

Francesco Montalenti's CV

Personal data

Montalenti Francesco (Cimbrotta)

Born in Torino, June 22nd 1970.

Nationality: italian

Marital status: married, father of two twin boys.

Office address

Prof. Francesco Montalenti, Phd

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Formation/career

1989: Scientific high-school diploma, Liceo Salvador Allende, Milano. Grade: 60/60.

1990-1995: Undergraduate physics student, University of Milano.

1995: Laurea in Physics, University of Milano. Thesis' title: He and Ne interaction with simple metals: ab initio results. Advisor: Prof. G.P. Brivio. Grade: 110/110 cum laude.

1997: Civil Service at Mario Negri Institute for Pharmacological Research, Milano. Duty: development of cellular-cycle simulation algorithms.

1996-1999: Graduate student in Physics, University of Genova.

1999: PHD in Physics, University of Genova. Thesis' title: Diffusion on channeled metal surfaces. Advisor: Prof. R. Ferrando.

2000-2001: Directorial-funded POST-DOC, Los Alamos National Laboratory, Theoretical Division.

2002-2012: University Researcher in Physics of Matter, Materials Science Department, University of Milano-Bicocca. Tenured Researcher since 2005.

2012: Associate Professor (starting from October 1st) of Physics of Matter, Materials Science Department, University of Milano-Bicocca (habilitation to associate professor obtained in August 2010).

2013: Full-professor habilitation in Theoretical Physics of Matter

Affiliations and duties

Associate Professor of Physics of Matter, Università degli Studi di Milano-Bicocca,

Materials Science Department,

Vice-coordinator of the PHD program in Materials Science and Nanotechnology.

Member of the Scientific Board of L-NESS, Laboratory for Epitaxial Nanostructures Nanostrutture on Silicon and for Spintronics, a inter-university center Politecnico di Milano and Università di Milano-Bicocca.

Research interests

Theoretical/Computational modeling of semiconductor heteroepitaxial growth: surface diffusion, growth modeling, investigation of elastic and plastic misfit-strain relaxation. Expertise in several synergic techniques, ranging from continuum models (Phase-field approach, Finite Element Methods, Dislocation Dynamics) to atomistic ones (classical MD, ab initio calculations).

International collaborations

Prof. A. Voigt, TU Dresden. Development of codes for continuum simulations of growth.

Dr. B. Devincre e Dr. R. Gatti. ONERA/CNRS, Châtillon, Francia. Dislocation dynamics simulations based on the MicroMegas code; code development.

Dr. P. Storck, Siltronic AG (Burghausen, Germania). Joint theoretical and experimental effort devoted to reducing the threading dislocation density in Ge/Si films.

Dr. G. Capellini, IHP Frankfurt (Oder). Design, growth, and modeling of Ge/Si nanostructures for optics and microelectronics.

Publications

ORCID-ID 0000-0001-7854-8269; ResearcherID: A-7738-2010; Scopus Author ID: 7003456432

115 publications on international peer-reviewed journals, around 3000 citations (around 2500 excluding self-citing). h-index: 27.

45 invited talks and seminars,

Conference organization

Organizer (with Prof. F. Schäffler) of the symposium Growth of Heteroepitaxial islands in group IV and III/V semiconductors, 26th ECOSS Conference (Parma, Italy, 2009).

Member of the Program Committee for the VIII international workshop ESPS-NIS (Epitaxial Semiconductors on Patterned Substrates and Novel Index Surfaces), Como, Italy, 2010.

Member of the Scientific Committee for the conference ICSII-VII/ISTDM (Nagoya, Japan, 2016).

Member of the Scientific Committee for the symposium "Integration of novel materials and devices on silicon for future technologies"; E-MRS Fall Meeting (Warsaw, 2016).

Organizer (with I. Fischer, C. Merklings, and D. Landru) of the symposium "Material and device integration on silicon for advanced applications"; E-MRS Fall Meeting (Warsaw, 2017).

Organizer (with I. Fischer, C. Merklings, and D. Landru) of the symposium "Monolithic and heterogeneous integration of advanced materials & devices on silicon"; E-MRS Fall Meeting (Warsaw, 2018).

Funded projects and research contracts (ended)

1) Epitaxial technologies on silicon for electronics and optoelectronics), funded by Fondazione Cariplo. Role: partner.

2) NANOCrystalline silicon films for PHOTOvoltaic and optoelectronic applications, EU STREP project, contract # 013944. Role: partner.

3) Disposable DOT Field Effect Transistor for high speed si integrated circuits, EU STREP project, contract # 12150. Role: partner.

4) EU COST ACTION P19 "Multiscale modeling of materials" (2006-2010). Role: representative of Italy in the management committee.

5) SiGe Optical Waveguides: Design, Fabrication, Characterization, and Application to Raman Amplification, Italian PRIN (Programmi di ricerca Rilevante Interesse Nazionale) project. Role: partner.

