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 10 *CONTENTS* **MARCH 2007-1(II)**

RAPID COMMUNICATIONS

Structure, structural phase transitions, mechanical properties, defects

Role of electron capture in ion-induced electronic sputtering of insulators *(4 pages)* . . . . . 100101(R)
M. Famá, B. D. Teolis, D. A. Bahr, and R. A. Baragiola

He diffusion in irradiated α-Fe: An *ab-initio*-based rate theory model *(4 pages)* . . . . . 100102(R)
C. J. Ortiz, M. J. Caturla, C. C. Fu, and F. Willaime

Magnetism

Commensurate fluctuations in the pseudogap and incommensurate spin-Peierls phases of TiOCl *(4 pages)* . . . . 100401(R)
J. P. Clancy, B. D. Gaulin, K. C. Rule, J. P. Castellan, and F. C. Chou

Oscillatory tunneling magnetoresistance caused by antiferromagnetic Mn layers *(4 pages)* . . . . . 100402(R)
P. Bose, I. Mertig, and J. Henk

Impurity-doping-induced ferroelectricity in the frustrated antiferromagnet $CuFeO_2$ *(4 pages)* . . . . . 100403(R)
S. Seki, Y. Yamasaki, Y. Shiomi, S. Iguchi, Y. Onose, and Y. Tokura

Superfluidity and superconductivity

Thermodynamics of a heavy-ion-irradiated superconductor: The zero-field transition *(4 pages)* . . . . . 100501(R)
C. J. van der Beek, Thierry Klein, René Brusetti, Christophe Marcenat, Mats Wallin, S. Teitel, and Hans Weber

Superharmonic Josephson relations in unconventional superconductor junctions with a ferromagnetic barrier *(4 pages)* . . . . . 100502(R)
R. Zikic and L. Dobrosavljević-Grujić

Confinement versus deconfinement of Cooper pairs in one-dimensional spin-3/2 fermionic cold atoms *(4 pages)* . . . . . 100503(R)
S. Capponi, G. Roux, P. Azaria, E. Boulat, and P. Lecheminant

Fully anisotropic superconducting transition in ion-irradiated $YBa_2Cu_3O_{7-\delta}$ with a tilted magnetic field *(4 pages)* . . . . . 100504(R)
B. Espinosa-Arronte, M. Andersson, C. J. van der Beek, M. Nikolaou, J. Lidmar, and M. Wallin

Checkerboard and stripe inhomogeneities in cuprates *(4 pages)* . . . . . 100505(R)
G. Seibold, J. Lorenzana, and M. Grilli

Copyright 2007 by The American Physical Society

(Continued)

1098-0121(20070301)75:10;1-#

PHYSICAL REVIEW B THIRD SERIES, VOLUME 75, NUMBER 10 MARCH 2007-1(II)

ARTICLES

Structure, structural phase transitions, mechanical properties, defects

Long-range empirical potential model: Application to fcc transition metals and alloys *(10 pages)* 104101
X. D. Dai, Y. Kong, and J. H. Li

Coherent diffractive imaging and partial coherence *(7 pages)* 104102
Garth J. Williams, Harry M. Quiney, Andrew G. Peele, and Keith A. Nugent

Ferroelectric polarization-leakage current relation in high quality epitaxial $Pb(Zr,Ti)O_3$ films *(14 pages)* 104103
L. Pintilie, I. Vrejoiu, D. Hesse, G. LeRhun, and M. Alexe

Identification of polar nanoclusters in $PbMg_{1/3}Nb_{2/3}O_3$ from NMR spectra *(5 pages)* 104104
M. Vijayakumar, Gina L. Hoatson, and Robert L. Vold

High shock release in ultrafast laser irradiated metals: Scenario for material ejection *(11 pages)* 104105
J. P. Colombier, P. Combis, R. Stoian, and E. Audouard

Electric field-induced phase transitions in (111)-, (110)-, and (100)-oriented $Pb(Mg_{1/3}Nb_{2/3})O_3$ single crystals *(12 pages)* 104106
X. Zhao, W. Qu, X. Tan, A. A. Bokov, and Z.-G. Ye

