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INPAC activity report 2006 - 2007

Group Performance analysis

Presented to the Advice Committee by

- Group 1: **Moshchalkov Victor**, Institute for Nanoscale Physics and Chemistry, Director
Vanacken Johan, Scientific Secretary
 - Group 2: **Ceulemans Arnout**, Quantum Chemistry, Department of Chemistry
 - Group 3: **Van der Auweraer Mark**, Photochemistry and Spectroscopy, Department of Chemistry
 - Group 4: **Van Haesendonck Chris**, Nanophysics with Scanning Probes,
Solid-State Physics and Magnetism Section, Department of Physics and Astronomy
 - Group 5: **Vantomme André**, Nuclear Solid State Physics,
Nuclear and Radiation Physics Section, Department of Physics and Astronomy
 - Group 6: **Clays Koen**, Molecular Electronics and Photonics, Department of Chemistry
 - Group 7: **Lievens Peter**, Clusters and Laser Spectroscopy,
Solid-State Physics and Magnetism Section, Department of Physics and Astronomy
 - Group 8: **Stesmans Andre**, Semiconductor Electron Spectroscopy,
Department of Physics and Astronomy
 - Group 9: **Vanderleyden Jos**, Centre for Microbial and Plant Genetics,
Department of Microbial and Molecular Systems
-

Moshchalkov Victor

Nanoscale Superconductivity and Magnetism & Pulsed Fields

1.1. Composition of the team

Staff

V. V. Moshchalkov

Post-doc

J. Vanacken
 K. Vervaeke
 J. Van de Vondel
 A.V. Silhanek
 D. Saurel
 M. Menghini
 T. Nishio
 R. Kramer
 V. Gladilin
 A. Aladyshkin (till 31.09.2007)
 D. Taylor (till 31.07.2007)

Ph.D. students

N. Verellen
 W. Decelle
 K. De Keyser
 T. Nuytten
 W. Gillijns
 B. Willems
 J. Fritzche
 N. Schilderman
 ChinHua Chen
 A. Gebremedhin
 S. Godefroo

1.2. Ph.D. students

Current (Ph.D. in progress)

W. Gillijns "Superconductor/Ferromagnet hybrid heterostructures"
 (Nov 2004 -)
 N. Schilderman "Rectification effects in mesoscopic structures"
 (Nov 2004 -)
 K. de Keyser *on the topic of SHPM*
 (Nov 2006 -)
 B. Willems *on the topic of percolation in nanosuperconductors*
 (Nov 2004 -)
 J. Fritzche "Domain-wall superconductivity in S/F hybrids: scanning laser microscopy"
 (Nov 2004 -)
 T. Nuytten *on the topic of III-V nanostructures (QDots, Qdonuts, Qwires, ...)*
 (Nov 2004 -)
 Chinhua Chen *on the topic of Ginzburg-Landau calculations in nanosuperconductors*
 (Nov 2005 -)
 N. Verellen *on the topic of guided vortex motion in S/F hybrid nanosuperconductors*
 (Nov 2007)
 A. Ataklti *on the topic of metamaterials*
 (Nov 2007)

Ph.D. attained

- J. Van de Vondel (2007)
Vortex dynamics and rectification effects in superconducting films with periodic pinning
- K. Vervaeke (2006)
Microscopic Hall sensors for magnetometry and local magnetic imaging
- W. Vinckx (2007)
Vortex pinning in superconductors laterally modulated by nanoscale self-assembled arrays
- S. Godefroo (2007)
Photoluminescence of Semiconductor Nanostructures in high magnetic fields

1.3. Main achievements

- **Origin of the multiple reversals in ratchet systems.** The direction of easy flow of vortices in asymmetric periodic pinning landscapes depends on the density of vortices. We demonstrate that the ultimate condition to obtain sign reversals is a strong vortex-vortex interaction with a characteristic interaction length larger than the period of the pinning landscape. [Souza Silva et al., Nature 440, 651 (2006), W. Gillijns et al., Phys. Rev. Lett. In press (2007)]
- **Magnetic Ratchet.** Asymmetric pinning landscapes have been so far introduced via micropatterning plain films. We have recently shown that arrays of micromagnets break the inversion symmetry of the system and also give rise to an effective ratchet potential. [Souza Silva et al., Phys.Rev.Lett. 98, 117005 (2007), A.V.Silhanek et al., Appl. Phys. Lett. 90, 182501 (2007)]
- **Alternative mechanism for voltage rectification** in superconducting systems. It is widely accepted that vortices submitted to ac excitations in an asymmetric pinning landscape will give rise to a rectification of the dc output voltage signal. Interestingly we have recently found that this is not the only mechanism leading to this kind of behavior. Similar rectification effects can result from the interplay between external currents and persistent currents in superconductors. [M. Morelle et al., Appl. Phys. Lett. 89, 112512 (2006), N. Schildermans et al., Phys. Rev. B (2007), J. Van de Vondel et al., Eur. Phys. Lett. (2007)]
- **From Domain Wall Superconductivity to Field Induced Superconductivity.** Domain wall superconductivity refers to the preferential nucleation of the superconducting condensate on top of ferromagnetic domain walls in superconductor/ferromagnet hybrids. This effect has been thought to be apparently disconnected from that which leads to the nucleation of superconductivity at finite magnetic fields. In this work, we have established a clear theoretical link between these phenomena and which have been corroborated experimentally. [W. Gillijns et al., Phys. Rev. B (R) 76, 60503 (2007)]
- **Tunable pinning centers.** We have recently demonstrated the possibility to control the strength of vortex pinning by using either multiply-connected magnetic structures or superconducting rings. The unprecedented flexibility of these systems might have an important impact in the ongoing development of fluxonic devices. [A.V. Silhanek et al., Appl.Phys.Lett. 89, 182505]
- **Development of vortex-antivortex pairs in magnetic dots.** For the first time, using transport measurements we unveiled the way in which vortex-antivortex pairs are created as the magnetization of small magnetic dots is progressively increased. This effect leads to clear oscillations of the superconducting phase diagram which is in good agreement with previous theoretical estimates. [W. Gillijns et al., Phys. Rev. B (R) 74, 220509 (2006), A.V. Silhanek et al., Phys. Rev. B (R) 76, 100502 (2007)]
- **Magnetic camera.** We successfully designed and developed a magnetic camera consisting of an array of very sensitive hall crosses which can be addressed individually. This device is under EU patent and USA patent N.....

- **Anisotropic avalanche regime induced by asymmetric pinning landscapes.** Avalanches of fluxons resulting from a subtle balance between self-heating and heat removal through the sample boundaries can be substantially altered by introducing asymmetric pinning arrays. This represents a clear direct evidence of the anisotropic critical current in these kind of systems [M. Menghini et al., Phys. Rev. B 76, 184515 (2007)]
- **Direct visualization of magnetic domain superconductivity.** Laser scanning microscopy has been used as a key technique to visualize the nucleation of superconducting condensate on top of ferromagnetic domains. [J. Fritzsche et al., Phys. Rev. Lett. 96, 247003 (2006)]
- **Nucleation of superconductivity in a mesoscopic disk** with a magnetic dot on top. By using the nonlinear Ginzburg-Landau equations, we investigate symmetry-breaking effects at temperatures well below the normal-superconducting phase boundary in a superconducting microsquare with a magnetic dot on. Vorticity values forbidden by the inhomogeneous field of the dot at the phase boundary are progressively recovered deep inside the superconducting state. This restoration of the increase of the fluxoid quantum number by 1 with decreasing temperature is achieved both by the conventional flux expulsion and by the spontaneous generation of additional vortices [Qinghua Chen et al., Phys.Rev.B 74, 214519 (2006)]
- **Time-resolved measurements of the magnetization reversal in single-crystals of Mn₁₂Ac in pulsed magnetic fields**, corresponding to high effective magnetic field sweep rates from 1.5kT/s up to 7kT/s, suggest a process that can not be scaled onto a deflagration-process driven by heat diffusion. The sweep rate dependence of the time-difference in between reversal of the magnetisation on both sides of the easy axis of a cylindrical single crystal of Mn₁₂Ac indicates the existence of two new regimes at the highest sweep rates, with a transition around 4kT/s. It is shown that if no propagation effects are involved, the data can be understood by assuming a collective reversal of spins in large regions of the crystal. If on the other hand propagation of magnetic avalanches from one side of the crystal to the other at a constant speed is assumed, it is shown that our data can be understood as the first observation of a magnetic deflagration-to-detonation transition. Both interpretations imply an enhanced radiative coupling of the Mn₁₂-molecules in the crystal in the high sweep rate regimes. [W. Decelle, submitted to PRL]
- By combining Electron Spin Resonance and photoluminescence (PL) in high magnetic fields, we were able to unambiguously determine the **origin of PL in these Si nanocrystals**. Moreover, we showed that the origin of PL in one sample can be switched between quantum confinement and defects: In the as-grown state, the PL is dominated by highly-localized defect states. After H-passivation, which removes the ESR-active defects, the PL is purely originating from quantum confinement. After subsequent irradiation with UV, the PL is again of defect-related origin. [M. Jivanescu et al., J. Optoelect. Adv. Mat. 9, 721 (2007)]
- **Excitonic Properties of Strain-Engineered InAs/InGaAs/GaAs Quantum Dots.** We have investigated the low temperature (10 K) photoluminescence (PL) of strain-engineered InAs/InGaAs/GaAs quantum dots (QDs) in pulsed magnetic fields. The lowering of the mismatch between the QDs and the lower confining layer (LCL) and, consequently, of the QD strain, induces a decrease in the exciton effective mass. This results in an expansion of the exciton wave-function, which is at first hampered by the spatial limitations of the nanostructure. However, as the lattice mismatch between the LCL and the QDs and the QD-LCL band discontinuities are further reduced, dramatic changes in the magneto-PL suggest that the exciton unbinds. [T. Nuytten et al., submitted to Phys. Rev. B.]
- Design of a Sample Stick for **Optically Detected Magnetic Resonance**. We have finished the design of the sample stick for ODMR measurements to be performed at LNCMP, Toulouse, France. The stick is currently being constructed in the KULeuven workshop, and will be installed as soon as it is ready. A number of experiments are planned, amongst others the investigation of InSe and AlP/GaP quantum wells [T. Nuytten et al., milestone achievement EuroMagNET EU-FP6]
- **Zeeman and possible quantum confinement effect on the 1.5 μm emission band in Er³⁺-doped nano-glass-ceramics.** A zero-phonon component of the 1.5 μm emission band of Er³⁺ in the nano-glass-ceramics 32(SiO₂)9(AlO_{1.5})31.5(CdF₂)18.5(PbF₂)5.5(ZnF₂):3.5(ErF₃) mol%, shifts to higher energy and splits in Zeeman doublet in external magnetic field. These effects

provide tools to flatten the amplification band of the Er^{3+} -doped amplifier. The high-energy shift may be ascribed to quantum confinement effect on the 1.5 μm emission band of Er^{3+} in nano-glass-ceramics, where most of the Er^{3+} -dopants are located in about 8 nm diameter PbF_2 nano-crystals. [D. Saurel et al.]

