

RAPID COMMUNICATIONS

Structure, structural phase transitions, mechanical properties, defects

- Structure of a 2° (010) Cu twist boundary interface and the segregation of vacancies and He atoms (4 pages) 060101(R)
Enrique Martínez, John P. Hirth, Michael Nastasi, and Alfredo Caro

Inhomogeneous, disordered, and partially ordered systems

- Short-range structural signature of excess specific heat and fragility of metallic-glass-forming supercooled liquids (5 pages) 060201(R)
Jun Ding, Yong-Qiang Cheng, Hongwei Sheng, and Evan Ma

Dynamics, dynamical systems, lattice effects:

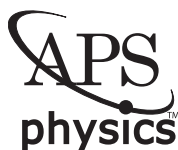
- High-temperature phonon stabilization of γ -uranium from relativistic first-principles theory (4 pages) 060301(R)
Per Söderlind, B. Grabowski, L. Yang, A. Landa, T. Björkman, P. Souvatzis, and O. Eriksson

Magnetism

- Pronounced first-order metamagnetic transition in the paramagnetic heavy-fermion system CeTiGe (5 pages) 060401(R)
M. Deppe, S. Lausberg, F. Weickert, M. Brando, Y. Skourski, N. Caroca-Canales, C. Geibel, and F. Steglich
- Ground-state phase diagram of the quantum $J_1 - J_2$ model on the honeycomb lattice (4 pages) 060402(R)
Fabio Mezzacapo and Massimo Boninsegni
- Cubic MnSb: Epitaxial growth of a predicted room temperature half-metal (5 pages) 060403(R)
James D. Aldous, Christopher W. Burrows, Ana M. Sánchez, Richard Beanland, Ian Maskery,
Matthew K. Bradley, Manuel dos Santos Dias, Julie B. Staunton, and Gavin R. Bell

Superfluidity and superconductivity

- Quasiclassical and ultraquantum decay of superfluid turbulence (4 pages) 060501(R)
A. W. Baggaley, C. F. Barenghi, and Y. A. Sergeev
- Size-induced melting and reentrant freezing in fullerene-doped helium clusters (4 pages) 060502(R)
F. Calvo
- Contrasts in electron correlations and inelastic scattering between LiFeP and LiFeAs revealed by charge transport (5 pages) 060503(R)
S. Kasahara, K. Hashimoto, H. Ikeda, T. Terashima, Y. Matsuda, and T. Shibauchi



CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 85, NUMBER 6

FEBRUARY 2012-1(II)

Mass of a vortex in a superconducting film measured via magneto-optical imaging plus ultrafast heating and cooling (<i>4 pages</i>)	060504(R)
Daniel Golubchik, Emil Polturak, and Gad Koren	
Superconducting gap structure of CeIrIn ₅ from field-angle-resolved measurements of its specific heat (<i>4 pages</i>)	060505(R)
Shunichiro Kittaka, Yuya Aoki, Toshiro Sakakibara, Akito Sakai, Satoru Nakatsuji, Yasumasa Tsutsumi, Masanori Ichioka, and Kazushige Machida	
Absolute value and temperature dependence of the magnetic penetration depth in Ba(Co _{0.074} Fe _{0.926}) ₂ As ₂ (<i>5 pages</i>)	060506(R)
Oren Ofer, J. C. Baglo, M. D. Hossain, R. F. Kiefl, W. N. Hardy, A. Thaler, H. Kim, M. A. Tanatar, P. C. Canfield, R. Prozorov, G. M. Luke, E. Morenzoni, H. Saadaoui, A. Suter, T. Prokscha, B. M. Wojek, and Z. Salman	
Low-energy subgap states in multichannel <i>p</i> -wave superconducting wires (<i>5 pages</i>)	060507(R)
G. Kells, D. Meidan, and P. W. Brouwer	
Anomalous magnetotransport in the heavy-fermion superconductor Ce ₂ PdIn ₈ (<i>4 pages</i>)	060508(R)
Daniel Gnida, Marcin Matusiak, and Dariusz Kaczorowski	

