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
500 Sunnyside Boulevard
Woodbury, NY 11797-2999

THIRD SERIES, VOLUME 56, NUMBER 23 ***CONTENTS*** **15 DECEMBER 1997-I**

BRIEF REPORTS

Electronic structure: wide-band, narrow-band, and strongly correlated systems

c/a anomalies and electronic topological transitions in Cd 14 871
B. K. Godwal, S. Meenakshi, and R. S. Rao

Temperature-dependent single-particle properties of the two-dimensional Hubbard model 14 875
V. Zlatić, S. Grabowski, and P. Entel

Lattice effects on the charge-ordering transition in $R_{0.5}Sr_{1.5}MnO_4$ 14 879
Y. Moritomo, A. Nakamura, S. Mori, N. Yamamoto, K. Ohoyama, and M. Ohashi

Positive magnetoresistance in quasi-one-dimensional conductors 14 883
Ivar Martin and Philip Phillips

Low-energy electron mean free path and its spin dependence in transition metals 14 886
Henri-Jean Drouhin

Semiconductors I: bulk

Anomalous temperature dependence of deep-level-transient-spectroscopy peak amplitude 14 890
D. Cavalcoli, A. Cavallini, and E. Gombia

WKB approximation of screened two-dimensional excitons 14 893
J. A. Reyes and M. del Castillo-Mussot

Midgap traps related to compensation processes in CdTe alloys 14 897
A. Castaldini, A. Cavallini, B. Fraboni, P. Fernandez, and J. Piqueras

Noncollinear interlayer coupling across a semiconductor spacer 14 901
Ke Xia, Weiyi Zhang, Mu Lu, and Hongru Zhai

Semiconductors II: surfaces, interfaces, microstructures, and related topics

Numerical analysis of eigenmodes localized at line defects in photonic lattices 14 905
Kazuaki Sakoda, Tsuyoshi Ueta, and Kazuo Ohtaka

Surface processes during heteroepitaxy of ZnSe on GaAs(111)*A* as observed by reflection high-energy electron diffraction 14 909
Akihiro Ohtake, Shiro Miwa, Li-Hsin Kuo, Kozo Kimura, Tetsuji Yasuda, Chengguo Jin, and Takafumi Yao

Thickness effect on impurity-bound polaronic energy levels in a parabolic quantum dot in magnetic fields 14 913
Chuan-Yu Chen, Pei-Wan Jin, Wai-Sang Li, and D. L. Lin

Nonlinear magnetoconductance of nanowires 14 917
E. N. Bogachek, A. G. Scherbakov, and Uzi Landman

Effects of interface morphology on Schottky-barrier heights: A case study on Al/GaAs(001) 14 921
A. Ruini, R. Resta, and S. Baroni

Quantum confinement effect in silicon quantum-well layers 14 925
Jian-Bai Xia and K. W. Cheah

Electronic spectrum of quantum-δ-wells superlattices in an electric field 14 929
P. Carpena, V. Gasparian, and M. Ortuño

(Continued)

0163-1829(19971215)56:23;1-V

PHYSICAL REVIEW B THIRD SERIES, VOLUME 56, NUMBER 23 15 DECEMBER 1997-I

Control of band discontinuities at (100) GaAs/AlAs interfaces by ZnSe insertion layers: Comparison with Si insertion layers 14 933
Toshio Saito
Phase breaking of nonequilibrium electrons in a ballistic quantum dot 14 937
H. Linke, J. P. Bird, J. Cooper, P. Omling, Y. Aoyagi, and T. Sugano
Composite fermions and the half-filled state 14 941
D. C. Marinescu, J. J. Quinn, P. Sitko, and K. S. Yi