6) Simulation, diagnostic and modeling of an innovative cvd growth process activated by a low-energy, high-density plasma, funded by Fondazione Cariplo. Role: partner.

7) Nano-MANipulation of misfit DISlocations for innovative approaches to heteroepitaxial integration in silicon, funded by Fondazione Cariplo. Role: partner.

8) GaAs based optoelectronic materials for C-MOS compatible integrated applications, Italian PRIN project. Role: partner.

9) Nanostructures for the controlled deformation of layers and membranes of group-IV semiconductors, funded by Fondazione Cariplo. Role: partner (responsible of the theoretical unit).

10) 12-months research contract with Siltronic AG (Burghausen, Germany): theoretical/computational investigation of dislocations in Ge/Si films. Year: 2016. Role: PI.

11) 12-months research contract with Siltronic AG (Burghausen, Germany): theoretical/computational investigation of dislocations in Ge/Si films. Year: 2017. Role: PI.

Funded projects and research contracts (active)

12) CHALLENGE (3C-SiC Hetero-epitaxiALLY grown on silicon compliancE substrates and 3C-SiC substrates for sustainAble wide-band-Gap powEr devices) project; Horizon2020 (Industrial Leadership). Role: partner.

13) MICRO-SPIRE (MICRO-crystals Single Photon InfraREd detectors) project; Horizon2020 (FET). Role: partner.

14) TEINVEIN project (Tecnologie per i veicoli intelligenti); funded by Regione Lombardia. Role: partner.

15) 12-months research contract with Siltronic AG (Burghausen, Germany): theoretical/computational investigation of dislocations in Ge/Si films. Year: 2018. Role: PI.

Supercomputing projects (financed in terms of free computing time).

(i) INFN project "Iniziativa Calcolo Parallelo 2003". Role: PI.

(ii) INFN project "Iniziativa Calcolo Parallelo 2004". Role: PI.

(iii) INFN project "Iniziativa Calcolo Parallelo 2005". Role: PI.

(iv) CNISM project "Iniziativa Calcolo Parallelo 2006", in collaboration with Prof. M.

Bernasconi.

(v) CNISM project "Iniziativa Calcolo Parallelo 2007", in collaboration with Prof. M.

Bernasconi.

(vi) CINECA/ISCRA class C project (2017). Role: PI.

Referee

Referee, on a regular basis, for the journals Phys. Rev. Lett., Phys. Rev. B, Phys. Rev. Mat., Nano Lett., Appl. Phys. Lett., Nanotechnology, and others.

Teaching at the University of Milano-Bicocca.

2002-present: Several courses taught for Physics and Materials Science students for both the Laurea Triennale (Bachelor) and Laurea Mafistrale (Master) programs.

Since 2013 in charge of the Courses "Struttura della Materia II" (Structure of Matter II) for Materials Science Laurea Triennale students and "Computational Statistical thermodynamics of Solids" for both Physics and Materials Science master students.

Invited lectures

1-3) Three lectures on the subject Standard and accelerated molecular dynamics simulations, Summer School Coarse graining in time and space: from microscopics to macroscopics, Sjukulla (Finlandia), 2001.

4-7) Four lectures on the subject Standard and accelerated molecular dynamics simulations, Nathiagali Summer College, Nathiagali (Pakistan), 2003.

8-9) Two lectures on the subject Simulation of crystal growth, PHD School in Materials Science, University of Milano-Bicocca, 2005.

10) Extending the time scale in atomistic simulations by temperature accelerated dynamics, lecture given at the International School of Solid State Physics, Erice (Sicily), 2006.

11) Crescita di film sottili eteroepitassiali: l'importanza del rilascio di energia elastica (Growth of thin heteroepitaxial films: the importance of strain release), lecture given at the University of Trieste (Italy), 2006.

12) Simulazioni atomistiche dei materiali: il problema della scala temporale (Atomistic simulation of materials: the time-scale problem), "master class", University of Trieste (Italy), 2006.

13-14) Two lectures on the subject Atomic-scale, theoretical modeling of surface phenomena: thin-film growth, 10th International Conference-School Advanced Materials and Technologies, Palanga (Lituania), 2008.

Students: Thesis supervisor

Master thesis in Materials Science: Silvia Cereda, Federico Gamba, Luca di Piazza, Marco Viridis, Roberto Bergamaschini.

Master Thesis in Physics: Fabrizio Gemma, Luca Laurin, Daniele Scopece, Dario Digiuni, Niccolò Castellani, Federica Riva, Marco Salvalaglio, Matteo Brunetto, Marco Albani, Fabrizio Rovaris, Luca Barbisan, Francesco Boccardo.

PhD in Materials Science: Silvia Cereda, Roberto Bergamaschini, Fabrizio Rovaris.

Bachelor thesis not listed.

Languages

English (TOEFL: 627/677), French (fair), Italian.