- **Disorder tuned superconductor insulator transition in electron and hole doped high temperature epitaxial $\text{La}_{2-x}(\text{Sr/Ce})_x\text{CuO}_4$ superconducting thin films.** In studying the magneto-resistivity $\rho(B)$ in high pulsed magnetic fields up to 55 T, it is often observed that the $\rho(B)$ curves for different temperatures in the vicinity of the critical temperature cross at the same field value $B=B_{\text{cross}}$. The work shows how the crossing field changes as function of the hole (or electron) doping x , showing similarity with the $T_c(x)$ phase line. The resistivity ρ and the magnetic field B at different temperatures may be scaled as R/R_{cross} and $|B-B_{\text{cross}}|/T^\gamma$, respectively. This kind of scaling behaviour was earlier observed earlier in beryllium thin films, where the critical exponent $1/\gamma=1.35$, identical to the case in our $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ thin films. This value is in good agreement with the predictions of theories based on dirty boson model, with renormalization group theories and Monte Carlo simulations [B. Leridon et al., submitted to PRB]

- **Direct observation of the high magnetic field effect on the Jahn-Teller state in TbVO_4 .** We report an x-ray powder diffraction study of the Jahn-Teller effect of TbVO_4 under pulsed magnetic fields up to 30 T. Contrary to spectroscopic and magnetic methods X-ray diffraction directly measures the Jahn-Teller distortion; the splitting between the (311)/(131) and (202)/(022) pairs of Bragg reflections is proportional to the order parameter. Our powder diffraction data are compared to detailed mean field calculations, taking into account all possible orientations of the powder grains relative to the applied magnetic field. We find that magnetic fields along [001] suppress the Jahn-Teller distortion, whereas fields along [100] increase it. Although these effects of the magnetic field on the JT state have long been predicted by theory, they have never been observed directly. [C. Detlefs et al., submitted to PRB]

- **Vortex pinning in Nb thin films modulated by nanospheres.** Superconducting Nb thin films deposited on top of self-assembled spherical nanoparticles have been investigated by transport measurements. Colloid polystyrene nanospheres have been organized by convective self-assembly into colloid crystals. These crystals serve as modulation templates for the Nb thin films which are deposited on top. These periodic arrays provide a natural topographic pattern to modulate laterally the superconducting order parameter in deposited Nb films. The nanoparticle diameter effectively controls the matching fields and flux pinning properties of these films. The superconducting phase boundary and matching effects have been studied for Nb films grown on the templates formed by polystyrene particles with diameter $d=202$ and $d=357$ nm. The triangular colloid lattice geometry induces strong modulation in thin Nb layers. In combination with the short range crystalline order of the templates, this leads to geometrical vortex ordering effects and vortex density dependent matching phenomena. [W. Vinckx et al., Journ. of Appl. Phys. 100 (2006) 044307]

- **Vortex pinning in superconducting Nb thin films deposited on nanoporous alumina templates.** We present a study of magnetization and transport properties of superconducting Nb thin films deposited on nanoporous aluminium oxide templates. Periodic oscillations in the critical temperature vs. field, matching effects in fields up to 700 mT and strongly enhanced critical currents were observed. These fields are considerably higher than those typical for periodic pinning arrays made by lithographic techniques, which reflects the benefits of nanostructuring superconductors by using self-organized growth. This method provides a periodic pinning potential with sub-100 nm spacing between the pinning centers, which enhances vortex pinning in broad field and temperature ranges. [W. Vinckx et al, Eur. Phys. J. B (2006)]

1.4. Publications

1. Holmberg H, Lebedeva N, Novikov S, et al.
Magnetotransport of holes through an AIAs/GaAs/AIAs resonant tunnelling quantum well with a ferromagnetic Ga_{1-x}Mn_xAs emitter
PHYSICA STATUS SOLIDI A-APPLICATIONS AND MATERIALS SCIENCE 204 (10): 3463-3477
OCT 2007
2. Silhanek AV, Gillijns W, Milosevic MV, et al.
Optimization of superconducting critical parameters by tuning the size and magnetization of arrays of magnetic dots
PHYSICAL REVIEW B 76 (10): Art. No. 100502 SEP 2007
3. Silhanek A, Van Look L, Jonckheere R, et al.
Enhanced vortex trapping by a composite antidot lattice in a superconducting Pb film
PHYSICA C-SUPERCONDUCTIVITY AND ITS APPLICATIONS 460: 1434-1435 Part 2 SEP 1 2007
4. Leridon B, Vanacken J, Wambecq T, et al.
Paraconductivity of underdoped La_{2-x}Sr_xCuO₄ thin-film superconductors using high magnetic fields
PHYSICAL REVIEW B 76 (1): Art. No. 012503 JUL 2007
5. Gillijns W, Aladyshkin AY, Silhanek AV, et al.
Magnetic confinement of the superconducting condensate in superconductor-ferromagnet hybrid composites
PHYSICAL REVIEW B 76 (6): Art. No. 060503 AUG 2007
6. Vinckx W, Vanacken J, Moshchalkov VV, et al.
High field matching effects in superconducting Nb porous arrays catalyzed from anodic alumina templates
PHYSICA C-SUPERCONDUCTIVITY AND ITS APPLICATIONS 459 (1-2): 5-10 AUG 1 2007
7. Sulka GD, Moshchalkov V, Borghs G, et al.
Electrochemical impedance spectroscopic study of barrier layer thinning in nanostructured aluminium
JOURNAL OF APPLIED ELECTROCHEMISTRY 37 (7): 789-797 JUL 2007
8. Aladyshkin AY, Ryzhov DA, Samokhvalov AV, et al.
Localized superconductivity and Little-Parks effect in superconductor/ferromagnet hybrids
PHYSICAL REVIEW B 75 (18): Art. No. 184519 MAY 2007
9. Popovic ZV, Moshchalkov VV, Isobe M, et al.
Raman scattering study of η -Na_{1.3}V₂O₅ in the charge disordered and ordered phases
SOLID STATE COMMUNICATIONS 142 (7): 385-388 MAY 2007
10. Silhanek AV, Gillijns W, Moshchalkov VV, et al.
Manipulation of the vortex motion in nanostructured ferromagnetic/superconductor hybrids
APPLIED PHYSICS LETTERS 90 (18): Art. No. 182501 APR 30 2007
11. Holmberg H, Lebedeva N, Novikov S, et al.
Electrical transport in Mn-doped GaAs pn-diodes
PHYSICA STATUS SOLIDI A-APPLICATIONS AND MATERIALS SCIENCE 204 (3): 791-804
MAR 2007
12. Silva CCD, Silhanek AV, de Vondel JV, et al.
Dipole-induced vortex ratchets in superconducting films with arrays of micromagnets
PHYSICAL REVIEW LETTERS 98 (11): Art. No. 117005 MAR 16 2007

13. Moshchalkov VV
Ginzburg-Landau theory: A powerful tool to study vortex matter in nanostructured superconductors
JOURNAL OF SUPERCONDUCTIVITY AND NOVEL MAGNETISM 19 (3-5): 409-416 JUL 2006

14. Li Z, Bender H, Malfait M, et al.
MBE growth of MgGeAs₂: Mn on GaAs substrate
PHYSICA STATUS SOLIDI A-APPLICATIONS AND MATERIALS SCIENCE 204 (1): 152-158
JAN 2007

15. Chen QH, Carballeira C, Moshchalkov VV
Symmetry-breaking effects and spontaneous generation of vortices in hybrid superconductor-ferromagnet nanostructures
PHYSICAL REVIEW B 74 (21): Art. No. 214519 DEC 2006

16. Gillijns W, Silhanek AV, Moshchalkov VV
Tunable field-induced superconductivity
PHYSICAL REVIEW B 74 (22): Art. No. 220509 DEC 2006

17. Cornet C, Hayne M, Caroff P, et al.
Increase of charge-carrier redistribution efficiency in a laterally organized superlattice of coupled quantum dots
PHYSICAL REVIEW B 74 (24): Art. No. 245315 DEC 2006

18. Malfait M, Vervaeke K, Fritzsche J, et al.
Direct local observation of magnetic anisotropy in microscopic Ga_{1-x}Mn_xAs dots
APPLIED PHYSICS LETTERS 89 (19): Art. No. 192502 NOV 6 2006

19. Silhanek AV, Gillijns W, Moshchalkov VV, et al.
Tunable pinning in superconducting films with magnetic microloops
APPLIED PHYSICS LETTERS 89 (18): Art. No. 182505 OCT 30 2006

20. Carballeira C, Teniers G, Moshchalkov VV, et al.
Vortex states inside the superconducting phase of a thin microtriangle
EUROPHYSICS LETTERS 75 (6): 936-942 SEP 2006

21. Vinckx W, Vanacken J, Moshchalkov VV, et al.
Vortex pinning in superconducting Nb thin films deposited on nanoporous alumina templates
EUROPEAN PHYSICAL JOURNAL B 53 (2): 199-203 SEP 2006

22. Silhanek AV, Gillijns W, Moshchalkov VV, et al.
Enhanced pinning and proliferation of matching effects in a superconducting film with a Penrose array of magnetic dots
APPLIED PHYSICS LETTERS 89 (15): Art. No. 152507 OCT 9 2006

23. Holmberg H, Lebedeva N, Novikov S, et al.
Magnetotransport in ferromagnetic (Ga, Mn)As and (Ga, Mn)N Pn-diodes
IEEE TRANSACTIONS ON MAGNETICS 42 (10): 2712-2714 OCT 2006

24. Hikavy A, Clauws P, Maes J, et al.
An investigation of structural and electrical properties of boron doped and undoped nanocrystalline diamond films
PHYSICA STATUS SOLIDI A-APPLICATIONS AND MATERIALS SCIENCE 203 (12): 3021-3027
SEP 2006

25. Golubovic DS, Moshchalkov VV
Hard magnetic-dots for flux bias of DC SQUIDS
IEEE TRANSACTIONS ON APPLIED SUPERCONDUCTIVITY 16 (3): 1908-1912 SEP 2006

26. Morelle M, Schildermans N, Moshchalkov VV
Rectification effects in superconducting triangles
APPLIED PHYSICS LETTERS 89 (11): Art. No. 112512 SEP 11 2006

