

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 61, NUMBER 13

CONTENTS

1 APRIL 2000-I

BRIEF REPORTS

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

- Distorted-wave approach to reference-beam x-ray diffraction in transmission cases 8593
Qun Shen
- Transient ordered states in the Fe-Co-Al ternary alloy 8598
Jun Ni and Binglin Gu
- Intermediate scaling regime for multilayer epitaxial growth 8602
Richard S. Ross and Mark F. Gyure

Inhomogeneous, disordered, and partially ordered systems

- Analytical approximation for calculation of the short-range order in disordered alloys with nonpair atomic interactions 8606
R. V. Chepurskii
- Dependence of the conductivity on the concentration and the hopping frequency of charge carriers in fluoride glasses 8610
M. Sural and A. Ghosh
- Tight-binding models on branched structures 8614
R. Burioni, D. Cassi, I. Meccoli, and S. Regina

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

- Quadratic solitons in nonlinear dynamical lattices 8618
Vladimir V. Konotop and Boris A. Malomed
- Debye-Waller factors of copper, silver, and lead 8622
C. K. Shepard, J. G. Mullen, and G. Schupp
- Ab initio* lattice dynamics of sapphire 8625
R. Heid, D. Strauch, and K.-P. Bohnen
- Phonon spectral function for an interacting electron-phonon system 8628
J. E. Han and O. Gunnarsson
- Effective mass of the $\mathbf{E} \otimes \mathbf{e}$ Jahn-Teller polaron in comparison with the Holstein polaron 8631
Yasutami Takada

Magnetism

- Magnetism and spin dynamics in the cluster compound $[\text{Cr}_4\text{S}(\text{O}_2\text{CCH}_3)_8(\text{H}_2\text{O})_4](\text{NO}_3)_2 \cdot \text{H}_2\text{O}$ 8635
Y. Furukawa, M. Luban, F. Borsa, D. C. Johnston, A. V. Mahajan, L. L. Miller, D. Mentrup, J. Schnack,
and A. Bino



Quantum tunneling and quantum-classical transitions in large spin systems	8639
Bambi Hu, De-gang Zhang, and Bo-zang Li	
Stability under pressure and magnetic field of the ferromagnetic-insulating phase in lightly doped $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ crystals	8643
B. Martínez, R. Senis, Ll. Balcells, V. Laukhin, J. Fontcuberta, L. Pinsard, and A. Revcolevschi	
Magnetic anisotropy energy and the anisotropy of the orbital moment of Ni in Ni/Pt multilayers	8647
F. Wilhelm, P. Pouloupoulos, P. Srivastava, H. Wende, M. Farle, K. Baberschke, M. Angelakeris, N. K. Flevaris, W. Grange, J.-P. Kappler, G. Ghiringhelli, and N. B. Brookes	
Critical behavior in $\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_3$	8651
S. Mukherjee, P. Raychaudhuri, and A. K. Nigam	
Microscopic derivation of the Landau-Lifschitz equation for ferromagnetic relaxation	8654
D. R. Fredkin and A. Ron	
Smart structure for tailoring the magneto-optical Kerr effect	8656
Z. Liu, S. M. Zhou, G. Q. Xia, S. Y. Wang, R. J. Zhang, Y. X. Zheng, L. Y. Chen, and J. T. Song	

Superfluidity and superconductivity

Role of confined phonons in thin-film superconductivity	8659
E. H. Hwang, S. Das Sarma, and M. A. Stroscio	
Spin-charge recombination and superconductivity in the t - J model	8663
Sanjoy K. Sarker	
Quasiparticle resonant states induced by a unitary impurity in a d -wave superconductor	8667
Jian-Xin Zhu, T. K. Lee, C. S. Ting, and Chia-Ren Hu	
Coherence effects in conventional layered superconductors	8671
S. P. Zhao	
Magnetoresistance properties of $\text{Bi}_2\text{Sr}_{2-x}\text{La}_x\text{CuO}_{6+\delta}$ superconducting thin films grown on vicinal substrates	8675
Y. Z. Zhang, R. Deltour, J.-F. de Marneffe, Y. L. Qin, L. Li, Z. X. Zhao, A. G. M. Jansen, and P. Wyder	
Electronic properties of CePd_2Si_2 under pressure	8679
S. Raymond and D. Jaccard	
Pseudogap phase in the U(1) gauge theory with incoherent spinon pairs	8683
Xi Dai, Yue Yu, Tao Xiang, and Zhao-bin Su	