Surface physics, low-dimensional systems, and related topics

Isotope effect in hydrogen surface diffusion 14 944
Thomas R. Mattsson and Göran Wahnström
Anomalous thermal behavior of the Fe(100) surface observed by grazing ion-surface scattering 14 948
R. Pfandzelter, T. Igel, and H. Winter
Adsorbed states of H on Ni(111) at 100 K: A vibrational study 14 952
H. Yanagita, J. Sakai, T. Aruga, N. Takagi, and M. Nishijima
Conductance eigenchannels in nanocontacts 14 956
Mads Brandbyge, Mads R. Sørensen, and Karsten W. Jacobsen
General crossovers from two-dimensional Mott $T^{-1/3}$ to soft-gap $T^{-\nu}$ variable-range hopping 14 960
Nguyen V. Lien and Ralph Rosenbaum

ARTICLES

Electronic structure: wide-band, narrow-band, and strongly correlated systems

Point-contact spectroscopy of $YbBe_{13}$ 14 964
A. Nowack, S. Wasser, W. Schlabitz, O. E. Kvitnitskaya, and Z. Fisk
Supercell technique for total-energy calculations of finite charged and polar systems 14 972
M. R. Jarvis, I. D. White, R. W. Godby, and M. C. Payne
Adaptive-coordinate electronic structure of $3d$ bands: TiO_2 ..... 14 979
D. R. Hamann
Momentum-matrix-element calculation using pseudopotentials 14 985
Hiroyuki Kageshima and Kenji Shiraishi
Electronic, structural, and optical properties of crystalline yttria 14 993
Yong-Nian Xu, Zhong-quan Gu, and W. Y. Ching
Charge and spin structures of a $d_{x^2-y^2}$ superconductor in the proximity of an antiferromagnetic Mott insulator 15 001
F. F. Assaad, M. Imada, and D. J. Scalapino
Aspects of the ground state of the $U=\infty$ Hubbard ladder 15 015
Masanori Kohno
Excitons and optical absorption in one-dimensional extended Hubbard models with short- and long-range interactions 15 025
F. B. Gallagher and S. Mazumdar
Configuration-dependent hybridization in electron spectroscopies of Ce-based compounds 15 040
N. Witkowski, F. Bertran, and D. Malterre
High-energy Ce-$3d$ photoemission: Bulk properties of CeM_2 (M=Fe,Co,Ni) and Ce_7Ni_3 ..... 15 047
L. Braicovich, N. B. Brookes, C. Dallera, M. Salvietti, and G. L. Olcese
Spectroscopy of metallic and insulating V_2O_3 ..... 15 056
O. Müller, J. P. Urbach, E. Goering, T. Weber, R. Barth, H. Schuler, M. Klemm, S. Horn, and M. L. denBoer

(Continued)

PHYSICAL REVIEW B THIRD SERIES, VOLUME 56, NUMBER 23 15 DECEMBER 1997-I

Crystalline electric field of the bromo-elpasolites Cs_2NaRBr_6 (R=rare earth) determined by inelastic neutron scattering 15 062
Albert Furrer and Hans-Ueli Güdel
Transport properties of Ce-doped $RMnO_3$ (R=La, Pr, and Nd) manganites 15 073
P. Mandal and S. Das
Filled skutterudite antimonides: Electron crystals and phonon glasses 15 081
B. C. Sales, D. Mandrus, B. C. Chakoumakos, V. Keppens, and J. R. Thompson
Optical nonlinear response of a single nonlinear dielectric layer sandwiched between two linear dielectric structures 15 090
E. Lidorikis, K. Busch, Qiming Li, C. T. Chan, and C. M. Soukoulis
Infrared intensity and local vibrations of charged solitons 15 100
Anna Painelli, Alberto Girlando, Luca Del Freo, and Zoltan G. Soos
Ce^{3+} luminescent centers of different symmetries in $KMgF_3$ single crystals 15 109
R. Francini, U. M. Grassano, L. Landi, A. Scacco, M. D'Elena, M. Nikl, N. Cechova, and N. Zema
Effect of valley-spin degeneracy on the screening of charged-impurity centers in two- and three-dimensional electronic devices 15 115
C. Bulutay, I. Al-Hayek, and M. Tomak
Observation of universal conductance-fluctuation crossovers in mesoscopic Li wires 15 124
J. S. Moon, Norman O. Birge, and Brage Golding