Structural studies of $Ni_{2+x}Mn_{1-x}Ga$ by powder x-ray diffraction and total energy calculations *(9 pages)* 104107
S. Banik, R. Ranjan, A. Chakrabarti, S. Bhardwaj, N. P. Lalla, A. M. Awasthi, V. Sathe, D. M. Phase, P. K. Mukhopadhyay, D. Pandey, and S. R. Barman

Dimensionality of interstitial cluster motion in bcc-Fe *(13 pages)* 104108
D. A. Terentyev, L. Malerba, and M. Hou

Steric quenching of the switchable mirror effect *(3 pages)* 104109
Troy C. Messina, Casey W. Miller, and John T. Markert

Ab initio study of monoclinic iridium nitride as a high bulk modulus compound *(6 pages)* 104110
Yuan Xu Wang, Masao Arai, Taizo Sasaki, and Chang Zeng Fan

Shear-strain-induced structural and electronic modifications of the molecular crystal 1,1-diamino-2,2-dinitroethylene: Slip-plane flow and band gap relaxation *(10 pages)* 104111
Maija M. Kuklja and Sergey N. Rashkeev

First-principles study of native point defects in hafnia and zirconia *(7 pages)* 104112
J. X. Zheng, G. Ceder, T. Maxisch, W. K. Chim, and W. K. Choi

Global space-group optimization problem: Finding the stablest crystal structure without constraints *(8 pages)* 104113
Giancarlo Trimarchi and Alex Zunger

Elastic constants and tensile properties of Al_2OC by density functional calculations *(5 pages)* 104114
R. Yu, X. F. Zhang, L. C. De Jonghe, and R. O. Ritchie

Phonon and elastic instabilities in rocksalt alkali hydrides under pressure: First-principles study *(8 pages)* 104115
Jingyun Zhang, Lijun Zhang, Tian Cui, Yan Li, Zhi He, Yanming Ma, and Guangtian Zou

Defect kinetics in spinels: Long-time simulations of $MgAl_2O_4$, $MgGa_2O_4$, and $MgIn_2O_4$ *(13 pages)* 104116
B. P. Uberuaga, D. Bacorisen, Roger Smith, J. A. Ball, R. W. Grimes, A. F. Voter, and K. E. Sickafus

Transferable force-constant modeling of vibrational thermodynamic properties in fcc-based Al-*TM* (*TM*=Ti, Zr, Hf) alloys *(15 pages)* 104117
Jefferson Z. Liu, G. Ghosh, A. van de Walle, and M. Asta

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 75, NUMBER 10** **MARCH 2007-1(II)**

Raman spectroscopy of ordered double perovskite La_2CoMnO_6 thin films *(6 pages)* 104118
M. N. Iliev, M. V. Abrashev, A. P. Litvinchuk, V. G. Hadjiev, H. Guo, and A. Gupta

Bond-order potential for simulations of extended defects in tungsten *(16 pages)* 104119
M. Mrovec, R. Gröger, A. G. Bailey, D. Nguyen-Manh, C. Elsässer, and V. Vitek

Inhomogeneous, disordered, and partially ordered systems

Intermediate states of GeO_2 glass under pressures up to 35 GPa *(5 pages)* 104201
Xinguo Hong, Guoyin Shen, Vitali B. Prakapenka, Matt Newville, Mark L. Rivers, and Stephen R. Sutton

Time-dependent universal conductance fluctuations in mesoscopic Au wires: Implications *(7 pages)* 104202
A. Trionfi, S. Lee, and D. Natelson

First-principles prediction of phase-segregating alloy phase diagrams and a rapid design estimate of their transition temperatures *(12 pages)* 104203
N. A. Zarkevich, Teck L. Tan, and D. D. Johnson

Piezoresistivity and tunneling-percolation transport in apparently nonuniversal systems *(9 pages)* 104204
N. Johner, P. Ryser, C. Grimaldi, and I. Balberg