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

Tetragonal-to-monoclinic phase transition in a ferroelectric perovskite: The structure of $\text{PbZr}_{0.52}\text{Ti}_{0.48}\text{O}_3$	8687
B. Noheda, J. A. Gonzalo, L. E. Cross, R. Guo, S.-E. Park, D. E. Cox, and G. Shirane	
Full <i>ab initio</i> geometry optimization of all known crystalline phases of Si_3N_4	8696
W. Y. Ching, Lizhi Ouyang, and Julian D. Gale	
Transition to a crystalline high-pressure phase in α - GeO_2 at room temperature	8701
J. Haines, J. M. Léger, and C. Chateau	
Stress concentration near a surface step and shear localization	8707
S. Brochard, P. Beauchamp, and J. Grilhé	
Dislocation pinning by glissile interstitial loops in a nickel crystal: A molecular-dynamics study	8714
D. Rodney and G. Martin	
Pressure-induced structural changes in ZnS	8726
Serge Desgreniers, Luc Beaulieu, and Ian Lepage	
Explicit Gibbs free energy equation of state applied to the carbon phase diagram	8734
Laurence E. Fried and W. Michael Howard	

Proposal for a hardness measurement technique without indenter by gas-cluster-beam bombardment	8744
Zinetulla Insepov, Rafael Manory, Jiro Matsuo, and Isao Yamada	
Thermal and elastic properties of solid neon	8753
Dominic Acocella, George K. Horton, and E. Roger Cowley	
Anomalous metallic lithium phases: Identification by ESR, ENDOR, and the bistable Overhauser effect	8759
C. Vigreux, P. Loiseau, L. Binet, and D. Gourier	
Inhomogeneous, disordered, and partially ordered systems	
Modeling the electrical conductivity of icosahedral quasicrystals	8771
Enrique Maciá	
Role of low-frequency vibrations on sound propagation in glasses at intermediate temperature	8778
A. Criado, M. Jiménez-Ruiz, C. Cabrillo, F. J. Bermejo, M. Grimsditch, H. E. Fischer, S. M. Bennington, and R. S. Eccleston	
Direct computation of the free volume fraction in amorphous polymers from positron lifetime measurements	8784
P. Bandžuch, J. Krištiak, O. Šauša, and J. Zrubcová	
Dynamics, dynamical systems, lattice effects, quantum solids, etc.	
High-pressure lattice dynamics and thermoelasticity of MgO	8793
B. B. Karki, R. M. Wentzcovitch, S. de Gironcoli, and S. Baroni	
High-pressure infrared spectroscopy of solid oxygen	8801
Yuichi Akahama and Haruki Kawamura	
<i>Ab initio</i> structure and zone-center phonons in LiNbO ₃	8806
V. Caciuc, A. V. Postnikov, and G. Borstel	
Electron diffraction studies of phonon and static disorder in SrTiO ₃	8814
Renhui Wang, Yimei Zhu, and S. M. Shapiro	
Condensation kinetics for bosonic excitons interacting with a thermal phonon bath	8823
L. Bányai, P. Gartner, O. M. Schmitt, and H. Haug	
Kinks in a periodically modulated disordered system	8835
Eva Majerníková, Jaroslav Riedel, and Boris A. Malomed	
Magnetism	
Modulated magnetic structure and spin waves in hexagonal CsCuCl ₃ -type antiferromagnets	8843
A. L. Sukstanskii, E. P. Stefanovskii, S. A. Reshetnyak, and V. N. Varyukhin	
Spin Hamiltonians for small Ni clusters	8851
E. Viitala, H. Häkkinen, M. Manninen, and J. Timonen	
Quantum phase interference for quantum tunneling in spin systems	8856
J.-Q. Liang, H. J. W. Müller-Kirsten, D. K. Park, and F.-C. Pu	
Phase diagrams of mixed-spin chains with period 4 using the nonlinear σ model	8863
Ken'ichi Takano	
Fate of spinons in spontaneously dimerized spin- $\frac{1}{2}$ ladders	8871
Dave Allen, Fabian H. L. Essler, and Alexander A. Nersesyan	
Disorder to order transition in the magnetic and electronic properties of URh ₂ Ge ₂	8878
S. Süllow, S. A. M. Mentink, T. E. Mason, R. Feyerherm, G. J. Nieuwenhuys, A. A. Menovsky, and J. A. Mydosh	
Angular dependence and interfacial roughness in exchange-biased ferromagnetic/antiferromagnetic bilayers	8888
Joo-Von Kim, R. L. Stamps, B. V. McGrath, and R. E. Camley	