Publication list

A) International, peer-reviewed journals

1. F. Montalenti, M.I. Trioni, G.P. Brivio, and S. Crampin, Ab initio results for the adiabatic atom-surface interaction for helium and neon on a simple metal, *Surf. Sci.* 364, L595 (1996). DOI: 10.1016/0039-6028(96)00791-1
2. M.I. Trioni, F. Montalenti, and G.P. Brivio, Charge transfer in chemisorption: N and Si on Al, *Solid State Comm.* 99, 7 (1996). DOI: 10.1016/0038-1098(96)00247-5
3. M.I. Trioni, F. Montalenti, and G.P. Brivio, Ab initio adiabatic noble gas-metal interaction: the role of the induced polarization charge, *Surf. Sci.* 401, L383 (1998). DOI: 10.1016/S0039-6028(98)00073-9
4. F. Montalenti, G. Sena, P. Cappella, and P. Ubezio, Simulating cancer-cell kinetics after drug treatment: application to cisplatin on ovarian carcinoma, *Phys. Rev. E* 57, 5877 (1998). DOI: 10.1103/PhysRevE.57.5877
5. F. Montalenti and R. Ferrando, Competing mechanisms in adatom diffusion on a channeled surface: jumps versus metastable walks, *Phys. Rev. B* 58, 3617 (1998). DOI: 10.1103/PhysRevB.58.3617
6. F. Montalenti and R. Ferrando, Jumps and concerted moves in Cu, Ag, and Au(110) self-diffusion, *Phys. Rev. B* 59, 5881 (1999). DOI: 10.1103/PhysRevB.59.5881
7. F. Montalenti and R. Ferrando, Leapfrog diffusion mechanism for one-dimensional chains on missing-row reconstructed surfaces, *Phys. Rev. Lett.* 82, 1498 (1999). DOI: 10.1103/PhysRevLett.82.1498
8. F. Montalenti and R. Ferrando, Dimers diffusion on (110)(1x2) metal surfaces, *Surf. Sci.* 432, 27 (1999). DOI: 10.1016/S0039-6028(99)00496-3
9. F. Montalenti and R. Ferrando, An MD study of adatom self-diffusion on Au(110) surfaces, *Surf. Sci.* 433-435, 445 (1999). DOI: 10.1016/S0039-6028(99)00633-0

10. G. Sena, C. Onado, P. Cappella, F. Montalenti, and P. Ubezio, Measuring the complexity of cell cycle arrest and killings of drugs: kinetics of phase-specific effects induced by Taxol, *Cytometry* 37, 113 (1999). DOI: 10.1002/(SICI)1097-0320(19991001)37:2<113::AID-CYTO4>3.0.CO;2-M
11. F. Montalenti and R. Ferrando, Universal law for piecewise dimer diffusion, *Phys. Rev. B* 60, 11102 (1999). DOI: 10.1103/PhysRevB.60.11102
12. R. Ferrando, F. Montalenti, G. Spadacini, and G.E. Tommei, Long-jump probabilities in a BGK model for surface diffusion, *Chem. Phys. Lett.* 315, 153 (1999). DOI: 10.1016/S0009-2614(99)01254-3
13. F. Montalenti and R. Ferrando, Probability of dimer reassociation in two dimensions, *Phys. Rev. E* 61, 3411 (2000). DOI: 10.1103/PhysRevE.61.3411
14. F. Montalenti, F. Baletto, and R. Ferrando, Diffusion of one-dimensional clusters on Au and Pt(110)(1x2), *Surf. Sci.* 454-456, 575 (2000). DOI: 10.1016/S0039-6028(00)00094-7
15. F. Montalenti and R. Ferrando, Mobility of atomic chains in channeled surfaces, *J. Chem. Phys.* 113, 349 (2000). DOI: 10.1063/1.481799
16. R. Ferrando, F. Montalenti, G. Spadacini, and G.E. Tommei, Long jumps in the strong collision model, *Phys. Rev. E* 61, 6344 (2000). DOI: 10.1103/PhysRevE.61.6344
17. F. Montalenti and R. Ferrando, Comment on scaling behavior of one-dimensional Pt chains migration on Pt(110)(1x2) surface, *Phys. Lett. A* 277, 185 (2000). DOI: 10.1016/S0375-9601(00)00707-6
18. P. Cappella, D. Tomasoni, M. Faretta, M. Lupi, F. Montalenti, F. Viale, F. Banzato, M. D'Incalci, and P. Ubezio, Cell cycle effects of gemcitabine, *Int. J. of Cancer* 93, 401 (2001). DOI: 10.1002/ijc.1351
19. F. Montalenti and A.F. Voter, Applying accelerated molecular dynamics to crystal growth, *Phys. Status Solidi B* 226, 21 (2001). DOI: 10.1002/1521-3951(200107)226:1<21::AID-PSSB21>3.0.CO;2-Q
20. F. Montalenti and A.F. Voter, Normal incidence steering effect in crystal growth: Ag/Ag(100), *Phys. Rev. B* 64, 081401(R) (2001). DOI: 10.1103/PhysRevB.64.081401
21. F. Montalenti, M.R. Sorensen, and A.F. Voter, Closing the gap between experiment and theory: crystal growth by temperature accelerated dynamics, *Phys. Rev. Lett.* 87, 126101 (2001). DOI: 10.1103/PhysRevLett.87.126101
22. F. Montalenti and A.F. Voter, Exploiting past visits or minimum-energy knowledge to gain further boost in the temperature-accelerated dynamics method, *J. Chem. Phys.* 116, 4819 (2002). DOI: 10.1063/1.1449865
23. F. Baletto, R. Ferrando, A. Fortunelli, F. Montalenti, and R. Ferrando, Crossover between structural motifs in transition and noble-metal clusters, *J. Chem. Phys.* 116, 3856 (2002). DOI: 10.1063/1.1448484
24. A.F. Voter, F. Montalenti, and T.C. Germann, Extending the time scale in atomistic simulation of materials, *Annu. Rev. Mater. Res.* 32, 321 (2002). DOI: 10.1146/annurev.matsci.32.112601.141541