ARTICLES

Structure, structural phase transitions, mechanical properties, defects

Trends in the elastic response of binary early transition metal nitrides (<i>9 pages</i>)	064101
David Holec, Martin Friák, Jörg Neugebauer, and Paul H. Mayrhofer	
Evidence of oxygen-dependent modulation in LuFe ₂ O ₄ (<i>10 pages</i>)	064102
J. Bourgeois, M. Hervieu, M. Poienar, A. M. Abakumov, E. Elkaïm, M. T. Sougrati, F. Porcher, F. Damay, J. Rouquette, G. Van Tendeloo, A. Maignan, J. Haines, and C. Martin	
Shear modulus of an elastic solid under external pressure as a function of temperature: The case of helium (<i>6 pages</i>)	064103
Felipe Barra, Fernando Lund, Nicolás Mujica, and Sergio Rica	
Regular nanodomain vertex arrays in BiFeO ₃ single crystals (<i>7 pages</i>)	064104
A. Berger, D. Hesse, A. Hähnel, M. Arredondo, and M. Alexe	
Systematic study of ferroelectric, interfacial, oxidative, and doping effects on conductance of Pt/BaTiO ₃ /Pt ferroelectric tunnel junctions (<i>8 pages</i>)	064105
Lei Shen (沈雷), Tiejun Zhou, Zhaoqiang Bai, Minggang Zeng, Jing Qiang Goh, Zhi-min Yuan, Guchang Han, Bo Liu, and Yuan Ping Feng	
Atomistic modeling of As diffusion in ZnO (<i>8 pages</i>)	064106
B. Puchala and D. Morgan	
EXAFS evidence for a primary Zn _{Li} dopant in LiNbO ₃ (<i>12 pages</i>)	064107
F. Bridges, J. Castillo-Torres, B. Car, S. Medling, and M. Kozina	
Probing grain boundary sink strength at the nanoscale: Energetics and length scales of vacancy and interstitial absorption by grain boundaries in α -Fe (<i>21 pages</i>)	064108
M. A. Tschopp, K. N. Solanki, F. Gao, X. Sun, M. A. Khaleel, and M. F. Horstemeyer	
Flexibility windows and compression of monoclinic and orthorhombic silicalites (<i>5 pages</i>)	064109
Asel Sartbaeva, Julien Haines, Olivier Cambon, Mario Santoro, Federico Gorelli, Claire Levelut, Gaston Garbarino, and Stephen A. Wells	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 85, NUMBER 6

FEBRUARY 2012-1(II)

