

PHYSICAL REVIEW B

CONDENSED MATTER

THIRD SERIES, VOLUME 54, NUMBER 16

CONTENTS

15 OCTOBER 1996-II

RAPID COMMUNICATIONS

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

- Experimental and theoretical studies of the electronic structure of TiS_2 R11 009
Z. Y. Wu, F. Lemoigno, P. Gressier, G. Ouvrard, P. Moreau, J. Rouxel, and C. R. Natoli
- Direct calculation of the two-photon line strength of a Γ_{1g} - Γ_{1g} transition in octahedral symmetry R11 014
Michael Chua and Peter A. Tanner
- Competition between the Mott transition and Anderson localization in one-dimensional disordered interacting electron systems R11 018
Satoshi Fujimoto and Norio Kawakami
- Bandwidth dependence of insulator-metal transitions in perovskite cobalt oxides R11 022
S. Yamaguchi, Y. Okimoto, and Y. Tokura
- Mott transition in degenerate Hubbard models: Application to doped fullerenes R11 026
Olle Gunnarsson, Erik Koch, and Richard M. Martin
- Optical absorption of CuGeO_3 R11 030
M. Bassi, P. Camagni, R. Rolli, G. Samoggia, F. Parmigiani, G. Dhalenne, and A. Revcolevschi
- Optical conductivity of strongly correlated electron systems R11 034
R. Eder, P. Wróbel, and Y. Ohta

Semiconductors I: bulk

- Titanium-hydrogen defects in silicon R11 038
W. Jost and J. Weber
- Optical detection of electron nuclear double resonance on a residual donor in wurtzite GaN R11 042
F. K. Koschnick, K. Michael, J.-M. Spaeth, B. Beaumont, and P. Gibart
- Nondiffusive excitonic transport in GaAs and the effects of momentum scattering R11 046
A. C. Schaefer, J. Erland, and D. G. Steel
- Observation of compensating Ga vacancies in highly Si-doped GaAs R11 050
T. Laine, K. Saarinen, J. Mäkinen, P. Hautojärvi, C. Corbel, L. N. Pfeiffer, and P. H. Citrin

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

- Reconstruction transitions during molecular-beam epitaxy on GaAs(111)*B* vicinal surfaces studied by scanning electron microscopy R11 054
Hong-Wen Ren and Tatau Nishinaga
- Step dynamics and equilibrium structure of monoatomic steps on Si(100)-2×1 R11 058
J. R. Sánchez and C. M. Aldao
- Structure and properties of clean and In-covered Ge(103) surfaces R11 062
L. Seehofer, G. Falkenberg, and R. L. Johnson
- Surface unwetting during growth of Ag on Si(001) R11 066
J. C. Glueckstein, M. M. R. Evans, and J. Nogami
- Topological characterization of delocalization in a spin-orbit coupling system R11 070
D. N. Sheng and Z. Y. Weng
- Zero-dimensional excitons in (Zn,Cd)Se quantum structures R11 074
M. Lowisch, M. Rabe, B. Stegmann, F. Henneberger, M. Grundmann, V. Türec, and D. Bimberg