Semiconductors I: bulk

Generation of amorphous silicon structures by rapid quenching: A molecular-dynamics study 15 133
Manabu Ishimaru, Shinji Munetoh, and Teruaki Motooka
Microscopic structure and reorientation kinetics of B-H complexes in silicon 15 139
José C. Noya, Carlos P. Herrero, and Rafael Ramírez
Polariton effects in reflectance and emission spectra of homoepitaxial GaN 15 151
R. Stępniewski, K. P. Korona, A. Wysmołek, J. M. Baranowski, K. Pakuła, M. Potemski, G. Martinez, I. Grzegory, and S. Porowski

Semiconductors II: surfaces, interfaces, microstructures, and related topics

Surface diffusion mechanism for step bunching 15 157
Mats I. Larsson
Dopant spatial distributions: Sample-independent response function and maximum-entropy reconstruction 15 167
D. P. Chu and M. G. Dowsett
Electronic and atomic structure of two-dimensional $ErSi_2$ (1×1)-H on Si(111) 15 171
P. Sonnet, L. Stauffer, S. Saintenoy, C. Pirri, P. Wetzel, G. Gewinner, and C. Minot
Single-electron transport in a one-dimensional channel by high-frequency surface acoustic waves 15 180
V. I. Talyanskii, J. M. Shilton, M. Pepper, C. G. Smith, C. J. B. Ford, E. H. Linfield, D. A. Ritchie, and G. A. C. Jones
Theory of X^- at high magnetic fields 15 185
D. M. Whittaker and A. J. Shields
Quantum transport in square and triangular antidot arrays with various periods 15 195
Satoshi Ishizaka and Tsuneya Ando
Excitonic properties in (111)B-grown (In,Ga)As/GaAs piezoelectric multiple quantum wells 15 202
P. Ballet, P. Disseix, J. Leymarie, A. Vasson, A-M. Vasson, and R. Grey
Exciton Rydberg in T-shaped quantum wires 15 211
Dirk Brinkmann and Guy Fishman
Measurements with a noninvasive detector and dephasing mechanism 15 215
S. A. Gurvitz

(Continued)

PHYSICAL REVIEW B THIRD SERIES, VOLUME 56, NUMBER 23 15 DECEMBER 1997-I

Acoustic phonon modulation of the electron response in tunnel-coupled quantum wells 15 224
F. T. Vasko and V. V. Mitin
Line junctions in the quantum Hall effect 15 231
C. L. Kane and Matthew P. A. Fisher
Magnetic-field-induced insulator-quantum Hall conductor-insulator transitions in doped GaAs/$Al_xGa_{1-x}As$ quantum wells 15 238
C. H. Lee, Y. H. Chang, Y. W. Suen, and H. H. Lin
Theory of potential modulation in lateral surface superlattices. II. Piezoelectric effect 15 242
Ivan A. Larkin, John H. Davies, Andrew R. Long, and Ramon Cuscó
Photoexcited carrier diffusion near a Si(111) surface: Non-negligible consequence of carrier-carrier scattering ... 15 252
Chun-Mao Li, Theodore Sjodin, and Hai-Lung Dai
Laser emission from semiconductor microcavities: Transition from nonperturbative to perturbative regimes 15 256
Xudong Fan, Hailin Wang, H. Q. Hou, and B. E. Hammons
Biexciton formation in $Cd_xZn_{1-x}Se$/ZnSe quantum-dot and quantum-well structures 15 261
K. Herz, T. Kümmell, G. Bacher, A. Forchel, B. Jobst, D. Hommel, and G. Landwehr
Time-resolved photoluminescence of all-porous-silicon microcavities 15 264
M. Cazzanelli and L. Pavesi
P *LVV* and *LMM* Auger emission induced by Ar^+ impact on the InP(110) surface 15 272
S. Valeri, M. Liberi, and R. Verucchi
Reflectance anisotropy spectra from Si δ-doped GaAs(001): Correlation of linear electro-optic effect with integrated surface field 15 277
Z. Sobiesierski, D. I. Westwood, and M. Elliott
Transport of superradiant excitons in GaAs single quantum wells 15 282
P. Vledder, A. V. Akimov, J. I. Dijkhuis, J. Kusano, Y. Aoyagi, and T. Sugano
Electrical and thermal transport of composite fermions 15 289
V. C. Karavolas, G. P. Triberis, and F. M. Peeters
Acoustoconductance in a nonuniform quantum channel 15 299
H. Totland, Ø. L. Bø, and Y. M. Galperin
Calculations of the electron-energy-loss spectra of silicon nanostructures and porous silicon 15 306
C. Delerue, M. Lannoo, and G. Allan