27. Aladyshkin AY, Moshchalkov VV
Thin-film superconductor-ferromagnet hybrids: Competition between nucleation of superconductivity at domain walls and domains' centers
PHYSICAL REVIEW B 74 (6): Art. No. 064503 AUG 2006
28. Vinckx W, Vanacken J, Moshchalkov VV
Vortex pinning in Nb thin films modulated by nanospheres
JOURNAL OF APPLIED PHYSICS 100 (4): Art. No. 044307 AUG 15 2006
29. Vavra O, Gazi S, Golubovic DS, et al.
0 and pi phase Josephson coupling through an insulating barrier with magnetic impurities
PHYSICAL REVIEW B 74 (2): Art. No. 020502 JUL 2006
30. Williams OA, Daenen M, D'Haen J, et al.
Comparison of the growth and properties of ultrananocrystalline diamond and nanocrystalline diamond
DIAMOND AND RELATED MATERIALS 15 (4-8): 654-658 Sp. Iss. SI APR-AUG 2006
31. Yang ZR, Van de Vondel J, Gillijns W, et al.
Effect of reversed magnetic domains on superconductivity in Pb/BaFe₁₂O₁₉ hybrids
APPLIED PHYSICS LETTERS 88 (23): Art. No. 232505 JUN 5 2006
32. Yang ZR, Vervaeke K, Moshchalkov VV, et al.
Modulation of superconductivity by a magnetic template in Nb/BaFe₁₂O₁₉ hybrids
PHYSICAL REVIEW B 73 (22): Art. No. 224509 JUN 2006
33. Fritzsche J, Moshchalkov VV, Eitel H, et al.
Local observation of reverse-domain superconductivity in a superconductor-ferromagnet hybrid
PHYSICAL REVIEW LETTERS 96 (24): Art. No. 247003 JUN 23 2006
34. Gheorghie DG, Menghini M, Wijngaarden RJ, et al.
Anisotropic avalanches and flux penetration in patterned superconductors
PHYSICA C-SUPERCONDUCTIVITY AND ITS APPLICATIONS 437-38: 69-72 MAY 15 2006
35. Gillijns W, Aladyshkin AY, Van Bael MJ, et al.
Domain-wall superconductivity in a ferromagnet/superconductor/ferromagnet trilayer
PHYSICA C-SUPERCONDUCTIVITY AND ITS APPLICATIONS 437-38: 73-76 MAY 15 2006
36. Golubovic DS, Moshchalkov VV
Soft magnetic dot as a linear flux amplifier
PHYSICA C-SUPERCONDUCTIVITY AND ITS APPLICATIONS 437-38: 82-85 MAY 15 2006
37. Villar R, Pryadun VV, Sierra J, et al.
Magnetic field induced suppression of vortex flow resistance in superconductors with periodic pinning centers
PHYSICA C-SUPERCONDUCTIVITY AND ITS APPLICATIONS 437-38: 345-348 MAY 15 2006
38. Raedts S, Silhanek AV, Moshchalkov VV, et al.
Crossover from intravalley to intervalley vortex motion in type-II superconductors with a periodic pinning array
PHYSICAL REVIEW B 73 (17): Art. No. 174514 MAY 2006
39. Sidor Y, Partoens B, Peeters FM, et al.
High-field magnetoexcitons in unstrained GaAs/Al_xGa_{1-x}As quantum dots
PHYSICAL REVIEW B 73 (15): Art. No. 155334 APR 2006
40. Morelle M, Moshchalkov VV
Enhanced critical currents through field compensation with magnetic strips
APPLIED PHYSICS LETTERS 88 (17): Art. No. 172507 APR 24 2006

41. Vavra O, Gazi S, Vavra I, et al.
Integration method for visualization of the suppressed Josephson supercurrent
PHYSICA C-SUPERCONDUCTIVITY AND ITS APPLICATIONS 435 (1-2): 92-95 MAR 15 2006

42. Solis PJC, Garcia-Santiago A, Tejada J, et al.
Magnetic characterisation of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ at microwave frequencies
JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS 67 (1-3): 419-423 JAN-MAR 2006

43. Moshchalkov VV, Golubovic DS, Morelle M
Nucleation of superconductivity and vortex matter in hybrid superconductor/ferromagnet nanostructures
COMPTES RENDUS PHYSIQUE 7 (1): 86-98 JAN-FEB 2006

44. Silva CCD, de Vondel JV, Morelle M, et al.
Controlled multiple reversals of a ratchet effect
NATURE 440 (7084): 651-654 MAR 30 2006

45. Pryadun VV, Sierra J, Aliev FG, et al.
Plain superconducting films as magnetic field tunable two-dimensional rectifiers
APPLIED PHYSICS LETTERS 88 (6): Art. No. 062517 FEB 6 2006

46. Chen QH, Teniers G, Jin BB, et al.
Pinning properties and vortex dynamics in thin superconducting films with ferromagnetic and antiferromagnetic arrays of magnetic dots
PHYSICAL REVIEW B 73 (1): Art. No. 014506 JAN 2006

47. de Souza Silva CC, Van de Vondel J, Zhu BY, et al.
Vortex ratchet effects in films with a periodic array of antidots
PHYSICAL REVIEW B 73 (1): Art. No. 014507 JAN 2006

48. M. Jivanescu, A. Stesmans, S. Godefroo and M. Zacharias
Electron Spin Resonance analysis of Si nanocrystals embedded in a SiO_2 matrix
J. Optoelect. Adv. Mat. 9, 721 (2007)

Arnout Ceulemans

Quantum Chemistry

2.1. Composition of the team

Staff

Prof. Arnout Ceulemans
Prof. Minh Tho Nguyen
Prof. Marc Hendrickx
Prof. Liviu Chibotaru

Post-doc

Dao Hung Vu
Lijnen Erwin
Lin Ling
Ramaswamy Amutha
Soncini Alessandro
Wang Hongming
Yang Lijun

Ph.D. students

Gopanidan Pillai Gopakumar
Hörtl Tibor
Michielssens Servaas
Moors Samuel
Nguyen Vinh Son
Swinnen Saartje
Ungur Liviu
Van den Heuvel Willem
Vu Thi Ngan

2.2. Ph.D. students

Current (Ph.D. in progress)

Gopanidan Pillai Gopakumar
Hörtl Tibor
Michielssens Servaas
Moors Samuel
Nguyen Vinh Son
Swinnen Saartje
Ungur Liviu
Van den Heuvel Willem
Vu Thi Ngan

2.3. Main achievements

- In view of the ongoing experimental studies of confinement in 2D structures, a general analytical tool was developed to describe the **eigenstates in a quantum box of arbitrary shape**. The method uses the particle on a disk solutions, which are deformed to cover the shape of the box. A deformation functional was developed which provides convergence and smoothness of the

solutions. The method was successfully applied to the spectra of Co-islands in the form of a truncated triangle on a gold surface. In the near future extensions are planned to deal with superconducting pentagons and hexagons.

- A theoretical study was undertaken of **mesoscopic two-gap superconductors** with sizes of the order of the coherence length. Noncomposite vortices were found to be thermodynamically stable in a large domain of the T-H phase diagram. In these phases the vortex cores of one condensate are spatially separated from the other condensate ones, and their respective distributions can adopt distinct symmetries. The appearance of these vortex phases is caused by a non-negligible effect of the boundary of the sample on the superconducting order parameter and represents therefore a genuine mesoscopic effect. The calculations show that noncomposite vortices could be observed in thin mesoscopic samples of MgB₂.

- Using quantum chemical calculations, we have shown the strong **influence of doped-metal atoms on geometrical and electronic structures of the silicon, germanium, copper and silver clusters**. In some special cases, the doped clusters are stabilized due to the π -aromaticity or three-dimensional aromaticity.

2.4. Publications

1. S.L.C. Moors, M. Hellings, M. De Maeyer, Y. Engelborghs, A. Ceulemans Tryptophan rotamers as evidenced by X-ray. Fluorescence lifetimes and molecular dynamics modeling, *Biophysical Journal* 91, 816-823 (2006)
2. S. Cojocaru, V. Bărsan, A. Ceulemans Green's function and excitation spectrum of finite lattices, *Physica Status Solidi b* 243, 1963-1977 (2006)
3. S. Cojocaru, V. Bărsan, A. Ceulemans Spin excitations on finite lattices and the discrete Fourier transform *J. Magnetism and Magnetic Materials*, 307, 62-73 (2006)
4. S. Cojocaru, V. Barsan, A. Ceulemans Exact solution of the discrete Schrödinger equation for ferromagnetic chain *Philosophical Magazine* 86, 4983-4995 (2006)
5. S. Compemolle, L.F. Chibotaru, A. Ceulemans Novel type of magnetic response in carbon nanomaterials *Chem. Phys. Lett.* 428, 119-124 (2006)
6. C. Carballeira; G. Teniers, V.V. Moshchalkov, L.F. Chibotaru, A. Ceulemans Vortex states inside the superconducting phase of a thin mesoscopic triangle *Europhys. Lett.* 75, 936-942 (2006)
7. Q.-C. Qiu, E. Lijnen, A. Ceulemans Construction of the $\pi^9x(g+2h)$ Jahn Teller Hamiltonian *Mol. Phys.*, 104, 3173-3185 (2006)
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Mark Van der Auweraer

Photochemistry and Spectroscopy

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3.3. Main achievements

- **Dronpa-related projects.** The characterization of the photophysical properties of the photoswitchable fluorescent protein Dronpa and its mutants Dronpa2 and Dronpa3 at the ensemble level by partner 3 using femtosecond transient absorption spectroscopy, confirmed that the first and rate-limiting step for Dronpa photoswitching from dark to bright state transition involves excited-state proton transfer. The single-molecule experiments, allowed a better understanding of the photoswitching scheme by identification of several dark intermediates. Starting from this information partner 3 developed the methodology to use Dronpa and its mutants for imaging with resolution below the diffraction limit of light (“super-resolution” or “nanoscopy”). By means of photoactivation-localization microscopy (PALM), demonstrated the possibility of super-resolution imaging using Dronpa-labeled nano-objects of known dimensions (~50 nm). Introduction of a stroboscopic approach to PALM (S-PALM) reduced the noise and thus enhanced the spatial resolution. Furthermore Dronpa was used in a different experimental scheme to achieve super-resolution, by using a donut-mode depletion beam (known as RESOLFT microscopy: reversible saturable optical fluorescence transitions). The results were however limited due to severe photobleaching of Dronpa. In collaboration with partner 6 the nonlinear optical properties and, in particular, the first hyperpolarizability ($\chi^{(2)}$) of Dronpa was quantified and the influence of pH and photoswitching on this parameter was studied. When comparing the results with those of the model compounds (EGFP and the synthetic GFP fluorophore HBDI) unexpectedly a higher $\chi^{(2)}$ was observed for the neutral fluorophore than for the anionic one. This trend was attributed to important conformational changes upon protonation or photoswitching of Dronpa.

- **Self-assembled molecular and macromolecular structures.** Partner 3 probed the self-assembly of a variety of new functional molecular building blocks using scanning tunneling microscopy (STM). A first set of molecular systems is designed to arrange into nanoporous surface confined networks. By tuning the alkyl chain length of the molecular building blocks, the diameter of the pores can be tuned at will ranging from about 1 nm to more than 5 nm, under the proper experimental conditions as e.g. the concentration of the building blocks. For a given set of building blocks, specific surface patterns can be created on demand only depending on the concentration of the molecular building blocks. When these nanoporous surface-confined networks were probed to host a set of mainly aromatic guest molecules they turned out to be guest selective. Furthermore, the nature of the surface pattern, being porous or not, can be directed by the presence of appropriate guest molecules. In parallel, intrinsic porous molecular systems (macrocycles) are investigated as porous host matrices for the adsorption of a variety of guest molecules. Once their self-assembly properties are established, the adsorption of semiconducting (MoS) and metallic nanoparticles in the pores will be targeted, following a number of different deposition methods, including the size-selective pinning of gas-phase produced clusters (partner 7) and the in-situ generation of metallic clusters by reduction of the proper metal salt. When the self-assembly of a set of molecules under potential control has been probed by electrochemical STM partner 3 observed that the ordering of water-insoluble amphiphiles can be tuned by the potential at the interface between an aqueous electrolyte and a metallic substrate.