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 54, NUMBER 16

15 OCTOBER 1996-II

Quantum wells with zero valence-band offset: Drastic enhancement of forbidden excitonic transitions	R11 078
A. V. Kavokin, M. A. Kaliteevski, S. V. Goupalov, J. D. Berger, O. Lyngnes, H. M. Gibbs, G. Khitrova, A. Ribayrol, A. Bellabchara, P. Lefebvre, D. Coquillat, and J. P. Lascaray	
Evolution of the interband absorption threshold with the density of a two-dimensional electron gas	R11 082
S. A. Brown, Jeff F. Young, J. A. Brum, P. Hawrylak, and Z. Wasilewski	
Observation of a D^- triplet transition in GaAs/Al _x Ga _{1-x} As multiple quantum wells	R11 086
S. R. Ryu, Z. X. Jiang, W. J. Li, B. D. McCombe, and W. Schaff	
Frequency-dependent admittance of a two-dimensional quantum wire	R11 090
Jian Wang and Hong Guo	
Thermopower of quantum nanowires in a magnetic field	R11 094
E. N. Bogachev, A. G. Scherbakov, and Uzi Landman	
Folded and confined one-dimensional plasmons in modulated wires	R11 098
Florent Perez, Bernard Jusserand, Claus Dahl, Marcel Filoche, Laurence Ferlazzo-Manin, and Bernard Etienne	
Pressure and alloy-composition dependence of Al/Ga _{1-x} Al _x As (100) Schottky barriers	R11 102
J. Bardi, N. Binggeli, and A. Baldereschi	
Tunneling spectroscopy of hole plasmons in a valence-band quantum well	R11 106
B. R. A. Neves, T. J. Foster, L. Eaves, P. C. Main, M. Henini, D. J. Fisher, M. L. Lerch, A. D. Martin, and C. Zhang	
Nonlinear σ model for partially polarized quantum Hall states	R11 110
T. H. Hansson, A. Karlhede, and J. M. Leinaas	
Composite fermions with orbital magnetization	R11 114
Steven H. Simon, Ady Stern, and Bertrand I. Halperin	
p - and n -type cubic GaN epilayers on GaAs	R11 118
D. J. As, D. Schikora, A. Greiner, M. Lübbes, J. Mimkes, and K. Lischka	
Effects of contact metals on electroluminescence from embedded nanosize-Si-particle films	R11 122
G. G. Qin, A. P. Li, and Y. X. Zhang	
Optical transitions in β -FeSi ₂ films	R11 126
Lianwei Wang, M. Östling, Kai Yang, Linhong Qin, Chenglu Lin, Xiangdong Chen, Shichang Zou, Yuxiang Zheng, and Youhua Qian	
Thermally induced interface degradation in (111) Si/SiO ₂ traced by electron spin resonance	R11 129
A. Stesmans and V. V. Afanas'ev	

Surface physics, low-dimensional systems, and related topics

Grain boundary and surface energies of fcc metals	R11 133
D. Udler and D. N. Seidman	
Monte Carlo determination of heteroepitaxial misfit structures	R11 137
Jeff Baker and Per-Anker Lindgård	
π -bonded-trimer formation on the clean diamond C(111) surface	R11 141
M.-H. Tsai, J. C. Jiang, and S. H. Lin	
Structure and contrast in scanning tunneling microscopy of oxides: FeO monolayer on Pt(111)	R11 145
H. C. Galloway, P. Sautet, and M. Salmeron	
Mechanically stretched carbon nanotubes: Induction of chiral current	R11 149
Yoshiyuki Miyamoto	
Magnetically split sp -derived states in fcc-like Fe/Cu(001)	R11 153
B. Gubanka, M. Donath, and F. Passek	
Magnetism of thin Fe films on Cu(100)	R11 157
J. Hunter Dunn, D. Arvanitis, and N. Mårtensson	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 54, NUMBER 16

15 OCTOBER 1996-II

ARTICLES

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

Polarization dependence of Born effective charge and dielectric constant in KNbO_3	11 161
Cheng-Zhang Wang, Rici Yu, and Henry Krakauer	
Efficient iterative schemes for <i>ab initio</i> total-energy calculations using a plane-wave basis set	11 169
G. Kresse and J. Furthmüller	
Self-consistent relativistic full-potential Korringa-Kohn-Rostoker total-energy method and applications	11 187
S. Bei der Kellen and A. J. Freeman	
Estimates of electronic interaction parameters for LaMO_3 compounds ($M=\text{Ti-Ni}$) from <i>ab initio</i> approaches	11 199
Priya Mahadevan, N. Shanthi, and D. D. Sarma	
Spin- and charge-rotation invariant approach to the Hubbard model	11 207
J. J. Vicente Alvarez, C. A. Balseiro, and H. A. Ceccatto	
Differences between random-potential and random-magnetic-field localization in quasi-one-dimensional systems	11 213
W. L. Chan, X. R. Wang, and X. C. Xie	
Phase-conjugated signal induced and enhanced by weak localization of excitonic polaritons	11 219
Eiichi Hanamura	
ac-conductivity measurements on $\text{La}_2\text{NiO}_{4+\delta}$	11 224
H. Jhans, D. Kim, R. J. Rasmussen, and J. M. Honig	
Electrons, pseudoparticles, and quasiparticles in the one-dimensional many-electron problem	11 230
J. M. P. Carmelo and A. H. Castro Neto	
Large omnidirectional band gaps in metallodielectric photonic crystals	11 245
Shanhui Fan, Pierre R. Villeneuve, and J. D. Joannopoulos	
Electron scattering by a cut-off atomic potential: Application to electron properties in atomic liquids	11 252
V. M. Atrazhev and I. V. Timoshkin	
Electronic phase transitions in the spin- $\frac{1}{2}$ Falicov-Kimball model	11 261
Pavol Farkašovský	
Properties of the layered $\text{BaCo}_{1-x}\text{Ni}_x\text{S}_2$ alloy system	11 265
L. S. Martinson, J. W. Schweitzer, and N. C. Baenziger	
<i>Ab initio</i> optical conductivity in LaMO_3 ($M=\text{Ti-Cu}$)	11 271
S. Bouarab, A. Vega, and M. A. Khan	