Two different incorporation sites of manganese in single-crystalline monohydrated *L*-asparagine studied by electron paramagnetic resonance *(5 pages)* 104205
K. Krambrock, K. J. Guedes, L. O. Ladeira, M. J. B. Bezerra, T. M. Oliveira, G. A. Bezerra, B. S. Cavada, M. C. F. de Oliveira, M. Z. S. Flores, G. A. Farias, and V. N. Freire

Calorimetric study of the crystallization kinetics of $Cu_{47}Ti_{33}Zr_{11}Ni_8Si_1$ metallic glass *(9 pages)* 104206
S. Venkataraman, H. Hermann, C. Mickel, L. Schultz, D. J. Sordelet, and J. Eckert

Strong nuclear contribution to the optical Kerr effect in niobium oxide containing glasses *(6 pages)* 104207
Arnaud Royon, Lionel Canioni, Bruno Bousquet, Vincent Rodriguez, Michel Couzi, Clara Rivero, Thierry Cardinal, Evelyne Fargin, Martin Richardson, and Kathleen Richardson

Structure and dynamics of *l*-Ge: Neutron scattering experiments and *ab initio* molecular dynamics simulations *(9 pages)* 104208
Virginie Hugouvieux, Emmanuel Farhi, Mark R. Johnson, Fanni Juranyi, Philippe Bourges, and Walter Kob

X-ray reflectivity studies of atomic-level surface-segregation in a liquid eutectic alloy of AuSn *(7 pages)* 104209
Venkatachalapathy S. K. Balagurusamy, Reinhard Streitel, Oleg G. Shpyrko, P. S. Pershan, Mati Meron, and Binhua Lin

Theoretical assessment on the validity of the Wiedemann-Franz law for icosahedral quasicrystals *(5 pages)* 104210
Enrique Maciá and Rogelio Rodríguez-Oliveros

Dynamics, dynamical systems, lattice effects, quantum solids

Neutron scattering measurements of phonons in nickel at elevated temperatures *(7 pages)* 104301
M. Kresch, O. Delaire, R. Stevens, J. Y. Y. Lin, and B. Fultz

Franck-Condon higher order lattice excitations in the $LaFe_{1-x}Cr_xO_3$ (x=0, 0.1, 0.5, 0.9, 1.0) perovskites due to Fe-Cr charge transfer effects *(8 pages)* 104302
Jakob Andreasson, Joakim Holmlund, Christopher S. Knee, Mikael Käll, Lars Börjesson, Stefan Naler, Joakim Bäckström, Michael Rübhausen, Abul Kalam Azad, and Sten-G. Eriksson

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 75, NUMBER 10** **MARCH 2007-1(II)**

Hot-electron effect in palladium thin films *(5 pages)* 104303
Andrea Vinante, Paolo Falferi, Renato Mezzena, and Michael Mück

Impact of ring torsion on the intrachain mobility in conjugated polymers *(7 pages)* 104304
Magnus Hultell and Sven Stafström

Matrix product states algorithms and continuous systems *(15 pages)* 104305
S. Iblisdir, R. Orús, and J. I. Latorre

Lattice dynamics of CoO from first principles *(6 pages)* 104306
U. D. Wdowik and K. Parlinski

Magnetism

Sharp switching of the magnetization in $Fe_{1/4}TaS_2$ *(7 pages)* 104401
E. Morosan, H. W. Zandbergen, Lu Li, Minhyea Lee, J. G. Checkelsky, M. Heinrich, T. Siegrist, N. P. Ong, and R. J. Cava

Synthesis, structure, magnetism and specific heat of $YCrO_4$ and its zircon-to-scheelite phase transition *(7 pages)* 104402
Y. W. Long, L. X. Yang, Y. Yu, F. Y. Li, R. C. Yu, and C. Q. Jin

High-frequency ESR and frequency domain magnetic resonance spectroscopic studies of single molecule magnets in frozen solution *(5 pages)* 104403
F. El Hallak, J. van Slageren, J. Gómez-Segura, D. Ruiz-Molina, and M. Dressel