In order to control reactions at the liquid-solid interface on the nanoscale the ordering and reactivity of diacetylene containing amphiphiles is currently being investigated under electrochemical control, aiming at optimizing the polymerisation conditions of this particular system, potentially giving rise to surface confined conjugated polymers. Partner 3 realized another approach to create a conductive 1D nanosystems by the self-assembly of carefully designed tetrathiofulvalene derivatives at the liquid-solid interface. Scanning tunneling spectroscopy experiments hand in hand with theoretical studies predict high charge carrier mobilities in these self-assembled structures. Efforts to extend these principles to the third dimension are in progress.

Using scanning probe microscopy techniques as AFM and electrical force microscopy (EFM) partner 3 investigated in collaboration with partner 4 the origin of the high conductivity of poly(3,4-Ethylene-dioxy-thiophene)- polystyrenesulfonate (PEDOT-PSS) plastic electrodes. These experiments showed that in the presence of diethylene glycol PEDOT-PSS appears to form a three-dimensional conducting network explaining the improvement of its electrical property. Together with partner 8 the model for the carrier mobility as a function of temperature and carrier density, was worked out for a 2D-system starting from a model developed earlier by partner 8 for a 3D-system. This approach allowed to explain literature data obtained by Sirringhaus et al. for a poly-3-hexylthiophene thin film FET.

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72. B. Kolaric; K. Baert; R.A.L. Vallée; M. Van der Auweraer; K. Clays; 'Controlling the fluorescence resonant energy transfer by photonic crystal bandgap engineering',
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STM, STS and Bias Dependent Imaging on Organic Monolayers at the Solid-Liquid Interface,
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Supramolecular Chemistry at the Liquid/Solid Interface, a Scanning Tunneling Microscopy Approach,
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J. Am. Chem. Soc., 2007, accepted
79. Anca Margineanu, Steven De Feyter, Sergey Melnikov, Patrick Chaltin, Arthur van Aerschot, Piet Herdewijn, Satoshi Habuchi, Frans C. De Schryver, Johan Hofkens ,
Complexation between lipofectamine and cholesterol-modified DNA sequences studied by single molecule fluorescence techniques, *Biomacromolecules*, 2007, accepted

Chris Van Haesendonck

Nanophysics with Scanning Probes

4.1. Composition of the team

Staff

Chris Van Haesendonck

Post-doc

Steven Brems
Manish Pal Chowdhury
Jyoti Mohanty
Sudipta Sarkar Pal
Johan Snauwaert (part-time, 30%)
Alexander Volodin
Qing-feng Zhan

Ph.D. students

Maarten Gysemans
Alexander Malesevic
Tom Moorkens
Cristina Toma
Koen Schouteden
Stijn Vandezande

4.2. Ph.D. students

Current (Ph.D. in progress)

Cristina Toma
"Nanoscale characterization and modification of the electronic properties of hydrogen terminated diamond surfaces"
Promoters: Chris van Haesendonck and Alexander Volodin
(Start October 2002)

Stijn Vandezande
"Influence of surface morphology on the hysteretic properties of magnetic films and microstructures"
Promoters: Chris Van Haesendonck and Kristiaan Temst
(start October 2003)

Maarten Gysemans
"Production and properties of electronic systems based on self-assembling biological nanostructures"
Promoters: Chris Van Haesendonck and Johan Snauwaert
(Start October 2004)

Koen Schouteden
"Tunnel microscopy and tunnel spectroscopy of self-assembled metal islands and of deposited metallic clusters on single-crystal metal surfaces"
Promoters: Chris Van Haesendonck and Peter Lievens
(Start October 2004)

Alexander Malesevic
“Production and application of carbon nanostructures prepared by plasma based techniques”
Promoters: Chris Van Haesendonck and Annick Vanhulsel (VITO Mol)
(Start December 2004)

Tom Moorkens
“Structural and electronic properties of graphene based layers before and after modification with organic molecules”
Promoters: Chris Van Haesendonck and Alexander Volodin
(Start September 2007)

Koen Lauwaet
“Growth of novel nanostructures with cluster deposition”
Promoters: Peter Lievens and Chris Van Haesendonck
(Start September 2007)

Ph.D. attained

Steven Brems
“Magnetization reversal and domain structure in the polycrystalline Co/CoO system”
Promoters: Chris Van Haesendonck and Alexander Volodin
October 2007

4.3. Main achievements

- Important progress has been achieved with respect to **understanding the exchange bias effect in polycrystalline Co/CoO bilayers**. Using high-resolution measurements of the anisotropic magnetoresistance and of the magnetization, we have studied in detail the exchange bias effect as a function of both the magnitude and direction of the applied magnetic field. CoO/Co is selected for its large training effect and initial asymmetry of the magnetic hysteresis after field cooling, which is removed after training. Applying a magnetic field perpendicular to the cooling field largely restores the untrained state with pronounced asymmetry. The possibility to re-induce asymmetry strongly depends on the magnitude of the perpendicular field, providing the key to identify the origin of training and removal of asymmetry. These effects result from misalignment between ferromagnetic Co magnetization and uncompensated magnetization of the granular CoO antiferromagnet. The training effect has been further investigated with low-temperature magnetic force microscopy (MFM). After field cooling, no MFM contrast is detected, but clear contrast becomes visible after the first magnetization reversal of the Co layer. Ferromagnetic domains are detectable even at saturation and cannot be annihilated by the application of a magnetic field parallel to the cooling field. On the other hand, the magnetic domains can be partially removed by applying a perpendicular hysteresis loop.

- The **setup for UHV scanning tunneling microscopy (STM) and spectroscopy (STS) at low temperatures has been further optimized**, including the possibility for in situ flash heating of the STM tips, surface reconstruction by combined heating and ion bombardment, and controlled deposition of submonolayer metal films for island growth. We have performed detailed STM/STS measurements on nanosize Co islands on Au(111) films. By means of mapping of the local density of states with lock-in detection, electron standing wave patterns have been resolved on top of the atomically flat islands. The patterns are found to nicely fit to the calculated wave functions for a single electron in a box having the corresponding island symmetry. The observed standing wave patterns are identified either as individual eigenstates or as a mixture of two or more close-lying individual eigenstates. STM/STS has also been performed of ring-like features that appear around Co metal clusters deposited on a clean (110) oriented surface of cleaved p-type InAs crystals. These features are visible in spectroscopic images within a certain range of negative tunneling bias voltages due to the presence of a negative differential conductance in the current-voltage dependence. A theoretical model has been introduced to take into account non-equilibrium effects in the small tunneling junction. The ring-like features can be explained in terms of interference

between electrons tunneling directly and indirectly (via a Co island) between the tip and the InAs surface.

- **A new method based on electrostatic force microscopy (EFM) has been developed** for separate mapping of the surface potential and of the surface conductivity on a sub-100 nm scale. The technique has been applied for imaging the voltage distribution in current-carrying H-terminated diamond films. The uniform linear voltage drop in highly conductive H-terminated diamond surface layers indicates that the layers behave as homogeneous, diffusive conductors with a well-defined value of the sheet resistance. On the other hand, we observe conductive as well as insulating regions that coexist for not perfectly H-terminated diamond surfaces with poor electrical conductivity.

- The EFM technique has also been applied for investigating the **voltage distribution in banded individual carbon nanotubes** (CNTs) that are deposited on oxidized silicon wafers and to which electrical contacts are attached using electron beam lithography. The CNTs, which are grown by chemical vapor deposition (CVD), have also been investigated with atomic resolution STM/STS after deposition on atomically flat Au(111) surfaces. Plasma enhanced CVD has been successfully used for the preparation of high-quality carbon nanowall (CNW) samples on quartz substrates. The atomic-scale structure of the CNWs with a thickness around ten graphene monolayers has been investigated by both STM and transmission electron microscopy. We are now proceeding with attaching electrical contacts to individual CNWs for magnetotransport measurements.

4.4. Publications

1. Size and shape dependences on magnetization reversal in ferromagnetic/antiferromagnetic bilayer patterned into nano-dot arrays

E. Girgis, R.D. Portugal, K. Temst, C. Van Haesendonck
J. Phys. D - Appl. Phys. 39, 1733-1738 (2006)

2. Characterization of commercial nanofiltration membranes and comparison with self-made polyethersulfone membranes

K. Boussu, B. Van der Bruggen, A. Volodin, C. Van Haesendonck, J.A. Delcour,
P. Van der Meeren, C. Vandecasteele
Desalination 191, 245-253 (2006)

3. Wetting of self-assembled 1,4-benzendimethanethiol monolayer on gold and silver: An adhesion force spectroscopy study

Nele Vandamme, Koen Schouteden, Johan Snauwaert, Peter Lievens,
Chris Van Haesendonck
Surface Science 600, 2894-2899 (2006)

4. The influence of finite size and shape anisotropy on exchange bias: A study of patterned Co/CoO nanostructures

K. Temst, E. Popova, H. Loosvelt, M.J. Van Bael, S. Brems, Y. Bruynseraede,
C. Van Haesendonck, H. Fritzsche, M. Gierlings, L.H.A. Leunissen, R. Jonckheere
J. Magn. Magn. Mater. 304, 14-18 (2006)

5. Characterization of polymeric nanofiltration membranes for systematic analysis of membrane performance

K. Boussu, Y. Zhang, J. Cocquyt, P. Van der Meeren, A. Volodin,
C. Van Haesendonck, J.A. Martens, B. Van der Bruggen
Journal of Membrane Science 278, 418-427 (2006)

6. Microtubule binding and clustering of human tau-4R and tau-P301L proteins isolated from yeast deficient in orthologues of glycogen synthase kinase-3 β or cdk5

Tom Vandebroek, Dick Terwel, Thomas Vanhelmont, Maarten Gysemans,
Chris Van Haesendonck, Yves Engelborghs, Joris Winderickx, Fred Van Leuven
Journal of Biological Chemistry 281, 25388-25397 (2006)