Semiconductors I: bulk

Shallow electron centers in silver halides	11 276
M. T. Bennebroek, A. Arnold, O. G. Poluektov, P. G. Baranov, and J. Schmidt	
Nature of the bulk defects in GaAs through high-temperature quenching studies	11 290
C. V. Reddy, S. Fung, and C. D. Beling	
Single-site approximation for the <i>s-f</i> model in ferromagnetic semiconductors	11 298
Masao Takahashi and Kazuhiro Mitsui	
Isotopic effects on the lattice constant in compound semiconductors by perturbation theory: An <i>ab initio</i> calculation	11 305
Alberto Debernardi and Manuel Cardona	
Ultrafast kinetics of evolution of optical phonons in a photoinjected highly excited plasma in semiconductors	11 311
Antonio C. S. Algarte, Aurea R. Vasconcellos, and Roberto Luzzi	
Hall factor in strained <i>p</i> -type doped $\text{Si}_{1-x}\text{Ge}_x$ alloy	11 317
Y. Fu, K. B. Joelsson, K. J. Grahn, W.-X. Ni, G. V. Hansson, and M. Willander	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 54, NUMBER 16

15 OCTOBER 1996-II

Al-H and Al-D complexes in Si: A uniaxial-stress study of the hydrogen vibrational modes	11 322
Michael Stavola, Y. Michael Cheng, and Gordon Davies	
Semiconductors II: surfaces, interfaces, microstructures, and related topics	
Origin of buckling-dimer-row formation of Si(001) surfaces	11 331
T. Hoshino, M. Hata, S. Oikawa, M. Tsuda, and I. Ohdomari	
Evidence for three surface components in the 3d core-level photoemission spectra of Ge(100)-(2×1) surface	11 340
A. Goldoni, S. Modesti, V. R. Dhanak, M. Sancrotti, and A. Santoni	
Carrier relaxation and electronic structure in InAs self-assembled quantum dots	11 346
K. H. Schmidt, G. Medeiros-Ribeiro, M. Oestreich, P. M. Petroff, and G. H. Döhler	
Self-consistent density of states for a single- and double-quantum-well structure in a parallel magnetic field	11 354
Godfrey Gumbs	
Magneto-optical experiments on GaAs/In _x Ga _{1-x} As/Al _y Ga _{1-y} As modulation-doped single quantum wells	11 360
F. Iikawa, M. L. F. Abbade, J. A. Brum, A. A. Bernussi, R. G. Pereira, and G. Borghs	
Nature of one-dimensional excitons in polysilanes	11 365
T. Hasegawa, Y. Iwasa, T. Koda, H. Kishida, Y. Tokura, S. Wada, H. Tashiro, H. Tachibana, and M. Matsumoto	
Quasi-two-dimensional electron-hole plasma in a quantum well: Hartree, exchange, and correlation energies	11 375
O. Betbeder-Matibet and M. Combescot	
Systematics of properties of the electron gas in deep-etched quantum wires	11 386
J. Martorell and D. W. L. Sprung	
Magnetoexcitons and correlated electrons in quantum dots in a magnetic field	11 397
Pawel Hawrylak, Arkadiusz Wojs, and José A. Brum	
Classical chaos and ballistic transport in a mesoscopic channel	11 410
G. A. Luna-Acosta, A. A. Krokhn, M. A. Rodríguez, and P. H. Hernández-Tejeda	
Pseudopotential-based multiband k·p method for ~250 000-atom nanostructure systems	11 417
Lin-Wang Wang and Alex Zunger	
Dynamical response of double parabolically graded quantum wells	11 436
L. Wendler and T. Kraft	
Plasmon dispersion in strongly correlated superlattices	11 457
Dexin Lu, K. I. Golden, G. Kalman, P. Wyns, L. Miao, and X-L. Shi	
Effects of nonlocal response and level quantization on electronic excitations of a bimetallic jellium film in an Al _x Ga _{1-x} As heterostructure	11 467
E. L. Yuh, E. G. Gwinn, P. R. Pinsukanjana, W. L. Schaich, K. L. Campman, P. F. Hopkins, and A. C. Gossard	
Conductance fluctuations in a double-barrier resonant-tunneling structure with three-dimensional electrodes	11 479