25. F. Montalenti, A.F. Voter, and R. Ferrando, Spontaneous atomic shuffle in flat terraces: Ag(100), *Phys. Rev. B* 66, 205404 (2002). DOI: 10.1103/PhysRevB.66.205404
26. J.A. Sprague, F. Montalenti, B.P. Uberuaga, J.D. Kress, and A.F. Voter, Simulation of growth of Cu on Ag(001) at experimental deposition rates, *Phys. Rev. B* 66, 205415 (2002). DOI: 10.1103/PhysRevB.66.205415
27. F. Montalenti, Transition-path spectra at metal surfaces, *Surf. Sci.* 543, 141 (2003). DOI: 10.1016/j.susc.2003.08.003
28. B.P. Uberuaga, R. Smith, A.R. Cleave, F. Montalenti, G. Henkelman, R.W. Grimes, A.F. Voter, and K.E. Sickafus, Structure and mobility of defects formed from collision cascades in MgO, *Phys. Rev. Lett.* 92, 115505 (2004). DOI: 10.1103/PhysRevLett.92.115505
29. L. Martinelli, A. Marzegalli, P. Raiteri, M. Bollani, F. Montalenti, L. Miglio, D. Chrastina, G. Isella, and H. von Kaenel, Formation of strain-induced Si-rich and Ge-rich nanowires at misfit dislocations in SiGe: a model supported by photoluminescence data, *Appl. Phys. Lett.* 84, 2895 (2004). DOI: 10.1063/1.1705727
30. D.B. Migas, S. Cereda, F. Montalenti, and L. Miglio, Electronic and elastic contributions in the enhanced stability of Ge(105) under compressive strain, *Surf. Sci.* 556, 121 (2004). DOI: 10.1016/j.susc.2004.03.023
31. M. Basham, P.A. Mulheran, and F. Montalenti, Diffusion and stability of small vacancy clusters on Cu(100) - a simulation study, *Surf. Sci.* 565, 289 (2004). DOI: 10.1016/j.susc.2004.07.019
32. A. Marzegalli, F. Montalenti, M. Bollani, L. Miglio, G. Isella, D. Chrastina, and H. von Kaenel, Relaxed SiGe heteroepitaxy on Si with very thin buffer layers: experimental LEPECVD indications and an interpretation based on strain-dependent dislocation nature, *Microelectron. Eng.* 76, 290 (2004). DOI: 10.1016/j.mee.2004.07.031
33. F. Hontinfinde, A. Videcoq, F. Montalenti, and R. Ferrando, Leapfrog induced selective faceting in the growth of missing-row (110) surfaces, *Chem. Phys. Lett.* 398, 50 (2004). DOI: 10.1016/j.cplett.2004.09.008
34. F. Montalenti, P. Raiteri, D.B. Migas, H. von Kaenel, A. Rastelli, C. Manzano, G. Costantini, U. Denker, O.G. Schmidt, K. Kern, and L. Miglio, Atomic-scale pathway of the pyramid-to-dome transition during Ge growth on Si(001), *Phys. Rev. Lett.* 93, 216102 (2004). DOI: 10.1103/PhysRevLett.93.216102
35. L. Giordano, L. Di Piazza, M.I. Trioni, and F. Montalenti, Theoretical evidence for fast H-divacancy rotation on H/Pd(111), *Chem. Phys. Lett.* 565, 289 (2004). DOI: 10.1016/j.cplett.2004.10.085
36. F. Montalenti, D.B. Migas, F. Gamba, and L. Miglio, Fast isotropic adatom diffusion on Ge(105) dot facets, *Phys. Rev. B* 70, 245315 (2004). DOI: 10.1103/PhysRevB.70.245315
37. A. Marzegalli, F. Montalenti, and L. Miglio, Stability of shuffle and glide dislocations segments with increasing misfit in Ge/Si_{1-x}Gex(001) epitaxial layers, *Appl. Phys. Lett.* 86, 041912 (2005). DOI: 10.1063/1.1856145
38. S. Cereda, F. Montalenti, and L. Miglio, Atomistic modeling of step formation and step bunching at the Ge(105) surface, *Surf. Sci.* 591, 23 (2005). DOI: 10.1016/j.susc.2005.06.016