7. The origin of the high conductivity of poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) (PEDOT- PSS) plastic electrodes
X. Crispin, F.L.E. Jakobsson, A. Crispin, P.C.M. Grim, P. Andersson, A. Volodin,
C. Van Haesendonck, M. Van der Auweraer, W.R. Salaneck, M. Berggren
Chemistry of Materials 18, 4354-4360 (2006)
8. Magnetization cusp in a thin AuFe spin glass film in high magnetic fields
Helmut Fritzsche, John Root, Kristiaan Temst, Chris Van Haesendonck
Physica B 385-386, 378-380 (2006)
9. Bias voltage dependent shift of the atomic-scale structure of a Ge(111)-(2 x 1) reconstructed surface measured by low temperature scanning tunneling microscopy
P.I. Arseyev, N.S. Maslova, V.I. Panov, S.V. Savinov, C. Van Haesendonck
JETP Lett. 85, 277-282 (2007)
10. Observation of wetting-like phase transitions in a surface-enhanced type-I superconductor
V.F. Kozhevnikov, M.J. Van Bael, P.K. Sahoo, K. Temst, C. Van Haesendonck,
A. Vantomme, J.O. Indekeu
New J. Phys. 9, art. No. 75, 7 pages (2007)
11. Influence of membrane and colloid characteristics on fouling of nanofiltration membranes
K. Boussu, A. Belpaire, A. Volodin, C. Van Haesendonck, P. Van der Meeren,
C. Vandecasteele, B. Van der Bruggen
Journal of Membrane Science 289, 220-230 (2007)
12. Origin of the training effect and asymmetry of the magnetization in polycrystalline exchange bias systems
Steven Brems, Kristiaan Temst, Chris Van Haesendonck
Phys. Rev. Lett 99, art. No. 067201, 4 pages (2007)
13. Determination of the size of Fe grains in Ag by Mössbauer spectroscopy
J. Balogh, D. Kaptás, I. Vincze, K. Temst, and C. Van Haesendonck
Phys. Rev. B 76, art. No. 052408, 4 pages (2007)
14. A polarized neutron reflectometry study of the spin glass freezing in a 29 nm thick AuFe film
H. Fritzsche, M. Saoudi, K. Temst and C. Van Haesendonck
Physica B 397, 47-49 (2007)
15. Study of the catalyst evolution during annealing preceding the growth of carbon nanotubes by microwave plasma enhanced chemical vapour deposition
Alexander Malesevic, Hong Chen, Tom Haufmann, Annick Vanhulsel,
Herman Terryn, Chris Van Haesendonck
Nanotechnology 18, art. No. 455602, 9 pages (2007)
16. Manipulation of in-plane uniaxial anisotropy in Fe/MgO(001) films by ion sputtering
Qing-feng Zhan, Stijn Vandezande, Chris Van Haesendonck, Kristiaan Temst
Appl. Phys. Lett. 91, art. No. 122510, 3 pages (2007)
17. Electrostatic force microscopy study of electrical conductivity of hydrogen-terminated CVD diamond films
A. Volodin, C. Toma, G. Bogdan, W. Deforme, K. Haenen, M. Nesládek,
C. Van Haesendonck
Phys. Stat. Sol. A 204, 2915-2919 (2007)
18. Voltage bias controlled local modification of hydrogenated diamond surface using atomic force microscopy
C. Toma, A. Volodin, G. Bogdan, W. Deforme, K. Haenen, M. Nesládek,
C. Van Haesendonck
Phys. Stat. Sol. A 204, 2920-2924 (2007)

19. Electrostatic force microscopy mapping of electrical conductivity of hydrogen-terminated diamond films
A. Volodin, C. Toma, G. Bogdan, W. Deferme, K. Haenen, M. Nesládek,
C. Van Haesendonck
Appl. Phys. Lett. 91, art. No.142111, 3 pages (2007)
20. Combined growth of carbon nanotubes and carbon nanowalls by plasma-enhanced chemical vapor deposition
Alexander Malesevic, Sorin Vizireanu, Raymond Kemps, Annick Vanhulsel,
Chris Van Haesendonck, Gheorghe Dinescu
Accepted for publication in Carbon
21. Single-electron tunneling phenomena on preformed gold clusters deposited on dithiol self-assembled monolayers
K. Schouteden, N. Vandamme, E. Janssens, P. Lievens, C. Van Haesendonck
Accepted for publication in Surface Science
22. XPS study of the assembling morphology of 3-hydroxy 3-phosphono-butiric acid ter-butyl ester on various pretreated Al surfaces
O. Blajiev, A. Ithurbide, A. Hubin, C. Van Haesendonck, H. Terryn
Accepted for publication in Progress in Organic Coatings

André Vantomme

Nuclear Solid State Physics

5.1. Composition of the team

Staff

André Vantomme
Kristiaan Temst

Post-doc

Cottenier Stefaan
Wahl Ulrich

Ph.D. students

Almeida Francisco
Decoster Stefan
Demeter Joost
Demeulemeester Jelle
Fleischmann Claudia
Kana Tomas
Laenens Bart
Paredis Kristof
Planckaert Nikie
Smeets Dries
Song Shu Fang
Vandervorst Wilfried (deeltijds)
Wang Huan
Zhao Qiang

5.2. Ph.D. students

Current (Ph.D. in progress)

Zhao Qiang, "Nuclear reaction analysis using energetic ion beams" (gestart 1-9-2001)

Malgorzata Kmiecik, "Investigation of Ir and NiSi₂ as gate materials for sub-micron CMOS technology" (gestart 1-1-2002, ism Prof. K. Maex, IMEC)

Vasco Matias, "Structural and optical properties of rare-earth doped group III-nitrides" (gestart 1-10-2002)

Francisco Almeida, "Exchange bias in Fe-Pt based heterostructured epitaxial thin films" (gestart 1-11-2003)

Simone Giangrandi, "Optimization of low-energy elastic recoil detection for the study of light impurities in ultra-thin films" (gestart 1-9-2003, ism Prof. W. Vandervorst, IMEC)

Stefan Decoster, "Studie van de roosterplaats van ingeplante onzuiverheden en stralingsschade in germanium" (gestart 1-10-2004)

Kristof Paredis, "Thermische en ionenbundeldepositie van ultradunne metaallagen op halfgeleiders" (gestart 1-9-2004)

Nikie Planckaert, "Magnetische eigenschappen van CsCl-FeSi/Fe multilagen bestudeerd met behulp van nucleaire resonante verstrooiing van synchrotron straling" (gestart 1-9-2005)

Bart Laenens, "Ontwikkeling van een circulair gepolariseerde Mössbauer bron" (gestart 1-9-2005)

Jelle Demeulemeester, "In-situ studie van de fasevorming en eigenschappen van silicidelegeringen met zeldzame aard elementen" (gestart 1-9-2006)

Ruben Verheyden, "De atoomprobe als routine 3D-analyse in halfgeleider technologie" (gestart 1-9-2006, ism Prof. W. Vandervorst, IMEC)

Wang Huan, "Magnetische eigenschappen van hybride nanostructuren" (gestart 1-9-2006)

Joost Demeter, "Exchange bias in granular systems" (gestart 10-09-2007)

Claudia Fleischmann, "Ge surface passivation" (gestart 10-10-2007)

Ph.D. attained

De Vries Bart (19-01-06)
Lattice site location of impurities in group III nitrides using emission channeling
A. Vantomme

Torumba Doru (27-09-06)
Density Functional Theory Studies in Nuclear Condensed Matter Physics: Hyperfine Interactions at Lanthanide Impurities in Fe and the Temperature Dependence of Electric-Field Gradients in Metals
S. Cottenier

Vanhoof Veerle (29-09-06)
Density Functional Theory Studies for Transition Metals: Small (Fe,Co)-clusters in fcc Ag, and the Spin Density Wave in bcc Chromium
S. Cottenier

Huygebaert Cedric (20-12-06)
Oxygen beam interactions during sputter profiling of Si, SiGe and Ge substrates
A. Vantomme

Smeets Dries (27-02-07)
Nucleation, diffusion and texture during growth of CoNi-silicides
A. Vantomme

Dobrynin Alexey (08-05-2006)
Exchange coupling in hybrid magnetic nanocluster systems
P. Lievens en K. Temst

5.3. Main achievements

- **Relation between implantation damage and luminescence in rare-earth doped GaN.** The lattice site location of the implanted impurities has been determined by emission channeling, whereby the effect of the nitride mosaicity was taken into account.
- Using the ternary **CoxNi1-xSi2** system as a vehicle, the **role of the lattice mismatch versus the growth kinetics on the epitaxial growth of thin films was studied.** The results show that the most abundant texture component is not necessarily the one with the smallest in plane lattice mismatch.
- **The role of surfactants (i.e. Ag, Au, Cu) on the growth of Fe(silicide) nanostructures on Si was studied in detail.** The surfactant modifies the surface reconstruction (hence the density of dangling bonds), thus decoupling the substrate temperature and the mobility of the deposited atoms. Hence, tailoring of the nanostructures becomes achievable.
- Using **DLTS, a number of new defect levels in the band gap of ion-implanted germanium were determined.** For ions heavier than B, no mass dependence of the implantation-induced damage was found. On the other hand, Ge surfaces were passivated by H₂S exposure. With a combination of surface sensitive experimental techniques (e.g. STM) and ab initio calculation, disulfide bridges interacting via hydrogen bonding were found to be at the origin of this passivation.
- **The Fe-Fe interlayer coupling across an FeSi spacer layer was directly probed with nuclear resonant scattering of synchrotron radiation.** Through comparison with macroscopic magnetization measurements, it is shown that static magnetic ordering in the spacer leads to suppression of the coupling at low temperatures. Above 150 K, fluctuating moments in the spacer result in biquadratic coupling.
- **The influence of ion irradiation on epitaxial Fe-films was studied using in-situ scanning tunneling microscopy and MOKE magnetization experiments.** It was found that the surface develops a ripple structure which has a profound effect on the in-plane magnetic anisotropy and providing a way to manipulate the easy and hard axes of the film. The resulting engineered anisotropy was successfully modeled.
- We applied new developments in **first principles methodology to the prototype problem of hyperfine fields at isolated impurities in Fe: the LDA+U method for strongly correlated lanthanides in Fe, and hybrid exchange-correlation functionals for actinides in Fe.** The experimentally controversial group of alkali impurities was treated with standard LDA/GGA.
- A new scheme based on first principles phonon calculations was applied to study another long-standing hyperfine problem: the **temperature dependence of the electric-field gradient at a Cd nucleus in hcp-Cd.** We show how this effect arises as an average of many phonon modes.