Lamy Ghenim, D. L. Sivco, A. Y. Cho, and G. Hill	
Signal propagation in electron waveguides: Transmission-line analogies	11 484
Jan-Olof J. Wesström	
First-order resonant Raman scattering under an electric field	11 492
A. García-Cristóbal, M. Kuball, M. Cardona, and A. Cantarero	
Phonons in semiconductor planar microcavities: A Raman scattering study	11 505
A. Fainstein and B. Jusserand	
Theory of Raman spectra of heavily doped semiconductor multiple quantum wells	11 517
Yia-Chung Chang and Huade Yao	
Carrier relaxation and thermal activation of localized excitons in self-organized InAs multilayers grown on GaAs substrates	11 528
Z. Y. Xu, Z. D. Lu, X. P. Yang, Z. L. Yuan, B. Z. Zheng, J. Z. Xu, W. K. Ge, Y. Wang, J. Wang, and L. L. Chang	
Rapid carrier relaxation in self-assembled In _x Ga _{1-x} As/GaAs quantum dots	11 532
B. Ohnesorge, M. Albrecht, J. Oshinowo, A. Forchel, and Y. Arakawa	

(Continued)

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 54, NUMBER 16

15 OCTOBER 1996-II

Numerically stable Hermitian secular equation for the envelope-function approximation for superlattices	11 539
Frank Szmulowicz	
State filling and time-resolved photoluminescence of excited states in $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ self-assembled quantum dots	11 548
S. Raymond, S. Fafard, P. J. Poole, A. Wojs, P. Hawrylak, S. Charbonneau, D. Leonard, R. Leon, P. M. Petroff, and J. L. Merz	
Fabrication and physical properties of radio frequency sputtered $\text{Cd}_{1-x}\text{Mn}_x\text{S}$ thin films	11 555
C. T. Tsai, S. H. Chen, D. S. Chuu, and W. C. Chou	
Quasiparticle lifetime in a two-dimensional electron system in the limit of low temperature and excitation energy	11 561
D. Menashe and B. Laikhtman	
Effective-mass theory for InAs/GaAs strained coupled quantum dots	11 575
Shu-Shen Li, Jian-Bai Xia, Z. L. Yuan, Z. Y. Xu, Weikun Ge, Xiang Rong Wang, Y. Wang, J. Wang, and L. L. Chang	
Polarized interacting exciton gas in quantum wells and bulk semiconductors	11 582
J. Fernández-Rossier, C. Tejedor, L. Muñoz, and L. Viña	
Numerical calculation of the optical absorption in semiconductor quantum structures	11 592
S. Glutsch, D. S. Chemla, and F. Bechstedt	
Conductance fluctuations near the ballistic-transport regime	11 602
Yasuhiro Asano and Gerrit E. W. Bauer	
Origin of conductance fluctuations in large circular quantum dots	11 612
Karl-Fredrik Berggren, Zhen-Li Ji, and Tomas Lundberg	
Single-impurity Anderson model out of equilibrium	11 622
Noam Sivan and Ned S. Wingreen	
Numerical confirmation of universality of transmission microsymmetry relations in a four-probe quantum dot	11 630
Ming Lei and Hong Guo	
Transport properties of ion-implanted and chemically doped polyaniline films	11 638
A. N. Aleshin, N. B. Mironkov, A. V. Suvorov, J. A. Conklin, T. M. Su, and R. B. Kaner	
Spontaneous interlayer coherence in double-layer quantum Hall systems: Symmetry-breaking interactions, in-plane fields, and phase solitons	11 644
Kun Yang, K. Moon, Lotfi Belkhir, H. Mori, S.M. Girvin, A. H. MacDonald, L. Zheng, and D. Yoshioka	
Mössbauer study of the magnetic character and ordering process of the cubic $\gamma\text{-FeSi}_2$ phase obtained by Fe implantation into a $\text{Si}(100)$ matrix	11 659
R. L. Maltez, L. Amaral, M. Behar, A. Vantomme, G. Langouche, and X. W. Lin	
Ultrafast ellipsometry of coherent processes and exciton-exciton interactions in quantum wells at negative delays	11 666
J. A. Bolger, A. E. Paul, and Arthur L. Smirl	