39. R. Marchetti, F. Montalenti, L. Miglio, G. Capellini, M. De Seta, and F. Evangelisti, Strain-induced ordering of small Ge islands in clusters at the surface of multilayered Si-Ge nanostructures, *Appl. Phys. Lett.* 87, 261919 (2005). DOI: 10.1063/1.2151250
40. A. Marzegalli, F. Montalenti, and L. Miglio, Atomistic simulation of a 60° shuffle dislocation segment migrating in Ge/SiGe(001) epitaxial films, *J. Phys.: Condens. Matter* 17, 7505 (2005). DOI: 10.1088/0953-8984/17/48/004
41. M. Basham, F. Montalenti, and P.A. Mulheran, Multiscale modeling of island nucleation and growth during Cu(100) homoepitaxy, *Phys. Rev. B* 73, 245315 (2006). DOI: 10.1103/PhysRevB.73.045422
42. G. Capellini, M. De Seta, F. Evangelisti, V.A. Zinovyev, G. Vastola, F. Montalenti, and L. Miglio, Self-ordering of a Ge island single layer induced by Si overgrowth, *Phys. Rev. Lett.* 96, 106102 (2006). DOI: 10.1103/PhysRevLett.96.106102
43. M. Ceriotti, R. Ferrando, and F. Montalenti, Impact-driven effects in thin-film growth: steering and transient mobility at the Ag(110) surface, *Nanotechnol.* 17, 3556 (2006). DOI: 10.1088/0957-4484/17/14/033
44. S. Cereda, F. Montalenti, M. Cogoni, D. Branduardi, M.W. Radny, P.V. Smith, and L. Miglio, Binding sites for SiH₂/Si(001): a combined ab initio, tight-binding and classical investigation, *Surf. Sci.* 600, 4445 (2006). DOI: 10.1016/j.susc.2006.07.009
45. V.A. Zinovyev, G. Vastola, F. Montalenti, and L. Miglio, Accurate and analytical strain mapping at the surface of Ge/Si(001) islands by an improved flat-island approximation, *Surf. Sci.* 600, 4777 (2006). DOI: 10.1016/j.susc.2006.07.047
46. M. De Seta, G. Capellini, F. Evangelisti, V.A. Zinovyev, G. Vastola, F. Montalenti, and L. Miglio, Spontaneous Ge island ordering promoted by partial silicon capping, *Mater. Sci. Semicond. Process* 9, 823 (2006). DOI: 10.1016/j.mssp.2006.08.071
47. F. Montalenti, A. Marzegalli, G. Capellini, M. De Seta, and L. Miglio, Vertical and lateral ordering of Ge islands grown on Si(001): theory and experiments, *J. Phys.: Condens. Matter* 19, 225001 (2007). DOI: 10.1088/0953-8984/19/22/225001
48. Z.Y. Zhong, W. Schwinger, F. Schaffler, G. Bauer, G. Vastola, F. Montalenti, and L. Miglio, Delayed plastic relaxation on patterned Si substrates: coherent SiGe pyramids with dominant {111} facets, *Phys. Rev. Lett.* 98, 176102 (2007). DOI: 10.1103/PhysRevLett.98.176102
49. S. Cereda and F. Montalenti, Atomic-scale modeling of next-layer nucleation and step flow at the Ge(105) rebonded-step surface, *Phys. Rev. B* 75, 195321 (2007). DOI: 10.1103/PhysRevB.75.195321
50. S. Cereda, M. Ceriotti, F. Montalenti, M. Bernasconi, and L. Miglio, Quantitative estimate of H abstraction by thermal SiH₃ on hydrogenated Si(001)(1x2), *Phys. Rev. B* 75, 235311 (2007). DOI: 10.1103/PhysRevB.75.235311