Magnetization reversal in orthovanadate RVO_3 compounds (R=La, Nd, Sm, Gd, Er, and Y): Inhomogeneities caused by defects in the orbital sector of quasi-one-dimensional orbital systems *(10 pages)* 104404
L. D. Tung, M. R. Lees, G. Balakrishnan, and D. McK. Paul

Deconfined quantum criticality in the two-dimensional antiferromagnetic Heisenberg model with next-nearest-neighbor Ising exchange *(6 pages)* 104405
J. Hove and A. Sudbø

Magnetic order in RMn_2Ge_2 (R=Y,Ca) compounds and their solid solutions with $LaMn_2Ge_2$ *(6 pages)* 104406
S. Di Napoli, A. M. Llois, G. Bihlmayer, and S. Blügel

Micromagnetics of derivative ring-shaped nanomagnets *(6 pages)* 104407
N. Singh, S. Goolaup, W. Tan, A. O. Adeyeye, and N. Balasubramaniam

Pressure-induced monoclinic distortion and charge and orbital ordering in $La_{0.5}Ca_{0.5}MnO_3$ *(6 pages)* 104408
D. P. Kozlenko, L. S. Dubrovinsky, I. N. Goncharenko, B. N. Savenko, V. I. Voronin, E. A. Kiselev, and N. V. Proskurnina

Transport mechanisms in manganite-titanate heterojunctions *(5 pages)* 104409
T. Susaki, N. Nakagawa, and H. Y. Hwang

Kondo physics and dissipation: A numerical renormalization-group approach to Bose-Fermi Kondo models *(23 pages)* 104410
Matthew T. Glossop and Kevin Ingersent

Spin-1 chain with spin-$\frac{1}{2}$ excitations in the bulk *(7 pages)* 104411
Diptiman Sen and Naveen Surendran

Structure, magnetism, and conductivity in epitaxial Ti-doped α-Fe_2O_3 hematite: Experiment and density functional theory calculations *(7 pages)* 104412
T. Droubay, K. M. Rosso, S. M. Heald, D. E. McCready, C. M. Wang, and S. A. Chambers

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 75, NUMBER 10** **MARCH 2007-1(II)**

Magnetic order and exchange interactions in monoatomic 3*d* transition-metal chains *(10 pages)* 104413
Y. Mokrousov, G. Bihlmayer, S. Blügel, and S. Heinze

Magnetic superelasticity and inverse magnetocaloric effect in Ni-Mn-In *(6 pages)* 104414
Thorsten Krenke, Eyüp Duman, Mehmet Acet, Eberhard F. Wassermann, Xavier Moya, Lluís Mañosa, Antoni Planes, Emmanuelle Suard, and Bachir Ouladdiaf

Spiral spin structure in the Heisenberg pyrochlore magnet $CdCr_2O_4$ *(6 pages)* 104415
M. Matsuda, M. Takeda, M. Nakamura, K. Kakurai, A. Oosawa, E. Lelièvre-Berna, J.-H. Chung, H. Ueda, H. Takagi, and S.-H. Lee

Domain-structure relaxation in the tetragonal-to-orthorhombic phase transition of the layered perovskite $Sr_{1.8}La_{0.2}Mn_{1-y}Fe_yO_4$ *(5 pages)* 104416
Wataru Norimatsu and Yasumasa Koyama

Structural phase transition and magnetism in hexagonal $SrMnO_3$ by magnetization measurements and by electron, x-ray, and neutron diffraction studies *(12 pages)* 104417
A. Daoud-Aladine, C. Martin, L. C. Chapon, M. Hervieu, K. S. Knight, M. Brunelli, and P. G. Radaelli

Local defect in a magnet with long-range interactions *(8 pages)* 104418
José A. Hoyos and Thomas Vojta

Metastable resistivity of $La_{0.8}Ca_{0.2}MnO_3$ manganite thin films *(8 pages)* 104419
V. Markovich, G. Jung, Y. Yuzhelevskii, G. Gorodetsky, F. X. Hu, and J. Gao