Temperature and field dependence of the phase separation, structure, and magnetic ordering in $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ ($x=0.47, 0.50$, and 0.53)	8895
Q. Huang, J. W. Lynn, R. W. Erwin, A. Santoro, D. C. Dender, V. N. Smolyaninova, K. Ghosh, and R. L. Greene	
First-principles calculations of magnetic interactions in correlated systems	8906
M. I. Katsnelson and A. I. Lichtenstein	
Evidence for fast oscillations vanishing at the spin-density-wave-metal transition in Bechgaard salts	8913
D. Vignolles, J. P. Ulmet, A. Audouard, M. J. Naughton, and J. M. Fabre	
Transport mechanism in polycrystalline $\text{La}_{0.825}\text{Sr}_{0.175}\text{Mn}_{1-x}\text{Cu}_x\text{O}_3$	8917
Li Pi, Lei Zheng, and Yuheng Zhang	
Magnetic excitations in heavy-fermion CePd_2Si_2	8922
N. H. van Dijk, B. Fåk, T. Charvolin, P. Lejay, and J. M. Mignot	
Observation of an exchange-split alloy surface state	8932
F. Schedin, L. Hewitt, P. Morrall, V. N. Petrov, G. Thornton, and G. Y. Guo	
Isotope effects and charge-gap formation in the charge-ordered phase of colossal magnetoresistance manganites ...	8936
Unjong Yu, Yu. V. Skrypnik, and B. I. Min	
Structural and magnetic properties of the colossal magnetoresistance perovskite $\text{La}_{0.85}\text{Ca}_{0.15}\text{MnO}_3$	8941
M. V. Lobanov, A. M. Balagurov, V. Ju. Pomjakushin, P. Fischer, M. Gutmann, A. M. Abakumov, O. G. D'yachenko, E. V. Antipov, O. I. Lebedev, and G. Van Tendeloo	
Effects of oxygen isotope and stoichiometry on the structural and transport properties of $\text{La}_{0.65}\text{Ca}_{0.35}\text{MnO}_{3-\delta}$	8950
A. K. Heilman, Y. Y. Xue, Y. Y. Sun, R. L. Meng, Y. S. Wang, B. Lorenz, C. W. Chu, J. P. Franck, and Weimin Chen	
Exchange biasing and low-field magnetoresistance in $\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3/\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ bilayers	8955
H. B. Peng, X. X. Zhang, Z. Xie, H. J. Tao, B. Xu, H. Liu, and B. R. Zhao	
Specific heat and optical birefringence of $\text{Fe}_{0.25}\text{Zn}_{0.75}\text{F}_2$	8960
W. C. Barber and D. P. Belanger	
Resonant x-ray scattering studies of the magnetic structure near the surface of an antiferromagnet	8966
G. M. Watson, Doon Gibbs, G. H. Lander, B. D. Gaulin, L. E. Berman, H. J. Matzke, and W. Ellis	
Magnetic microwires as macrospins in a long-range dipole-dipole interaction	8976
L. C. Sampaio, E. H. C. P. Sinnecker, G. R. C. Cernicchiaro, M. Knobel, M. Vázquez, and J. Velázquez	
Brillouin study of long-wavelength spin waves in quasimonatomic Co films with uniaxial perpendicular magnetic anisotropy	8984
Akihiro Murayama, Kyoko Hyomi, James Eickmann, and Charles M. Falco	
Evidence for nonclassical critical behavior of a one-dimensional incommensurately modulated crystal: A ^{35}Cl NQR study of bis(4-chlorophenyl)sulfone	8993
F. Decker and J. Petersson	
One-dimensional fermions with incommensuration	9001
Diptiman Sen and Siddhartha Lal	
High magnetic field study of lattice and magnetic effects on the charge-melting transition in $L_{1/2}\text{Ca}_{1/2}\text{MnO}_3$ perovskites	9014
M. Respaud, A. Llobet, C. Frontera, C. Ritter, J. M. Broto, H. Rakoto, M. Goiran, and J. L. García-Muñoz	
Triplet superconductivity in a one-dimensional ferromagnetic t - J model	9019
G. I. Japaridze and E. Müller-Hartmann	
Structural and magnetic properties of $\text{La}_{0.7}\text{Pb}_{0.3}(\text{Mn}_{1-x}\text{Fe}_x)\text{O}_3$ ($0 \leq x \leq 0.3$) giant magnetoresistance perovskites ...	9028
J. Gutiérrez, A. Peña, J. M. Barandiarán, J. L. Pizarro, T. Hernández, L. Lezama, M. Insausti, and T. Rojo	
Theory of scanning tunneling spectroscopy of a magnetic adatom on a metallic surface	9036
Avraham Schiller and Selman Hershfield	
Magnetoresistance in doped magnetic tunnel junctions: Effect of spin scattering and impurity-assisted transport	9047
R. Jansen and J. S. Moodera	