51. M. Rondanini, S. Cereda, F. Montalenti, L. Miglio, and C. Cavallotti, A multiscale model of the plasma assisted deposition of crystalline silicon, *Surf. & Coat. Technol.* 201, 8863 (2007). DOI: 10.1016/j.surfcoat.2007.04.104
52. S. Cereda, F. Montalenti, and L. Miglio, Interaction of SiH_x precursors with hydrogen-covered Si surfaces: impact dynamics and adsorption sites, *Surf. Sci.* 601, 3970 (2007). DOI: 10.1016/j.susc.2007.04.086
53. A. Marzegalli, V.A. Zinovyev, F. Montalenti, A. Rastelli, M. Stoffel, T. Merdzhanova, O.G. Schmidt, and L. Miglio, Critical shape and size for dislocation nucleation in Si_{1-x}Ge_x islands on Si(001), *Phys. Rev. Lett.* 99 235505 (2007). DOI: 10.1103/PhysRevLett.99.23550
54. S. Cereda, F. Zipoli, M. Bernasconi, L. Miglio, and F. Montalenti, Thermal-hydrogen promoted selective desorption and enhanced mobility of adsorbed radicals in silicon film growth, *Phys. Rev. Lett.* 100, 046105 (2008). DOI: 10.1103/PhysRevLett.100.046105
55. F. Zipoli, S. Cereda, M. Ceriotti, M. Bernasconi, L. Miglio, and F. Montalenti, First principles study of Ge/Si exchange mechanisms at the Si(001) surface, *Appl. Phys. Lett.* 92, 191908 (2008). DOI: 10.1063/1.2926683
56. R. Gatti, F. Uhlik, and F. Montalenti, Intermixing in heteroepitaxial islands: fast, self-consistent calculation of the concentration profile minimizing the elastic energy, *New J. Phys.* 10, 083039 (2008). DOI: 10.1088/1367-2630/10/8/083039
57. G. Vastola, F. Montalenti, and L. Miglio, Understanding the elastic relaxation mechanisms of strain in Ge islands on pit-patterned Si(001) substrates, *J. Phys.: Condens. Matt.* 20, 454217 (2008). DOI: 10.1088/0953-8984/20/45/454217
58. R. Gatti, A. Marzegalli, V.A. Zinovyev, F. Montalenti, and L. Miglio, Modeling the plastic relaxation onset in realistic SiGe islands on Si(001), *Phys. Rev. B* 78, 184104 (2008). DOI: 10.1103/PhysRevB.78.184104
59. T.U. Schüllli, G. Vastola, M.I. Richard, A. Malachias, G. Renaud, F. Uhlik, F. Montalenti, G. Chen, L. Miglio, F. Schäffler, and G. Bauer, Enhanced Relaxation and Intermixing in Ge Islands Grown on Pit-Patterned Si(001) Substrates, *Phys. Rev. Lett.* 102, 025502 (2009). DOI: 10.1103/PhysRevLett.102.025502
60. F. Uhlik, R. Gatti, and F. Montalenti, A fast computational method for determining equilibrium concentration profiles in intermixed nanoislands, *J. Phys.: Condens. Matt.* 21, 084217 (2009). DOI: 10.1088/0953-8984/21/8/084217
61. P.L. Novikov, A. Le Donne, S. Cereda, L. Miglio, S. Pizzini, S. Binetti, M. Rondanini, C. Cavallotti, D. Chrastina, T. Moiseev, H. von Känel, G. Isella, and F. Montalenti, Crystallinity and microstructure in Si films grown by plasma-enhanced chemical vapor deposition: A simple atomic-scale model validated by experiments, *Appl. Phys. Lett.* 94, 051904 (2009). DOI: 10.1063/1.3077187
62. M. Ceriotti, S. Cereda, F. Montalenti, L. Miglio, and M. Bernasconi, Ab initio study of the diffusion and decomposition pathways of SiH_x species on Si(100), *Phys. Rev. B* 79, 165437 (2009). DOI: 10.1103/PhysRevB.79.165437

63. G. Vastola, A. Marzegalli, F. Montalenti, and L. Miglio, Strain and strain-release engineering at epitaxial SiGe islands on Si(001) for microelectronic applications, *Mat. Sci Engin. B*, 159-160, 90 (2009). DOI: 10.1016/j.mseb.2008.05.011
64. D. Digiuni, R. Gatti, and F. Montalenti, Aspect-ratio-dependent driving force for nonuniform alloying in Stranski-Krastanow islands, *Phys. Rev. B* 80, 155432 (2009). DOI: 10.1103/PhysRevB.80.155436
65. M. Brehm, F. Montalenti, M. Grydlik, G. Vastola, H. Lichtenberger, N. Hrauda, M.J. Beck, T. Fromherz, F. Schäffler, L. Miglio, and G. Bauer, Key role of the wetting layer in revealing the hidden path of Ge/Si(001) Stranski-Krastanow growth onset, *Phys. Rev. B* 80, 205321 (2009). DOI: 10.1103/PhysRevB.80.205321
66. R. Bergamaschini, F. Montalenti, and L. Miglio, Optimal Growth Conditions for Selective Ge Islands Positioning on Pit-Patterned Si(001), *Nanoscale Res. Lett.* 5, 1873 (2010). DOI: 10.1007/s11671-010-9723-x
67. J.J. Zhang, F. Montalenti, A. Rastelli, N. Hrauda, D. Scopece, H. Groiss, J. Stangl, F. Pezzoli, F. Schäffler, O.G. Schmidt, L. Miglio, and G. Bauer, Collective Shape Oscillations of SiGe Islands on Pit-Patterned Si(001) Substrates: A Coherent-Growth Strategy Enabled by Self-Regulated Intermixing, *Phys. Rev. Lett.* 105, 166102 (2010). DOI: 10.1103/PhysRevLett.105.166102
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B) Book Chapters