SU(3) bosons and the spin nematic state on the spin-1 bilinear-biquadratic triangular lattice *(8 pages)* 104420
Peng Li, Guang-Ming Zhang, and Shun-Qing Shen

Disorder and double-exchange spin dynamics in $La_{0.7}Sr_{0.3}MnO_3$ and $La_{0.7}Sr_{0.3}CoO_3$ from NMR hyperfine couplings *(9 pages)* 104421
M. J. R. Hoch, P. L. Kuhns, W. G. Moulton, A. P. Reyes, M. A. Torija, J. F. Mitchell, and C. Leighton

Ab initio analysis of magnetovolume versus chemical effects in CeRuSi and its hydride *(6 pages)* 104422
Samir F. Matar

Electronic phase separation in manganite-insulator interfaces *(7 pages)* 104423
Luis Brey

Magnetic endohedral metallofullerenes with floppy interiors *(6 pages)* 104424
Meichun Qian, Stephen V. Ong, Shiv N. Khanna, and Mark B. Knickelbein

Magnetocaloric study of spin relaxation in dipolar spin ice $Dy_2Ti_2O_7$ *(8 pages)* 104425
M. Orendáč, J. Hanko, E. Čižmár, A. Orendáčová, M. Shirai, and S. T. Bramwell

Study of the structure, segregation, and magnetic properties of Ni-Rh clusters *(10 pages)* 104426
Tristana Sondón, Javier Guevara, and Andrés Saúl

Spin-density distribution in the partially magnetized organic quantum magnet F_2PNNNO *(4 pages)* 104427
A. Zheludev, V. O. Garlea, S. Nishihara, Y. Hosokoshi, A. Cousson, A. Gukasov, and K. Inoue

Bond algebraic liquid phase in strongly correlated multiflavor cold atom systems *(15 pages)* 104428
Cenke Xu and Matthew P. A. Fisher

Subtle competition between ferromagnetic and antiferromagnetic order in a Mn(II)-free radical ferrimagnetic chain *(11 pages)* 104429
E. Lhotel, V. Simonet, E. Ressouche, B. Canals, D. B. Amabilino, C. Sporer, D. Luneau, J. Veciana, and C. Paulsen

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 75, NUMBER 10** **MARCH 2007-1(II)**

Dynamics of molecular nanomagnets in time-dependent external magnetic fields: Beyond the Landau-Zener-Stückelberg model *(8 pages)* 104430
P. Földi, M. G. Benedict, J. Milton Pereira, Jr., and F. M. Peeters

Chiral magnetic ordering in two-dimensional ferromagnets with competing Dzyaloshinsky-Moriya interactions *(8 pages)* 104431
E. Y. Vedmedenko, L. Udvardi, P. Weinberger, and R. Wiesendanger

Role of diffused Co atoms in improving effective exchange coupling in Sm-Co/Fe spring magnets *(6 pages)* 104432
Y. Choi, J. S. Jiang, Y. Ding, R. A. Rosenberg, J. E. Pearson, S. D. Bader, A. Zambano, M. Murakami, I. Takeuchi, Z. L. Wang, and J. P. Liu

Superfluidity and superconductivity

Node-like excitations in superconducting $PbMo_6S_8$ probed by scanning tunneling spectroscopy *(4 pages)* 104501
C. Dubois, A. P. Petrovic, G. Santi, C. Berthod, A. A. Manuel, M. Decroux, Ø. Fischer, M. Potel, and R. Chevrel

Thermodynamics and phase diagrams of layered superconductor/ferromagnet nanostructures *(12 pages)* 104502
Paul H. Barsic, Oriol T. Valls, and Klaus Halterman

Theory of the Luttinger surface in doped Mott insulators *(9 pages)* 104503
Tudor D. Stanescu, Philip Phillips, and Ting-Pong Choy