5.4. Publications

1. M.F. Wu, S.Q. Zhou, A. Vantomme, Y. Huang, H. Wang, and H. Yang
"High-precision determination of lattice constants and structural characterization of InN thin film"
J. Vac. Sci. Technol. 24(2), 275-279, (2006)
2. K. Vanormelingen, B. Degroote, and A. Vantomme
"Quantitative characterization of the surface morphology using a height difference correlation function"
J. Vac. Sci. Technol. 24 (2), 725-729, (2006)

3. A. Martin Hoyas, Y. Travaly, J. Schuhmacher, T. Sajavaara, C.M. Whelan, B. Eyckens, O. Richard, S. Giangrandi, B. Brijs, W. Vandervorst, K. Maex, J.P. Clis, A.M. Jonas, and A. Vantomme
"The impact of the density and type of reactive sites on the characteristics of the atomic layer deposited WN_xC_y films"
J. Appl. Phys. 99, 063515, (2006)
4. B. Devries, A. Vantomme, U. Wahl, J.G. Correia, J.P. Araujo, W. Lojkowski, D. Kolesnikov, and ISOLDE collaboration
"Lattice site location and annealing behavior of implanted Ca and Sr in GaN"
J. Appl. Phys. 100, 023531, (2006)
5. M.A. Pawlak, A. Lauwers, T. Janssens, K.G. Anil, K. Opsomer, K. Maex, A. Vantomme, and J.A. Kittl
"Modulation of the workfunction of Ni fully silicided gates by doping: Dielectric and silicide phase effects"
Electron Dev. Lett. 27(2), 99-101, (2006)
6. A.N. Dobrynin, D.N. Ievlev, C. Hendrich, K. Temst, P. Lievens, U. Hormann, J. Verbeeck, G. Van Tendeloo, and A. Vantomme
"Influence of finite size effects on exchange anisotropy in oxidized Co nanocluster assembled films"
Phys. Rev. B 73, 245416, (2006)
7. S. Giangrandi, B. Brijs, T. Sajavaara, H. Bender, F. Iacope, A. Vantomme, and W. Vandervorst
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Koen Clays

Molecular Electronics and Photonics

6.1. Composition of the team

Staff

Koen Clays
Thierry Verbiest

Post-doc

Inge ASSELBERGHS (FWO)
Guy KOECKELBERGHS (FWO)
Javier PEREZ-MORENO (FWO)
Jagdish DADGE (DARPA)
Renaud VALLEE (FWO)
Branko KOLARIC (INPAC)
Janqiu YIANG (GOA)
Christina FLORS (INPAC)
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affiliated researcher
(KHogeschool Leuven)
Dr. Tom MORTIER

Ph.D. students

Sheng Ting HUNG (joint WSU)
Edith FRANZ
Stijn VANCLEUVENBERGEN
Kurt DEMEY
Ayele TESHOME
Wim LIBAERS
Kasper BAERT
Luis GONZALEZ

Jelle WOUTERS
Stijn FOERIER
Lieven DECREMER
Marnix VANGHELUWE
Wouter VANORMELINGEN
Monique VAN DER VEEN,
Caroline VAN ORSHOVEN,

6.2. Ph.D. students

Current (Ph.D. in progress)

promotor Koen Clays:

Sheng Ting HUNG, PhD student in the joint PhD program in Physics and Astronomy of Washington State University and Chemistry of K.U.Leuven, Promotors Mark G. Kuzyk WSU and Koen Clays KUL

Edith FRANZ

Stijn VANCLEUVENBERGEN

Kurt DEMEY

Ayele TESHOME

Wim LIBAERS

Kasper BAERT

Luis GONZALEZ

Promotor Thierry Verbiest:

Jelle WOUTERS

Stijn FOERIER

Lieven DECREMER

Marnix VANGHELUWE

Wouter VANORMELINGEN

Monique VAN DER VEEN, promotor Thierry Verbiest, co-promotor Dirk De Vos,
Centrum voor Oppervlaktechemie en Katalyse

Caroline VAN ORSHOVEN, promotor Thierry Verbiest, co-promotor Ivo Vankelecom,
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6.3. Main achievements

- **Adding magnetic contribution to the optical response.** A precise way of determining Faraday rotation from both thin molecular films and nanoparticles in a molecular polymer matrix has been developed and allows for the Faraday rotation spectra in the visible range. In addition, MSHG contrast from superparamagnetic nanoparticles was measured.
- **Nonlinear optics of DRONPA Green Fluorescent Protein.** We have finished the experimental study of the second-order nonlinear optical properties of the DRONPA protein, a protein very similar to Green Fluorescent Protein (GFP). Theory confirms the unexpected experimental findings.
- **Photonic crystal heterostructures.** We have succeeded in using photonic bandgap engineering for fluorescence suppression in both the temporal and spectral domain, for spectral narrowing of fluorescence and for enhancing the energy transfer in light harvesting systems. We have recently found strong influence of a weak external magnetic field (90 Gauss) on the fluorescence dynamics of magnetic quantum dots (and not for closed-shell organic chromophores) in colloidal photonic crystals

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Peter Lievens

Clusters and Laser Spectroscopy

7.1. Composition of the team

Staff

Peter Lievens
Roger Silverans
Margriet Van Bael

Post-doc

Marcel Di Vece
Ewald Janssens (until 31-08-
2007)
Aurélie Lando
Nele Veldeman

Ph.D. students

Pieterjan Claes
Jorg De Haeck
Jo Cuppens
Koen Lauwaet
Christian Pablo Romero Vieyra
Maja Stanisavljev
Sabina Wyczawska

7.2. Ph.D. students

Current (Ph.D. in progress)

Sabina Wyczawska
Energetic beam impact on surfaces covered with organic overlayers: a study of
desorption phenomena with laser ionization and mass spectrometry
promoters: Peter Lievens and Roger Silverans
(September 2008)

Koen Schouteden
Tunneling microscopy and spectroscopy of metallic and ferromagnetic nanoclusters
promoters: Chris Van Haesendonck and Peter Lievens
(September 2008)

Jorg De Haeck
Study of metalloic binary clusters with high resolution mass spectrometry
promoter: Peter Lievens
(June 2009)

Nico Vanhove
Zero-energy SIMS
promoters: Wilfried Vandervorst and Peter Lievens
(June 2009)

Pieterjan Claes
Physical and chemical properties of binary clusters
promoter: Peter Lievens
(June 2011)

Jo Cuppens
Superconducting nanosystems
promoter: Margriet Van Bael
(June 2011)

Koen Lauwaet
Growth of novel nanostructures with cluster deposition
promoter: Peter Lievens
(June 2011)

Ph.D. attained

Alexey Dobrynin
Exchange coupling in hybrid magnetic nanocluster systems,
promoters: Peter Lievens and Kristiaan Temst,
8 May 2006.

Xin Wang
Mass spectrometric study of metal-doped group IV clusters
promoters: Peter Lievens and Roger Silverans
25 August 2006

Nele Veldeman
The influence of doping on the physicochemical properties of coinage metal clusters:
enhanced stabilities and modified chemical activities
promoter: Peter Lievens
24 October 2007

7.3. Main achievements

- The **influence of doping of silver clusters on their physical properties** was investigated by combining mass spectrometric determination of size and composition dependent stability with quantum chemical (density functional theory) calculations. Dopant atoms included all 3d transition metal elements. Focus was on the interplay between 2D and 3D structures, which was found to be strongly dopant dependent.
- The **reactivity of neutral Au clusters and of Y- and Al-doped Au clusters with CO** was studied in the gas phase. Hereto a new collision cell was implemented in the cluster beam setup. Strong size-dependent reactivity was found, supporting a dominant role of the electronic structure on the cluster reactivity. Upon doping with Al, little influence is observed, while Y-doping induces drastic changes in the size range where cage-like endohedral gold clusters are predicted.
- A combined theoretical and experimental study revealed the evolution with size of the **structure and electronic properties of Cu clusters doped with Sc, Co and Fe**. In particular DFT computations showed Cu₁₆Sc⁺ to be a highly symmetric Frank-Kasper tetraheder, with a closed 18-electron shell structure. The neutral cluster Cu₇Sc was found to be planar and π -aromatic.
- **A mass spectrometric study of binary Ge_nLi_m provided evidence for Ge₅ and Ge₉ units as building blocks for larger clusters.** A detailed and systematic study of Ge-Li binary clusters elucidated the building-up scheme for small binary Ge-Li species. A multiconfigurational quasidegenerate perturbation approach based on complete active space self-consistent-field wave functions and density functional theory was used. An electron localization function analysis on

some small species supports the view that the Ge-Li bond is predominantly ionic, however, with a small covalent character.

- A systematic mass spectrometry study of doped clusters of group 14 elements in combination with quantum chemical computations provided evidence for a **determining role of the formation of cage-like endohedral clusters on the size dependent cluster stability**. A general principle based on NICS predictions of aromaticity and geometrical fitting of dopant atoms was proposed.

- An **element-dependent critical size for argon physisorption at 80 K on transition-metal doped Si clusters was found**. Argon does not attach to elemental Si clusters but only to surface-located transition-metal atoms. Thus physisorption provides structural information. Specifically, the minimal cluster size for the formation of endohedral singly metal-doped Si cages has been determined. The observed critical size for doubly doped Si clusters indicates that larger caged molecules can be formed, eventually leading to the growth of metal-doped Si nanorods.

- Using laser ionization and mass spectrometry, **ion-induced desorption of neutral particles from BPN self-assembled monolayers** were investigated. The effect of purely structural changes on emission yield and fragmentation pattern was found to reflect the structural polymorphism earlier discovered with STM studies. Substantial differences in the ratio between cleavage of the molecule-substrate and the C-S bonds were observed.

- A **double hysteresis loop behavior was observed in films consisting of ferromagnetic Co clusters embedded in a thin antiferromagnetic CoO matrix**. Such magnetization behavior is related to the presence of two ferromagnetic parts with antiparallel orientations of their magnetization vectors. While the loop shifts are provided via the exchange bias mechanism, the alignment of randomly oriented magnetization vectors of Co clusters in either of two directions suggests the presence of an exchange spring effect in the system.

- Structural and morphological changes occurring in an ensemble of vapor deposited palladium nanoclusters was studied upon several hydrogenation cycles with XRD, EXAFS, RBS and STM. A cluster size increase was observed upon initial hydrogenation, conceptually similar to **Ostwald ripening**.

7.4. Publications

1. Mass spectrometric and modeling investigations of bimetallic silver-cobalt clusters, E. Janssens, Th. Van Hoof, N. Veldeman, S. Neukermans, M. Hou, P. Lievens, International Journal of Mass Spectrometry 252 (2006) 38-46.
2. Mass spectrometric stability study of binary M_n clusters (S = Si, Ge, Sn, and Pb, M = Cr, Mn, Cu, and Zn), S. Neukermans, X. Wang, N. Veldeman, E. Janssens, R.E. Silverans, P. Lievens, International Journal of Mass Spectrometry 252 (2006) 145-150.
3. Tellen, de nauwkeurigste vorm van meten
Peter Lievens
Karakter 14 (2006) 19-21
4. The geometric, electronic, and magnetic properties of Ag₅X⁺ (X=Sc, Ti, V, Cr, Mn, Fe, Co, and Ni) clusters
Ewald Janssens, Xin Juan Hou, Minh Tho Nguyen, Peter Lievens
Journal of Chemical Physics 124 (2006) 184319
5. Wetting of a self-assembled 1,4-benzenedimethanethiol monolayer on gold and silver: An adhesion force spectroscopy study,
N. Vandamme, K. Schouteden, J. Snauwaert, P. Lievens, C. Van Haesendonck,
Surface Science 600 (2006) 2894-2899.