Pressure-induced group-subgroup phase transitions and post-cotunnite phases in actinide dioxides (<i>10 pages</i>)	064110
Hong X. Song, Hua Y. Geng, and Q. Wu	
Electronic origin of the anomalous segregation behavior of Cr in Fe-rich Fe-Cr alloys (<i>6 pages</i>)	064111
Maximilien Levesque, Michèle Gupta, and Raju P. Gupta	
First-principles study of structural and vibrational properties of SrZrO ₃ (<i>8 pages</i>)	064112
Safari Amisi, Eric Bousquet, Karume Katcho, and Philippe Ghosez	
Constraints on the phase diagram of molybdenum from first-principles free-energy calculations (<i>13 pages</i>)	064113
C. Cazorla, D. Alfè, and M. J. Gillan	
Intermolecular control of thermoswitching and photoswitching phenomena in two spin-crossover polymorphs (<i>9 pages</i>)	064114
M. Buron-Le Cointe, J. Hébert, C. Baldé, N. Moisan, L. Toupet, P. Guionneau, J. F. Létard, E. Freysz, H. Cailleau, and E. Collet	
Mechanisms for the decomposition and dehydrogenation of Li amide/imide (<i>12 pages</i>)	064115
Khang Hoang, Anderson Janotti, and Chris G. Van de Walle	
Evidence for diffuse ferroelectric phase transition and cooperative tricritical freezing of random-site dipoles due to off-centered Bi ³⁺ ions in the average cubic lattice of (Ba _{1-x} Bi _x)(Ti _{1-x} Fe _x)O ₃ (<i>8 pages</i>)	064116
Anar Singh, Chikako Moriyoshi, Yoshihiro Kuroiwa, and Dhananjai Pandey	
Phenomenological thermodynamic potential for CaTiO ₃ single crystals (<i>10 pages</i>)	064117
Yijia Gu, Karin Rabe, Eric Bousquet, Venkatraman Gopalan, and Long-Qing Chen	
Exploring the high-pressure behavior of superhard tungsten tetraboride (<i>8 pages</i>)	064118
Miao Xie, Reza Mohammadi, Zhu Mao, Matt M. Armentrout, Abby Kavner, Richard B. Kaner, and Sarah H. Tolbert	
First-principles investigation of the structural phases and enhanced response properties of the BiFeO ₃ -LaFeO ₃ multiferroic solid solution (<i>10 pages</i>)	064119
O. E. González-Vázquez, Jacek C. Wojdeł, Oswaldo Diéguez, and Jorge Íñiguez	
Inhomogeneous, disordered, and partially ordered systems	
Structure and triclustering in Ba-Al-O glass (<i>12 pages</i>)	064201
Lawrie B. Skinner, Adrian C. Barnes, Philip S. Salmon, Henry E. Fischer, James W. E. Drewitt, and Veijo Honkimäki	
Dynamics, dynamical systems, lattice effects:	
Extremal transmission through a microwave photonic crystal and the observation of edge states in a rectangular Dirac billiard (<i>8 pages</i>)	064301
S. Bittner, B. Dietz, M. Miski-Oglu, and A. Richter	
Analyzing the frequency shift of physisorbed CO ₂ in metal organic framework materials (<i>8 pages</i>)	064302
Yanpeng Yao, Nour Nijem, Jing Li, Yves J. Chabal, David C. Langreth, and T. Thonhauser	
Adaptive-boost molecular dynamics simulation of carbon diffusion in iron (<i>7 pages</i>)	064303
Akio Ishii, Shigenobu Ogata, Hajime Kimizuka, and Ju Li	

(Continued)