116. F. Montalenti and R. Ferrando, Diffusion of adatoms and small clusters on missing-row reconstructed surfaces, in *Collective Diffusion on Surfaces: Correlation Effects and Adatom Interaction*, Nato Science Series, Ed.: M.C. Tringides and Z. Chvoj, (Kluwer, NL, 2001). ISBN 0-7923-7115-1
117. B.P. Uberuaga, F. Montalenti, T.C. Germann, and A.F. Voter, Accelerated molecular dynamics methods, in *Handbook of Materials Modeling*, Ed. S. Yip, Springer (N.Y., USA, 2005). ISBN 978-1-4020-3287-5
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119. L. Miglio and F. Montalenti, Modelling the evolution of germanium islands on silicon(001) thin films, in *Silicon-germanium (SiGe) nanostructures: Production, properties and applications in electronics*, Ed. Shiraki and Usami, (Woodhead, UK, 2011). ISBN 978-1- 84569-689-4

C) Other publications.

120. P. Cappella, C. Onado, G. Sena, F. Montalenti, L. Spinelli, e P. Ubezio, Time- and dose-dependence of DNA fragmentation induced by anticancer agents: a flow cytometric study, *European Journal of Histochemistry* 41, 67 (1997).
121. F. Montalenti, Diffusion on Channeled Metal Surfaces, PHD Thesis (Univ. Genova, 1999).
122. F. Montalenti, Temperature-accelerated dynamics: introduction and application to crystal growth, Technical Proceedings of the Second International Conference on Computational Nanoscience and Nanotechnology (San Juan, Puerto Rico, 2002).
123. J.A. Sprague, F. Montalenti, e A.F. Voter, Growth of Cu on Ag(001) at experimental deposition rates using TAD, Technical Proceedings of the Second International Conference on Computational Nanoscience and Nanotechnology (San Juan, Puerto Rico, 2002).
124. D. Digiuni, R. Gatti, F. Uhlik, and F. Montalenti, Concentration profiles in heteroepitaxial nanoislands, Proceedings of the 2009 Conference Physics, Chemistry and Application of Nanostructures (Minsk, BLR, 2009).

List of invited talks and seminars

1. Leap-frog mechanism for 1D clusters on missing-row reconstructed surfaces, Brown University, Providence (RI, USA), 1998.
2. Diffusion of adatoms and 1D clusters on channeled metal surfaces, ICTP (Trieste, Italy), 1999.
3. New diffusion mechanisms for 1D clusters on metal surfaces, Università di Milano-Bicocca, Milano (Italy), 1999.
4. New diffusion mechanisms for dimers and longer chains diffusion on channeled metal surfaces, workshop Dynamical correlations in single-particle and collective diffusion on surfaces, Lyon (France), 1999.
5. Diffusion on channeled metal surfaces, Helsinki Institute of Physics, Helsinki (Finlandia), 1999.
6. Diffusion on channeled metal surfaces, Centre de recherche sur les mecanismes de la croissance cristalline, Marseille (France), 1999.
7. Diffusion on channeled metal surfaces, Akademie věd České republiky, Prague (Czech Republic), 1999.
8. Crystal growth by temperature accelerated dynamics, Sandia National Laboratory, Albuquerque (NM, USA), 2000.

9. Atomistic simulation of crystal growth at experimental deposition fluxes, PEC Conference, Taos (NM, USA), 2001.
10. Unraveling the complexity of surface phenomena by accelerated molecular dynamics, Los Alamos National Laboratory, Los Alamos (NM, USA), 2001.
11. Atomistic simulations of crystal growth at experimental deposition fluxes, International Conference on Computational Nanoscience, San Juan (Puerto Rico, USA), 2002.
12. Unraveling the complexity of surface phenomena by accelerated molecular dynamics, Fritz-Haber Institute, Berlin (Germany), 2002.
13. Unraveling the complexity of surface phenomena by accelerated molecular dynamics, Swiss Center for Scientific Computing, Manno (Switzerland), 2002.
14. Simulazione di processi di diffusione e crescita mediante dinamica molecolare accelerata (simulation of diffusion and growth processes by accelerated molecular dynamics), CAPI2002 Workshop, Milano (Italy), 2002.
15. Ge islands on Si(001): stability and morphological evolution, Los Alamos National Laboratory, Los Alamos (NM, USA), 2003.
16. Ge islands on Si(001): stability and morphological evolution, Nato Advanced Workshop 2003, Heraklion (Greece), 2003.
17. Ge islands on Si(001): stability and morphological evolution, Nathiagali Summer College 2003, Nathiagali (Pakistan), 2003.
18. Multiple time scale simulations of solids based on the dimer method, workshop Modelling Statistics and Dynamics in Catalysis: from ab initio potentials to rare events, Ringberg (Germany), 2003.
19. Simple systems, complex kinetics: accurate, long time-scale dynamics at metal surfaces, APS 2004 March Meeting, Montreal (Canada), 2004.
20. Atomic-scale pathway of the pyramid to dome transition in Ge/Si(001), workshop Growth, electronic and optical properties of semiconductor nanostructures, Kuhlungsborn (Germany), 2005.
21. Ge islands on Si(001): stability and morphological evolution, Università di Genova, Genova (Italy), 2005.
22. Tackling the time-scale problem in molecular dynamics simulations of rare events: the temperature-accelerated dynamics method, Psi-k 2005 Conference, Schwabish Gmund (Germany), 2005.
23. Tackling the time-scale problem in molecular dynamics simulations of rare events: the temperature-accelerated dynamics method, workshop Bridging time and length scales in materials science and biophysics, IPAM Institute, UCLA, Los Angeles (CA, USA), 2005.
24. Closing the gap between experimental and theoretical time scales for systems dominated by rare-event dynamics: the temperature-accelerated dynamics method, IPCMS-Gemme Institute, Strasbourg (France), 2006.