6. Interaction of diatomic germanium with lithium atoms: Electronic structure and stability
G. Gopakumar, Peter Lievens, Minh Tho Nguyen
Journal of Chemical Physics 124 (2006) 214312
7. Atomic scale modification of hybrid FePt cluster assembled films
A.N. Dobrynin, D.N. Ievlev, G. Verschoren, J. Swerts, M.J. Van Bael, K. Temst, P. Lievens, E. Piscopiello, G. Van Tendeloo, S.Q. Zhou, A. Vantomme
Physical Review B, 73 (2006) 104421.
8. Influence of finite size effects on exchange anisotropy in oxidized Co nanocluster assembled films
A. N. Dobrynin, D. N. Ievlev, C. Hendrich, K. Temst, P. Lievens, U. Hörmann, J. Verbeeck, G. Van Tendeloo, A. Vantomme
Physical Review B, 73 (2006) 245416.
9. Isomorphous Substitution in Bimetallic Oxide Clusters
E. Janssens, G. Santambrogio, M. Brümmer, L. Wöste, P. Lievens, J. Sauer, G. Meijer, K. R. Asmis
Physical Review Letters 96 (2006) 233401.
10. To Achieve Stable Spherical Clusters: General Principles and Experimental Confirmations
Zhongfang Chen, Sven Neukermans, Xin Wang, Ewald Janssens, Zhen Zhou, Roger E. Silverans, Bruce R. King, Paul von Rague Schleyer, Peter Lievens,
Journal of the American Chemical Society 128, (2006) 12829-12834.
11. Domain-wall superconductivity in a ferromagnet/superconductor/ferromagnet trilayer,
W. Gillijns, A. Aladyshkin, M. Van Bael, M. Lange, V. Moshchalkov,
Physica C 437-38 (2006) 73-76.
12. The influence of finite size and shape anisotropy on exchange bias: A study of patterned Co/CoO nanostructures,
K. Temst, E. Popova, H. Loosvelt, M. Van Bael, S. Brems, Y. Bruynseraede, C. Van Haesendonck, H. Fritzsche, M. Gierlings, L. Leunissen, R. Jonckheere,
J. Magn. Magn. Mater. 304 (2006) 14-18.
13. Exchange bias as a function of nanosize,
A.N. Dobrynin, K. Temst, P. Lievens,
in Nanomagnet Embedded In Matrix (NEIM), ed. V. Dupuis, 2006, Transworld Research Network, Kerala, India (ISBN: 81-7895-231-9), pp. 39-64.
14. Measurement of the size of embedded metal clusters by mass spectrometry, transmission electron microscopy, and small angle X-ray scattering,
Christian Hendrich, Luc Favre, Dmitriy N. Ievlev, Alexey N. Dobrynin, Wim Bras, Ute Hörmann, Emanuela Piscopiello, Gustaaf Van Tendeloo, Peter Lievens, Kristiaan Temst,
Applied Physics A: Materials Science & Processing, 86 (2007) 533-538.
15. The Exchange Coupling in Cr₃O_n (n = 0-3) Clusters
Ewald Janssens, Xin Juan Hou, Sven Neukermans, Xin Wang, Roger E. Silverans, Peter Lievens, Minh Tho Nguyen
Journal of Physical Chemistry A 111, 4150-4157 (2007)
16. Interaction of Triatomic Germanium with Lithium Atoms: Electronic Structure and Stability of Ge₃Li_n Clusters
G. Gopakumar, Peter Lievens, Minh Tho Nguyen
Journal of Physical Chemistry A 111 (2007) 4353-4361.
17. Observation of wetting-like phase transitions in a surface-enhanced type-I superconductor ,
V. F. Kozhevnikov, M. J. Van Bael, P. K. Sahoo, K. Temst, C. Van Haesendonck, A. Vantomme, and J. O. Indekeu,
New Journal of Physics 9 (2007) 75.

18. Magic numbers for shells of electrons and shells of atoms in binary clusters, S. Neukermans, E. Janssens, R.E. Silverans, P. Lievens, in *The Chemical Physics of Solid Surfaces: Volume 12, Atomic clusters: from gas phase to deposited*, editor Ph. Woodruff (Elsevier), pp. 271-298.
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20. Silane ligand exchange to make hydrophobic superparamagnetic nanoparticles water-dispersible, R. De Palma, S. Peeters, M.J. Van Bael, H. Van den Rul, K. Bonroy, W. Laureyn, J. Mullens, G. Borghs, G. Maes, *Chem. Mater.* 19 (2007) 1821-1831.
21. Observation of Co/CoO nanoparticles below the critical size for exchange bias, A.N. Dobrynin, K. Temst, P. Lievens, J. Margueritat, J. Gonzalo, C.N. Afonso, E. Piscopiello, G. Van Tendeloo, *Journal of Applied Physics* 101 (2007) 113913.
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Nele Veldeman, Tibor Höltzl, Sven Neukermans, Tamás Veszprémi, Minh Tho Nguyen, Peter Lievens
Physical Review A – Rapid Communication, A 76 (2007) 011201
23. Argon physisorption as a structural probe for endohedral doped silicon clusters
E. Janssens, P. Gruene, G. Meijer, L. Wöste, P. Lievens, A. Fielicke,
Physical Review Letters, 99 (2007) 063401 (4 pagina's)
24. Evidence for coexistence of exchange bias and exchange spring effects in oxidized Co nanocluster assembled films,
A. Dobrynin, M. Van Bael, K. Temst, P. Lievens,
New Journal of Physics 9 (2007) 258 (8 pages).
25. Combined experimental and theoretical study of small aluminum oxygen clusters
S. Neukermans, N. Veldeman, E. Janssens, P. Lievens, Z. Chen, P.v.R. Schleyer,
European Physical Journal D, 45 (2007) 301-308.
26. Hydrogen adsorption studies in micro-size cobalt dots,
C.P. Romero, J.I. Avila, E. Cisternas, G.B. Cabrera, A.L. Cabrera, K. Temst, M.J. Van Bael,
J. Mater. Sci. 42 (2007) 7667.
27. Stability and dissociation pathways of doped AunX⁺ clusters (X = Y, Er, Nb)
Nele Veldeman, Ewald Janssens, Klavs Hansen, Jorg De Haeck, Roger E. Silverans, Peter Lievens,
Faraday Discussions 138 (2008), DOI: 10.1039/b705920e (first published on web 14 september 2007).
28. Spin and magnetic moment of ³³Mg: evidence for a negative-parity intruder ground state
D.T. Yordanov, M. Kowalska, K. Blaum, M. De Rydt, K. Flanagan, M. Kowalska, P. Lievens, R. Neugart, G. Neyens, H.H. Stroke
Physical Review Letters 99 (2007) 212501.
29. Chromium-doped germanium clusters CrGe_n (n = 1-5): geometry, electronic structure and topology of chemical bonding
Xin-Juan Hou, G. Gopakumar, Peter Lievens, Minh Tho Nguyen
Journal of Physical Chemistry A, 2007

30. Development of magnetic materials for photonic applications,
K. Baert, W. Libaers, B. Kolaric, R.A.L. Vallée, M. Van der Auweraer, D. Grandjean, M. Di Vece, P. Lievens, K. Clays,
Journal of Nonlinear Optical Physics & Materials, 2007
31. Single-electron tunneling phenomena on preformed gold clusters deposited on dithiol self-assembled monolayers
K. Schouteden, N. Vandamme, E. Janssens, P. Lievens, C. Van Haesendonck,
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32. Electron scattering in Au films containing Co clusters,
G. Verschoren, A. N. Dobrynin, K. Temst, R.E. Silverans, C. Van Haesendonck, P. Lievens, B. Pipeleers, S.Q. Zhou, A. Vantomme, W. Bras,
Thin Solid Films, 2007
33. Surface modification of γ -Fe₂O₃@SiO₂ magnetic nanoparticles for the controlled interaction with biomolecules,
R. De Palma, J. Trekker, S. Peeters, M.J. Van Bael, K. Bonroy, R. Wirix-Speetjens, G. Reekmans, W. Laureyn, G. Borghs, G. Maes,
Journal of Nanoscience and Nanotechnology, 2007.
34. Gas phase aluminum oxide clusters: structure determination by ab initio genetic algorithm and infrared photodissociation spectroscopy
M. Sierka, J. Döbler, J. Sauer, G. Santambrogio, L. Wöste, E. Janssens, G. Meijer, K.R. Asmis,
Angewandte Chemie International Edition, 46 (2007) 3372-3375.
35. Co-deposition of atomic clusters of different size and composition,
M. Di Vece, N. Young, Z. Li, Y. Chen, R. Palmer
Small vol:2 (2006) 1270-1272.
36. Pinning of size-selected Pd nanoclusters on graphite,
S. Gibilisco, M. Di Vece, S. Palomba, G. Faraci, R. E. Palmer,
Journal of Chemical Physics 125 (2006) 084704 (3 pages).
37. Modeling the pinning of Au and Ni clusters on graphite,
R. Smith, C. Nock, S. Kenny, J. Belbruno, M. Di Vece, S. Palomba, R. Palmer,
Phys. Rev. B 73 (2006) 125429 (5 pages).
38. Chemically induced morphology change in cluster-based nanostructures, A. Lando, N. Kébaïli, Ph. Cahuzac, C. Colliex, M. Couillard, A. Masson, M. Schmidt, C. Bréchnignac,
European Physical Journal D 43 (2007) 151-154.
39. Coarsening and pearling instabilities in silver nano-fractals,
A. Lando, N. Kébaïli, Ph. Cahuzac, A. Masson and C. Bréchnignac,
Physical Review Letters 97 (2006) 133402 (4 pages).
40. Three dimensional atomic-scale structure of size-selected gold nanoclusters,
Z.Y. Li, N.P. Young, M. Di Vece, S. Palomba, R.E. Palmer, A. Bleloch, B.C. Curley, R.L. Johnston, J. Jiang, J. Yuan,
Nature, accepted for publication

André Stesmans

Semiconductor Electron Spectroscopy

8.1. Composition of the team

Staff

V. V. Afanas'ev
G. Borgs (deeltijds)
A. Stesmans

Post-doc

M. Badylevich

Ph.D. students

M. Jivanescu
K. Keunen
P. Somers
S. Shamulia

8.2. Ph.D. students

Current (Ph.D. in progress)

M. Jivanescu "ESR study of point defects in semiconductor/isolator nanostructures"
(Nov 2005)
K. Keunen "Point defects in semiconductor/isolator heterostructures using ESR"
(Nov 2006)
P. Somers "ESR analysis of strain effects in semiconductor insulator structures"
(Oct 2004)
S. Shamulia "IPE study of traps in semiconductor/high- κ isolator structures"
(Sept 2004)

Ph.D. attained

Katrijn Clémer (25/10/2007)
Electron spin resonance probing of point defects in functional oxides and high- κ Structures

8.3. Main achievements

- For the first time a comparison has been made between **atomically abrupt interfaces of Si single-crystals with nm-thin layers of transition metal (Sc₂O₃) or rare-earth (Lu₂O₃, Gd₂O₃) insulating oxides in amorphous and crystalline (bixbyite) phases**. The oxide crystallization is found to result only in a variation of the oxygen-derived valence band energy while

the conduction bands derived from the unoccupied d-states of metal cations remain at the same energy.