Magnetism

Numerical study of the thermodynamics of clinoatacamite (7 pages)	064401
Ehsan Khatami, Joel S. Helton, and Marcos Rigol	
Al doping effect on magnetic phase transitions of magnetoelectric hexaferrite $\text{Ba}_{0.7}\text{Sr}_{1.3}\text{Zn}_2(\text{Fe}_{1-x}\text{Al}_x)_{12}\text{O}_{22}$ (9 pages)	064402
Hun Chang, Hak Bong Lee, Young-Sang Song, Jae-Ho Chung, S. A. Kim, I. H. Oh, M. Reehuis, and J. Schefer	
Asymmetric magnetization reversal in dipolarly coupled spin valve structures with perpendicular magnetic anisotropy (6 pages)	064403
M. Gottwald, M. Hehn, D. Lacour, T. Hauet, F. Montaigne, S. Mangin, P. Fischer, M.-Y. Im, and A. Berger	
Decorated Shastry-Sutherland lattice in the spin- $\frac{1}{2}$ magnet $\text{CdCu}_2(\text{BO}_3)_2$ (15 pages)	064404
O. Janson, I. Rousochatzakis, A. A. Tsirlin, J. Richter, Yu. Skourski, and H. Rosner	
Anharmonic phonons and magnons in BiFeO_3 (7 pages)	064405
O. Delaire, M. B. Stone, J. Ma, A. Huq, D. Gout, C. Brown, K. F. Wang, and Z. F. Ren	
Interplay between crystal-field splitting and superexchange interaction in the t_{2g} orbital Mott insulator (15 pages)	064406
Sergey Krivenko	
Surface spin polarization of the nonstoichiometric Heusler alloy Co_2MnSi (10 pages)	064407
Jan-Peter Wüstenberg, Roman Fetzner, Martin Aeschlimann, Mirko Cinchetti, Jan Minár, Jürgen Braun, Hubert Ebert, Takayuki Ishikawa, Tetsuya Uemura, and Masafumi Yamamoto	
Theory of laser-induced demagnetization at high temperatures (9 pages)	064408
A. Manchon, Q. Li, L. Xu, and S. Zhang	
Dynamics of successive minor hysteresis loops (8 pages)	064409
Y. W. Windsor, A. Gerber, and M. Karpovski	
Transport spin polarization of the rare-earth transition-metal alloy $\text{Co}_{1-x}\text{Gd}_x$ (5 pages)	064410
A. D. Naylor, G. Burnell, and B. J. Hickey	
Nonlinear behavior for the uniform mode and horizontal standing spin-wave modes in metallic ferromagnetic microstrips: Experiment and theory (7 pages)	064411
M. P. Wismayer, B.W. Southern, X. L. Fan, Y. S. Gui, C.-M. Hu, and R. E. Camley	
Single-crystal study of the kagome antiferromagnet $\text{U}_3\text{Ru}_4\text{Al}_{12}$ (9 pages)	064412
R. Troć, M. Pasturel, O. Tougaard, A. P. Sazonov, A. Gukasov, C. Sułkowski, and H. Noël	
Block magnetism coupled with local distortion in the iron-based spin-ladder compound BaFe_2Se_3 (5 pages)	064413
Yusuke Nambu, Kenya Ohgushi, Shunpei Suzuki, Fei Du, Maxim Avdeev, Yoshiya Uwatoko, Koji Munakata, Hiroshi Fukazawa, Songxue Chi, Yutaka Ueda, and Taku J. Sato	
Transverse magneto-optical effects in nanoscale disks (11 pages)	064414
R. Alcaraz de la Osa, J. M. Saiz, F. Moreno, P. Vavassori, and A. Berger	
Magnetic field effect on the fractal cluster spin-glass phase of an Ising antiferromagnet near the first-neighbor percolation threshold: $\text{Fe}_{0.25}\text{Zn}_{0.75}\text{F}_2$ (10 pages)	064416
K. A. P. de Lima, J. B. Brito, P. H. R. Barbosa, E. P. Raposo, and M. D. Coutinho-Filho	

(Continued)

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 85, NUMBER 6

FEBRUARY 2012-1(II)