25. Extending the time scale in atomistic simulations by temperature accelerated dynamics, CECAM workshop Hybrid atomistic methods for materials and biological systems, Lyon (France), 2006.
26. Atomistic simulations of rare events: extending the time scale by temperature-accelerated dynamics, ACS National Meeting, San Francisco (CA, USA), 2006.
27. Multiscale modeling of Ge 3D islands on Si(001): stability, shape transformation, and ordering, workshop Droplet epitaxial quantum dots, Milano (Italy), 2006.
28. Ge islands on Si(001): stability, evolution, elastic relaxation, and dislocation injection, Tsukuba National Institute for Materials Science, Tsukuba (Japan), 2007.
29. Ge islands on Si(001): frustrated evolution towards high aspect ratios, Institute of semiconductor and solid state physics, Johannes Kepler Universität Linz (Austria), 2007.
30. Multiscale modelling of Ge islands on Si(001): stability, morphology, elastic relaxation, and dislocation injection, workshop Nanopatterning via Ions, Photon Beam, and Epitaxy, Sestri Levante (Italy), 2007.
31. Accurate atomic-scale modelling of a complex system: silicon films grown by (low energy) plasma enhanced chemical vapour deposition, Nanoforum meeting, Milano (Italy), 2007.
32. How hydrogen solves problems caused by other hydrogen: low/temperature Si(001) crystalline growth in plasma enhanced chemical vapour deposition, Università di Roma "Tor Vergata", Roma (Italy), 2007.
33. Local concentration profiles in heteroepitaxial SiGe islands: trying to solve a nice puzzle, Fritz-Haber Institute, Berlin (Germany), 2008.
34. Fast surface exchange processes determining local concentration profiles in heteroepitaxial nanometric islands, E-MRS fall meeting 2008, Warsaw (Poland), 2008.
35. Concentration profiles in heteroepitaxial nanoislands (plenary), 2009 Nanomeeting, Minsk (Belorussia), 2009.
36. Ge growth on patterned Si substrates: beyond ordering. ICMAT 2011 Conference, Singapore, 2011.
37. Ge growth on patterned Si substrates: beyond ordering. SemiconNano workshop, Traukirchen (Austria), 2011.
38. Heteroepitaxial islands on pit-patterned substrates: Beyond ordered positioning. ICSF Conference, Genova (Italy), 2012.
39. Heteroepitaxial growth on pit-patterned substrates: phenomenology, interpretation, and methodological issues, workshop From Atomistic to Coarse-Grained Modeling of Materials Properties, Helsinki, Finland (2013)
40. Towards a realistic, continuum modeling of heteroepitaxial growth: elastic

relaxation, surface-energy minimization, misfit dislocations, and intermixing", CECAM workshop "SimGrow" 2015, Schloss Rauischholzhausen/Germany.

41. Continuum Modeling of Ge/Si Heteroepitaxy: Interplay Between Elastic and Plastic

Relaxation, ISTDM VII - ICSI 2016 Conference, Nagoya (Japan).

42. Continuum Modeling of cyclic growth in Ge/Si(001) heteroepitaxy, GDR Pulse

Meeting, Marseille (Fr) 2016

43. Modeling simultaneous elastic and plastic relaxation during Ge deposition on

Si(001), EMRS Fall Meeting 2016, Warsaw (Poland).

44. Continuum modeling of heteroepitaxial growth including dislocations. Université de Lyon 1 (France, 2018).

45. Theoretical interpretation of tilting-angle maps in heteroepitaxial films, ISTDM/ICSI 2018 (Potsdam, Germany).

Contributed talks and posters are not listed.