Surface physics, low-dimensional systems, and related topics

Monte Carlo simulation of nonspecular x-ray scattering profiles from multilayers	11 672
G. Gladyszewski and Y. Bruynseraede	
Scaling behavior in submonolayer film growth: A one-dimensional model	11 681
J. A. Blackman and P. A. Mulheran	
Crystal growth and characterization of Cu-intercalated misfit-layer compounds	11 693
Youichi Ohno	
Amorphization in the vicinity of a grain boundary: A molecular-dynamics approach	11 701
Gonzalo Gutiérrez, Miguel Kiwi, and Ricardo Ramírez	
Observation of a superlattice in silver-intercalated NbSe_2 by scanning tunneling microscopy	11 706
B. Koslowski, W. Xu, B. Blackford, and M. H. Jericho	
Morphological stability of alloy thin films	11 710
J. E. Guyer and P. W. Voorhees	

(Continued)

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 54, NUMBER 16

15 OCTOBER 1996-II

Final-state magnetic dichroism in Fe 3s photoemission	11 725
W. J. Lademan and L. E. Klebanoff	
Low-energy electron microscopy study of step mobilities on Si(001)	11 731
N. C. Bartelt and R. M. Tromp	
Ostwald ripening of two-dimensional islands on Si(001)	11 741
N. C. Bartelt, W. Theis, and R. M. Tromp	
Brownian motion and shape fluctuations of single-layer adatom and vacancy clusters on surfaces: Theory and simulations	11 752
S. V. Khare and T. L. Einstein	
Evidence for a strain-stabilized bct phase of cobalt deposited on Pd{100}: An x-ray photoelectron diffraction study	11 762
Hélène Giordano, Andrea Atrei, Marco Torrini, Ugo Bardi, Michael Gleeson, and Colin Barnes	
Atomic and electronic structure of ideal and reconstructed α -Sn (111) surface	11 769
Zhong-Yi Lu, Guido L. Chiarotti, S. Scandolo, and E. Tosatti	
Electronic effects in scanning tunneling microscopy of graphite: A Green's-function calculation based on the tight-binding model	11 777
B. A. McKinnon and T. C. Choy	
Electronic structure of silver and copper ultrathin films on V(100): Quantum-well states	11 786
T. Valla, P. Pervan, M. Milun, A. B. Hayden, and D. P. Woodruff	
Structural and vibrational analysis of amorphous Au ₅₅ clusters	11 796
Ignacio L. Garzón and Alvaro Posada-Amarillas	
A dynamically and kinetically consistent mechanism for H ₂ adsorption/desorption from Si(100)-2×1	11 803
Michelle R. Radeke and Emily A. Carter	
Cumulative Author Index	11 818