Interfacial geometry dependence of the iron magnetic moment: The case of MgO/Fe/MgO (7 pages)	064417
Juan Ignacio Beltrán, Lluís Balcells, and Carlos Martínez-Boubeta	
Proposal for electron quantum spin Talbot effect (5 pages)	064418
W. X. Tang, D. M. Paganin, and W. Wan	
High domain wall velocities in in-plane magnetized (Ga,Mn)(As,P) layers (6 pages)	064419
L. Thevenard, S. A. Hussain, H. J. von Bardeleben, M. Bernard, A. Lemaître, and C. Gourdon	
Frustrated spin chains in strong magnetic field: Dilute two-component Bose gas regime (17 pages)	064420
A. K. Kolezhuk, F. Heidrich-Meisner, S. Greschner, and T. Vekua	
Magnetic excitations in L -edge resonant inelastic x-ray scattering from cuprate compounds (15 pages)	064421
Jun-ichi Igarashi and Tatsuya Nagao	
Magnetic excitations in L -edge resonant inelastic x-ray scattering from one-dimensional cuprates (10 pages)	064422
Jun-ichi Igarashi and Tatsuya Nagao	
Exact diagonalization results for resonant inelastic x-ray scattering spectra of one-dimensional Mott insulators (7 pages)	064423
Stefanos Kourtis, Jeroen van den Brink, and Maria Daghofer	
Superfluidity and superconductivity	
☞ Origin of the material dependence of T_c in the single-layered cuprates (12 pages)	064501
Hirofumi Sakakibara, Hidetomo Usui, Kazuhiko Kuroki, Ryotaro Arita, and Hideo Aoki	
Regimes of flux transport at microwave frequencies in nanostructured high- T_c films (6 pages)	064503
R. Wördenweber, E. Hollmann, J. Schubert, R. Kutzner, and G. Panaitov	
Structure of the oxygen-annealed chalcogenide superconductor $\text{Fe}_{1.08}\text{Te}_{0.55}\text{Se}_{0.45}\text{O}_x$ (6 pages)	064504
Hefei Hu, Jian-Min Zuo, Mao Zheng, James N. Eckstein, Wan Kyu Park, Laura H. Greene, Jinsheng Wen, Zhijun Xu, Zhiwei Lin, Qiang Li, and Genda Gu	
Domain structure and magnetic pinning in ferromagnetic/superconducting hybrids (15 pages)	064505
V. Vlasko-Vlasov, A. Buzdin, A. Melnikov, U. Welp, D. Rosenmann, L. Uspenskaya, V. Fratello, and W. Kwok	
Magnetic field dependence of the quantum tunneling of normal-superconductor interfaces in a type-I Pb superconductor (5 pages)	064506
Saül Vélez, Ricardo Zarzuela, Antoni García-Santiago, and Javier Tejada	
Pseudogap in the chain states of $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$ (7 pages)	064507
V. B. Zabolotnyy, A. A. Kordyuk, D. Evtushinsky, V. N. Strocov, L. Patthey, T. Schmitt, D. Haug, C. T. Lin, V. Hinkov, B. Keimer, B. Büchner, and S. V. Borisenko	
Velocity-induced reorientation of a fast driven Abrikosov lattice (5 pages)	064508
S. Okuma, D. Shimamoto, and N. Kokubo	
Magnetic-field tuned anisotropy in superconducting $\text{Rb}_x\text{Fe}_{2-y}\text{Se}_2$ (6 pages)	064509
S. Bosma, R. Puzniak, A. Krzton-Maziopa, M. Bendele, E. Pomjakushina, K. Conder, H. Keller, and S. Weyeneth	

(Continued)