Crystalline electric field contribution to the magnetoresistance of $Pr_{1-x}La_xOs_4Sb_{12}$ *(5 pages)* 104504
C. R. Rotundu, K. Ingersent, and B. Andraka

Anisotropic properties of the layered superconductor $Cu_{0.07}TiSe_2$ *(5 pages)* 104505
E. Morosan, Lu Li, N. P. Ong, and R. J. Cava

Depairing and Bose-Einstein-condensation temperatures in a simple boson-fermion model of superconductors *(12 pages)* 104506
T. A. Mamedov and M. de Llano

Combined effect of Rashba spin-orbit coupling and disorder on the symmetry of superconducting pairing *(6 pages)* 104507
Ben-Ling Gao and Shi-Jie Xiong

Investigation of the breakpoint region in stacks with a finite number of intrinsic Josephson junctions *(7 pages)* 104508
Yu. M. Shukrinov, F. Mahfouzi, and N. F. Pedersen

Josephson effect due to the long-range odd-frequency triplet superconductivity in SFS junctions with Néel domain walls *(12 pages)* 104509
Ya. V. Fominov, A. F. Volkov, and K. B. Efetov

Relationship between hole density and charge-ordering wave vector in $Sr_{14-x}Ca_xCu_{24}O_{41}$ *(5 pages)* 104510
A. Rusydi, M. Berciu, P. Abbamonte, S. Smadici, H. Eisaki, Y. Fujimaki, S. Uchida, M. Rübhausen, and G. A. Sawatzky

Evidence for very strong electron-phonon coupling in $YBa_2Cu_3O_6$ *(5 pages)* 104511
Guo-meng Zhao

Determining ethylene group disorder levels in κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br *(6 pages)* 104512
A. U. B. Wolter, R. Feyerherm, E. Dudzik, S. Süllow, Ch. Strack, M. Lang, and D. Schweitzer

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 75, NUMBER 10** **MARCH 2007-1(II)**

Magnetization of $RuSr_2GdCu_2O_8$ in pulsed magnetic fields up to 47 T *(4 pages)* 104513
T. P. Papageorgiou, E. Casini, Y. Skourski, T. Herrmannsdörfer, J. Freudenberger, H. F. Braun, and J. Wosnitza

Momentum-dependent relaxation rate and pseudogap in doped magnetic insulators *(5 pages)* 104514
M. M. Zemljič and P. Prelovšek

Symmetric and asymmetric states in a mesoscopic superconducting wire in the voltage-driven regime *(4 pages)* 104515
D. Y. Vodolazov and F. M. Peeters

Persistent single-photon production by tunable on-chip micromaser with a superconducting quantum circuit *(7 pages)* 104516
J. Q. You, Yu-xi Liu, C. P. Sun, and Franco Nori

Peltier effects in Andreev interferometers *(5 pages)* 104517
Pauli Virtanen and Tero T. Heikkilä

Doping dependence of the superconducting gap in $Tl_2Ba_2CuO_{6+\delta}$ from heat transport *(6 pages)* 104518
D. G. Hawthorn, S. Y. Li, M. Sutherland, Etienne Boaknin, R. W. Hill, C. Proust, F. Ronning, M. A. Tanatar, Johnpierre Paglione, Louis Taillefer, D. Peets, Ruixing Liang, D. A. Bonn, W. N. Hardy, and N. N. Kolesnikov

COMMENTS

Comment on "Raman spectroscopy study of Na_xCoO_2 and superconducting $Na_xCoO_2 \cdot yH_2O$" *(2 pages)* 106501
P. Lemmens, P. Scheib, Y. Krockenberger, L. Alff, F. C. Chou, C. T. Lin, H.-U. Habermeier, and B. Keimer

Comment on "Magnon wave forms in the presence of a soliton in two-dimensional antiferromagnets with a staggered field" *(2 pages)* 107401
Denis D. Sheka

Reply to "Comment on 'Magnon wave forms in the presence of a soliton in two-dimensional antiferromagnets with a staggered field' " *(1 page)* 107402
M. P. P. Fonseca and A. S. T. Pires