Surface physics, low-dimensional systems, and related topics

Ionicity of nickel oxide: Direct determination by reflection diffraction of high-energy electrons from the (100) surface 15 314
L.-M. Peng, S. L. Dudarev, and M. J. Whelan
Phonon scattering in reflection high-energy electron diffraction: Multiple-scattering theory and experiment 15 320
U. Korte
Ionic and electronic processes at ionic surfaces induced by atomic-force-microscope tips 15 332
Alexander L. Shluger, Lev N. Kantorovich, Alexander I. Livshits, and Michael J. Gillan
Simultaneous force and conduction measurements in atomic force microscopy 15 345
M. A. Lantz, S. J. O'Shea, and M. E. Welland
Structure and bonding in small neutral alkali halide clusters 15 353
Andrés Aguado, Andrés Ayuela, José M. López, and Julio A. Alonso
Deformation patterns in thin films under uniform laser irradiation 15 361
D. Walgraef, N. M. Ghoniem, and J. Lauzeral
Helium-atom diffraction study of the submonolayer structures of sodium on Cu(001) 15 378
Andrew P. Graham and J. Peter Toennies
Charge dynamics and time evolution of contact potential studied by atomic force microscopy 15 391
M. Saint Jean, S. Hudlet, C. Guthmann, and J. Berger

(Continued)

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 56, NUMBER 23** **15 DECEMBER 1997-I**

H_2 dissociative adsorption on Pd(111) 15 396
W. Dong and J. Hafner
Unoccupied electronic states of the Cs/Cu(100) and Cs/Cu(111) adsorption systems 15 404
D. A. Arena, F. G. Curti, and R. A. Bartynski
Photoemission and photoabsorption study of C_{60} adsorption on Cu(111) surfaces 15 412
Ku-Ding Tsuei, Jih-Young Yuh, Chyuan-Tsyr Tzeng, Ren-Yu Chu, Shih-Chun Chung, and King-Lung Tsang
Hydrodynamic theory of photon drag 15 421
John Eric Goff and W. L. Schaich
Isotope effect on the Raman spectrum of the pentagonal-pinch mode in C_{60} 15 431
S. Guha, J. Menéndez, J. B. Page, and G. B. Adams
Reduction of the reflected pressure wave in the molecular-dynamics simulation of energetic particle-solid collisions 15 439
Michael Moseler, Johannes Nordiek, and Hellmut Haberland
Layer growth of Cs on Si(100)$c(4\times2)$ studied with photoelectron spectroscopy 15 446
Y.-C. Chao, L. S. O. Johansson, and R. I. G. Uhrberg
Adsorption of hydrocarbon species on a stepped diamond (111) surface 15 452
K. Larsson
O-induced modification of growth of thin Cu films on Ru(0001) 15 459
H. Wolter, K. Meinel, Ch. Ammer, K. Wandelt, and H. Neddermeyer

COMMENTS

Reply to ''Comment on 'Step dynamics and equilibrium structure of monoatomic steps on Si(100)-2×1' '' 15 471
F. J. Williams, J. R. Sánchez, and C. M. Aldao

Cumulative Author Index 15 474