Reconstructing the bulk Fermi surface and superconducting gap properties from neutron scattering experiments (9 pages)	064510
Tanmoy Das, R. S. Markiewicz, and A. Bansil	
Upper critical fields and two-band superconductivity in $\text{Sr}_{1-x}\text{Eu}_x(\text{Fe}_{0.89}\text{Co}_{0.11})_2\text{As}_2$ ($x = 0.20$ and 0.46) (5 pages)	064511
Rongwei Hu, Eun Deok Mun, M. M. Altarawneh, C. H. Mielke, V. S. Zapf, S. L. Bud'ko, and P. C. Canfield	
Experimental and materials considerations for the topological superconducting state in electron- and hole-doped semiconductors: Searching for non-Abelian Majorana modes in 1D nanowires and 2D heterostructures (11 pages)	064512
Jay D. Sau, Sumanta Tewari, and S. Das Sarma	
Upper critical field and thermally activated flux flow in single-crystalline $\text{Tl}_{0.58}\text{Rb}_{0.42}\text{Fe}_{1.72}\text{Se}_2$ (7 pages)	064513
L. Jiao, Y. Kohama, J. L. Zhang, H. D. Wang, B. Maiorov, F. F. Balakirev, Y. Chen, L. N. Wang, T. Shang, M. H. Fang, and H. Q. Yuan	
Extraction of normal electron self-energy and pairing self-energy in the superconducting state of the $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ superconductor via laser-based angle-resolved photoemission (7 pages)	064514
Wentao Zhang, Jin Mo Bok, Jae Hyun Yun, Junfeng He, Guodong Liu, Lin Zhao, Haiyun Liu, Jianqiao Meng, Xiaowen Jia, Yingying Peng, Daixiang Mou, Shanyu Liu, Li Yu, Shaolong He, Xiaoli Dong, Jun Zhang, J. S. Wen, Z. J. Xu, G. D. Gu, Guiling Wang, Yong Zhu, Xiaoyang Wang, Qinjun Peng, Zhimin Wang, Shenjin Zhang, Feng Yang, Chuangtian Chen, Zuyan Xu, H.-Y. Choi, C. M. Varma, and X. J. Zhou	
Suppression of the melting line in a weakly disordered flux-line system (6 pages)	064515
Gautam I. Menon, G. Ravikumar, M. J. Higgins, and S. Bhattacharya	
Stability and Josephson effect of time-reversal-symmetry-broken multicomponent superconductivity induced by frustrated intercomponent coupling (5 pages)	064516
Xiao Hu and Zhi Wang	
Coexistence of superconductivity and magnetism in FeSe_{1-x} under pressure (11 pages)	064517
M. Bendele, A. Ichsanow, Yu. Pashkevich, L. Keller, Th. Strässle, A. Gusev, E. Pomjakushina, K. Conder, R. Khasanov, and H. Keller	
Cluster-based superconducting tunneling networks (3 pages)	064518
Yury N. Ovchinnikov and Vladimir Z. Kresin	
Anomalous dependence of c -axis polarized Fe B_{1g} phonon mode with Fe and Se concentrations in $\text{Fe}_{1+y}\text{Te}_{1-x}\text{Se}_x$ (10 pages)	064519
Y. J. Um, A. Subedi, P. Toulemonde, A. Y. Ganin, L. Boeri, M. Rahlenbeck, Y. Liu, C. T. Lin, S. J. E. Carlsson, A. Sulpice, M. J. Rosseinsky, B. Keimer, and M. Le Tacon	
Effective three-particle interactions in low-energy models for multiband systems (14 pages)	064520
Stefan A. Maier and Carsten Honerkamp	
Three-dimensional numerical analysis of terahertz radiation emitted from intrinsic Josephson junctions with hot spots (8 pages)	064521
Hidehiro Asai, Masashi Tachiki, and Kazuo Kadowaki	
Doping dependence of Hall coefficient and evolution of coherent electronic state in the normal state of the Fe-based superconductor $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ (5 pages)	064522
Kenya Ohgushi and Yoko Kiuchi	

(Continued)

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 85, NUMBER 6

FEBRUARY 2012-1(II)

COMMENTS

- Comment on “Rapid chemical and topological ordering in supercooled liquid $\text{Cu}_{46}\text{Zr}_{54}$ ” (3 pages) 066101
J.-P. Harvey and A. E. Gheribi
- Reply to “Comment on ‘Rapid chemical and topological ordering in supercooled liquid $\text{Cu}_{46}\text{Zr}_{54}$ ’” (5 pages) 066102
V. Wessels, A. K. Gangopadhyay, K. K. Sahu, R. W. Hyers, S. M. Canepari, J. R. Rogers, M. J. Kramer,
A. I. Goldman, D. Robinson, J. W. Lee, J. R. Morris, and K. F. Kelton

ERRATA

- Publisher’s Note: $B - T$ phase diagram of CoCr_2O_4 in magnetic fields up to 14 T
[Phys. Rev. B **85**, 012101 (2012)] (1 page) 069901(E)
A. V. Pronin, M. Uhlarz, R. Beyer, T. Fischer, J. Wosnitza, B. P. Gorshunov, G. A. Komandin,
A. S. Prokhorov, M. Dressel, A. A. Bush, and V. I. Torgashev