takenobu, Yoshihiro Iwasa, Takahiko Sasaki, Norio Kobayashi, Yuji Miyazaki, Kazuya Saito, FangZhun Guo, Keisuke Kobayashi, Keiichi Osaka, Kenichi Kato, Masaki Takata, and Katsumi Tanigaki

Evaluation of matrix elements in partially projected wave functions *(9 pages)* 144505
Noboru Fukushima, Bernhard Edegger, V. N. Muthukumar, and Claudius Gros

Distinct pairing symmetries in $Nd_{1.85}Ce_{0.15}CuO_{4-y}$ and $La_{1.89}Sr_{0.11}CuO_4$ single crystals: Evidence from comparative tunneling measurements *(9 pages)* 144506
L. Shan, Y. Huang, H. Gao, Y. Wang, S. L. Li, P. C. Dai, F. Zhou, J. W. Xiong, W. X. Ti, and H. H. Wen

Superconducting transition of a two-dimensional Josephson junction array in weak magnetic fields *(5 pages)* 144507
In-Cheol Baek, Young-Je Yun, Jeong-Il Lee, and Mu-Yong Choi

Irreversible properties of superconducting $HoNi_2B_2C$ single crystals *(7 pages)* 144508
C. Krutzler, R. Fuger, M. Eisterer, G. Fuchs, G. Behr, and H. W. Weber

Phase conversion and interface growth in phase-separated ^3He-^4He liquid mixtures *(16 pages)* 144509
Haruka Abe, Takeo Satoh, and Serguei N. Burmistrov

Mobile Zhang-Rice singlets: Electron correlations and bond-length fluctuations in copper oxides *(7 pages)* 144510
L. Hozoi, S. Nishimoto, and A. Yamasaki

Superconducting proximity effect and interface transparency in Nb/PdNi bilayers *(7 pages)* 144511
C. Cirillo, S. L. Prischepa, M. Salvato, C. Attanasio, M. Hesselberth, and J. Aarts

Peak effect and square-to-rhombic vortex lattice transition in $La_{2-x}Sr_xCuO_4$ *(11 pages)* 144512
B. Rosenstein, B. Ya. Shapiro, I. Shapiro, Y. Bruckental, A. Shaulov, and Y. Yeshurun

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 72, NUMBER 14** **OCTOBER 2005-1(II)**

Destruction of superconductivity by impurities in the attractive Hubbard model *(7 pages)* 144513
Daniel Hurt, Evan Odabashian, Warren E. Pickett, Richard T. Scalettar, Felipe Mondaini, Thereza Paiva, and Raimundo R. dos Santos

Tunable interactions between vortices and a magnetic dipole *(10 pages)* 144514
Gilson Carneiro

Generation of tunable terahertz out-of-plane radiation using Josephson vortices in modulated layered superconductors *(7 pages)* 144515
Sergey Savel'ev, Valery Yampol'skii, Alexander Rakhmanov, and Franco Nori

Combined experimental and theoretical study of field and current conditioning in magnetically shielded superconducting films *(12 pages)* 144516
Ch. Jooss, E. Brinkmeier, and H. Heese

Nonequilibrium thermodynamics of unsteady superfluid turbulence in counterflow and rotating situations *(11 pages)* 144517
D. Jou and M. S. Mongiovì

Inhomogeneous electronic states of $La_{2-x}Sr_xCuO_4$ probed by scanning tunneling spectroscopy *(4 pages)* 144518
T. Kato, S. Okitsu, and H. Sakata

Quasiparticle density of states of $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals probed using tunneling spectroscopy in the 30–50 mK temperature range in high magnetic fields *(7 pages)* 144519
S. I. Vedeneev and D. K. Maude

Domain wall effects in ferromagnet-superconductor structures *(5 pages)* 144520
I. S. Burmistrov and N. M. Chtchelkatchev

Stability of the modulated states in $ErNi_2B_2C$: A neutron diffraction study of chemically doped samples *(6 pages)* 144521
M. El Massalami, R.-M. Galera, D. Schmitt, B. Ouladdiaf, and H. Takeya

Transition between triplet and singlet pairing in two-dimensional superconductors *(5 pages)* 144522
J. Mráz and R. Hlubina

Atomic ordering of the fluorine dopant in the $HgBa_2CuO_{4+\delta}$ high-T_c superconductor *(10 pages)* 144523
J. G. Correia, H. Haas, the ISOLDE Collaboration, V. S. Amaral, A. M. L. Lopes, J. P. Araújo, S. Le Floch, P. Bordet, E. Rita, J. C. Soares, and W. Tröger

Integrable dynamics of coupled Fermi-Bose condensates *(9 pages)* 144524
Emil A. Yuzbashyan, Vadim B. Kuznetsov, and Boris L. Altshuler

Vortex glass transitions in disordered three-dimensional *XY* models: Simulations for several different sets of parameters *(13 pages)* 144525
Peter Olsson

Vortex radiation in long narrow Josephson junctions: Theory and experiment *(7 pages)* 144526
A. A. Abdumalikov, Jr., M. V. Fistul, and A. V. Ustinov

Nernst effect and superconducting fluctuations in Zn-doped $YBa_2Cu_3O_{7-\delta}$ *(5 pages)* 144527
Z. A. Xu, J. Q. Shen, S. R. Zhao, Y. J. Zhang, and C. K. Ong

Quasiclassical determination of the in-plane magnetic field phase diagram of superconducting Sr_2RuO_4 *(9 pages)* 144528
R. P. Kaur, D. F. Agterberg, and H. Kusunose

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 72, NUMBER 14** **OCTOBER 2005-1(II)**

Correlation-induced suppression of decoherence in capacitively coupled Cooper-pair boxes *(5 pages)* 144529
J. Q. You, Xuedong Hu, and Franco Nori

Equilibrium magnetization in the vicinity of the Bragg glass to vortex glass transition in V_3Si *(7 pages)* 144530
G. Ravikumar and H. Küpfer

COMMENTS

Comment on "Nodeless pairing state in single-crystal $YBa_2Cu_3O_7$" *(3 pages)* 146501
J. E. Sonier, D. A. Bonn, J. H. Brewer, W. N. Hardy, R. F. Kiefl, and Ruixing Liang

Reply to "Comment on 'Nodeless pairing state in single-crystal $YBa_2Cu_3O_7$' " *(5 pages)* 146502
Dale R. Harshman, W. J. Kossler, X. Wan, Anthony T. Fiory, A. J. Greer, D. R. Noakes, C. E. Stronach, E. Koster, and John D. Dow

ERRATA

Publisher's Note: Inverse tunneling magnetoresisance in nanoscale magnetic tunnel junctions [Phys. Rev. B **72**, 024401 (2005)] *(1 page)* . . . . . 149901(E)
Tae-Suk Kim

Erratum: Condensation energy in Eliashberg theory: From weak to strong coupling [Phys. Rev. B **71**, 184513 (2005)] *(1 page)* . . . . . 149902(E)
Evelina Tsoncheva and Andrey V. Chubukov