Effects of dilute Zn impurities on the uniform magnetic susceptibility of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$	9051
N. Bulut	
Superfluidity and superconductivity	
Path-integral Monte Carlo simulation of helium at negative pressures	9055
Gregory H. Bauer, David M. Ceperley, and Nigel Goldenfeld	
Distribution functions in nonequilibrium theory of superconductivity and Andreev spectroscopy in unconventional superconductors	9061
Matthias Eschrig	
Quantum fluctuations and the c -axis optical conductivity of high- T_c superconductors	9077
L. B. Ioffe and A. J. Millis	
Microwave conductivity due to impurity scattering in a d -wave superconductor	9088
A. J. Berlinsky, D. A. Bonn, R. Harris, and C. Kallin	
Incommensurate charge fluctuations in a d -wave superconductor	9095
Khee-Kyun Voo, W. C. Wu, Jian-Xin Li, and T. K. Lee	
Dynamics of adiabatic Andreev levels in microwave-irradiated superconducting single-mode contacts	9101
N. I. Lundin	
Loss of π -junction behavior in an interacting impurity Josephson junction	9109
Aashish A. Clerk and Vinay Ambegaokar	
Irreversibility line of overdoped $\text{Bi}_{2+x}\text{Sr}_{2-(x+y)}\text{Cu}_{1+y}\text{O}_{6\pm\delta}$ at ultralow temperatures and high magnetic fields	9113
A. Morello, A. G. M. Jansen, R. S. Gonnelli, and S. I. Vedenev	
Metastability line in the phase diagram of vortices in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$	9118
B. Sas, F. Portier, K. Vad, B. Keszei, L. F. Kiss, N. Hegman, I. Puha, S. Mészáros, and F. I. B. Williams	
Josephson vortices at tricrystal boundaries	9122
V. G. Kogan, J. R. Clem, and J. R. Kirtley	
Magnetoelastic model for the relaxation of lanthanide ions in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ observed by neutron scattering	9130
Stephen W. Lovesey and Urs Staub	
Electronic structure of $\text{YBa}_2\text{Cu}_3\text{O}_x$ and $\text{YBa}_2\text{Cu}_4\text{O}_8$ studied by soft-x-ray absorption and emission spectroscopies	9140
J.-H. Guo, S. M. Butorin, N. Wassdahl, J. Nordgren, P. Berastegut, and L.-G. Johansson	
Magnetoresistance of granular superconducting metals in a strong magnetic field	9145
I. S. Beloborodov, K. B. Efetov, and A. I. Larkin	
c -axis tunneling in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}/\text{PrBa}_2\text{Cu}_3\text{O}_{7-\delta}$ superlattices	9162
J. C. Martínez, A. Schattke, M. Jourdan, G. Jakob, and H. Adrian	
Confinement and Bose condensation in gauge theory of high- T_c superconductors	9166
Naoto Nagaosa and Patrick A. Lee	
Simulation and study of the percolation effect in the magnetic susceptibility of high-temperature superconducting composites	9176
E. Bruneel, A. J. Ramirez-Cuesta, I. Van Driessche, and S. Hoste	
Cumulative Author Index	9181