- **The effect of crystallization on the band structure** is observed in the non-oxide insulator (AlN) deposited on Si upon transition from the amorphous to the hexagonal phase, using IPE, PC, and SE spectroscopy. The conduction band energy is found to be the same as in deposited amorphous alumina, indicating the states derived from s and p states of Al cations are insensitive to the kind of cation involved.

- Demonstration by ESR of the **absence of an SiO₂-type interlayer in the (100)Si/a-LaAlO₃ entity**. As this is maintained up to ~850 °C, revealing a thermally most stable and abrupt interface, the LaAlO₃ high- κ insulator would thus on these grounds qualify as a suitable insulator for future technological applications.

- **Mapping of paramagnetic point defects in phase separated SiO/SiO₂ superstructures composed of regular arrays of crystalline Si nanoparticles (~2 nm across) embedded in an a-SiO₂ matrix** reveals the presence of a dominant Pb-type interface trap system. Identification of the latter as a purely Pb₀/Pb₁ system suggests the nanocrystalline particles to be principally bordered by (100)-type facets. Controlled suppression of these centers has enabled to incontestably demonstrate the QC origin of photoluminescence, which can reversibly switched between QC or defect originated.

- The **intrinsic point defect density in Si/SiO₂ entities thermally grown on biaxially tensile strained Si is found to be distinctly reduced as compared to standard entities**, providing a fundamental explanation for the observed enhancement in the strained-Si channel mobility as well reduction in 1/f noise.

- **Detection of a first dopant (donor) impurity in a high- κ insulator (HfO₂) currently being introduced in the 45-nm technology node**. On the basis of revealed Hf structure, it has been identified as P2-type defect, a P substituting a Hf atom in the monoclinic HfO₂ phase, which center will inherently operate as a detrimental charge trap.

8.4. Publications

1. Characterization of electron states in high-k insulators and their interfaces using internal photo-emission spectroscopy
V. V. Afanas'ev and A. Stesmans
Intern. Workshop on Gate Stack Technology and Physics 2006, p. 67-72 (2006) (JSAP Nr. AP062204)
2. H₂/D₂ isotopic effect on negative bias temperature instabilities in SiO_x/HfSiON/TaN gate stacks
M. Houssa, M. Aoulaiche, S. De Gendt, G. Groeseneken, M. M. Heyns, and A. Stesmans
Electrochem. and Solid State Lett. 9, G10-12 (2006)
3. Probing point defects and traps in stacks of ultrathin hafnium oxides on (100)Si by electron spin resonance: interfaces and N incorporation
A. Stesmans and V. V. Afanas'ev
In Defects in high- κ Gate Dielectric Stacks, edited by E. Gusev (Springer, Dordrecht, 2006), p. 215-227 (ISBN: 1-4020-4366-X)
4. Band alignment between (100) Si and amorphous LaAlO₃, LaScO₃, and Sc₂O₃: Atomically abrupt versus interlayer-containing interfaces
V. V. Afanas'ev, A. Stesmans, L. F. Edge, D.G. Schlom, T. Heeg, and J. Schubert
Appl. Phys. Lett. 88, 032104 (3 pp) (2006)
5. Electron spin resonance probing of E'-type defects in fumed silica nanoparticles
K. Cl  mer, A. Stesmans and V. V. Afanas'ev
Mat. Sci. and Eng. C26, 766-770 (2006)

6. Electron energy band alignment at interfaces of (100)Ge with rare-earth oxide insulators
V. V. Afanas'ev, S. Shamuilia, A. Stesmans,
A. Dimoulas, Y. Panayiotatos, and A. Sotiropoulos
M. Houssa and D. P. Brunco
Appl. Phys. Lett. 88, 132111 (3pp) (2006)

7. Ruthenium gate electrodes on SiO₂ and HfO₂: sensitivity to hydrogen and oxygen ambients
L. Pantisano, T. Schram, Z. Li, J. G. Lisoni, G. Pourtois, S. De Gendt, and D. P. Brunco, A.
Akheyar, V. V. Afanas'ev, S. Shamuilia, and A. Stesmans,
Appl. Phys. Lett. 88, 243514 (3 pp) (2006)

8. Sources of optical absorption between 5.7 and 5.9 eV in silica implanted with Si or O
R. H. Magruder III, A. Stesmans, K. Clémer, R. A. Weeks, R. A. Weller,
J. Appl. Phys. 100, 033517 (8 pp) (2006)

9. Electron energy barriers at interfaces of GaAs(100) with LaAlO₃ and Gd₂O₃
V. V. Afanas'ev, and A. Stesmans,
R. Droopad, M. Passlack, L. F. Edge, and D. G. Schlom
Appl. Phys. Lett. 89, 092103 (3 pp) (2006)

10. Origins of optical absorption between 4.8 and 4.9 eV in silica implanted with Si and with O ions
R. H. Magruder III, A. Stesmans, K. Clémer, R. A. Weeks, R. A. Weller,
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11. Effective work function modulation by controlled dielectric monolayer deposition
L. Pantisano, T. Schram, B. O'Sullivan, T. Conard, S. De Gendt, G. Groeseneken, P. Zimmerman,
A. Akheyar, and M. Heyns
S. Shamuilia, V. V. Afanas'ev, and A. Stesmans,
Appl. Phys. Lett. 89, 113505 (3 pp) (2006)

12. Inherent density of point defects in thermal tensile strained (100)Si/SiO₂ entities probed by
electron spin resonance
A. Stesmans, P. Somers, V. V. Afanas'ev, C. Claeys, and E. Simoen
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L. Camel, I. Gordon, D. Van Gestel, G. Beaucarne, J. Poortmans, and A. Stesmans
J. Appl. Phys. 100, 063702 (8 pp) (2006)

14. Internal photoemission of electrons at interfaces of metals with low- κ insulators
S. Shamuilia, V. V. Afanas'ev, P. Somers, A. Stesmans, Y.-L. Li, Zs. Tökei, G. G. Groeseneken,
and K. Maex
Appl. Phys. Lett. 89, 202909 (1-3) (2006)

15. Paramagnetic intrinsic point defects in nm-sized silica particles: Interaction with SiO at elevated
temperatures
K. Clémer, A. Stesmans, and V. V. Afanas'ev
Mat. Sci. and Eng. C (2006)

16. Amorphous lanthanum lutetium oxide thin films as alternative high- κ gate dielectrics
J. M. J. Lopes, M. Roeckrath, T. Heeg, E. Rije, J. Schubert, S. Mantl, V. V. Afanas'ev, S.
Shamuilia, A. Stesmans, Y. Jia, and D. G. Schlom
Appl. Phys. Lett. 89, 222902 (1-3) (2006)

17. High performance Ge pMOS devices using a Si-compatible process flow
P. Zimmerman, G. Nicholas, B. De Jaeger, B. Kaczer, A. Stesmans, L.-A. Ragnarsson, D. P.
Brunco, F. E. Leys, M. Caymax, G. Winderickx, K. Opsomer, M. Meuris, and M. M. Heyns,
IEDM (2006)

18. Inherent point defects in thermal biaxially tensile strained-(100)Si/SiO₂ probed by electron spin resonance
A. Stesmans, P. Somers, V. V. Afanas'ev, C. Claeys, and E. Simoen
Mat. Sci. Eng. B 135, 195-198 (2006)
19. Nature and stability of the (100)Si/LaAlO₃ interface probed by paramagnetic defects
A. Stesmans, K. Clémer, and V. V. Afanas'ev
Appl. Phys. Lett. 89, 112121 (3 pp) (2006)
20. Spectroscopy of electron states at interfaces of (100)Ge with high- κ insulators
V. V. Afanas'ev and A. Stesmans
Mat Sci. Semicond. Process. 9, 764-771 (2006)
21. Impact of defects on the high-k/MG stack: The electrical characterization challenge
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Mat. Sci. Semicond. Proc. 9, 880-884 (2006)
22. Analysis of the (100)Si/LaAlO₃ structure by electron spin resonance: nature of the interface
K. Clémer, A. Stesmans, V. V. Afanas'ev, L. F. Edge, and D. G. Schlom
J. Mater. Sci: Mater. in Electron. 18, 735-741 (2007)
23. Comment on "Nitridation effects on Pb1 center structures at the SiO₂/Si(100) interfaces"
A. Stesmans and V. V. Afanas'ev
J. Appl. Phys. 101, 026106 (2p) (2007)
24. Flatband voltage shift of ruthenium gated stacks and its link with the formation of a thin ruthenium oxide layer at the ruthenium/dielectric interface
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J. Appl. Phys. 101, 034503 (3) (2007)
25. Electron spin resonance analysis of Si nanocrystals embedded in a SiO₂ matrix
M. Jivanescu, A. Stesmans, S. Godefroo, and M. Zacharias
J. Optoelectron. Adv. Mat. 9, 721-724 (2007)
26. Insights on the physical mechanism behind negative bias temperature instabilities
M. Houssa, V. V. Afanas'ev, A. Stesmans, M. Aoulaiche, G. Groeseneken, and M. M. Heyns,
Appl. Phys. Lett. 90, 043505 (2007)
27. Observation of a P-associated defect in HfO₂ nanolayers on (100)Si by electron spin resonance
K. Clémer, A. Stesmans, and V. V. Afanas'ev
Appl. Phys. Lett. 90 No. 142116 (2007)
28. Electron spin resonance observation of a P-associated defect in HfO₂ films on (100)Si
A. Stesmans, K. Clémer, and V. V. Afanas'ev
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29. Electronic structure of silicon interfaces with amorphous and epitaxial insulating oxides: Sc₂O₃, Lu₂O₃, LaLuO₃
V. V. Afanas'ev, S. Shamuilia, A. Badylevich, A. Stesmans, L. F. Edge, W. Tian, D. G. Schlom, J. M. J. Lopes, R. Roeckerath, and J. Schubert
Microelectron. Eng. 84, 2278-2281 (2007)
30. Forming gas anneal induced flat-band voltage shift of metal-oxide-semiconductor stacks and its link with hydrogen incorporation in metal gates
Z. Li, T. Schram, L. Pantisano, T. Witters, A. Stesmans, A. Akheyar, V. V. Afanas'ev, N. Yamada, T. Takaaki, S. De Gendt, and K. De Meyer
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31. Investigation of the electronic structure at interfaces of crystalline and amorphous Gd₂O₃ thin layers with silicon substrates of different orientations
M. Badylevich, S. Shamuilia, V. V. Afanas'ev, A. Stesmans, et al.
Appl. Phys. Lett. 90, No. 252101 (2007)
32. Paramagnetic point defects in (100)Si/LaAlO₃ structures: Nature and stability of the interface
K. Clémer, A. Stesmans, and V. V. Afanas'ev
L. F. Edge, and D. G. Schlom
J. Appl. Phys. 102, 034516 (8) (2007)
33. Paramagnetic intrinsic point defects in nm-sized silica particles: Interaction with SiO at elevated temperatures
K. Clémer, A. Stesmans and V.V. Afanas'ev
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34. Internal photoemission at interfaces of high-kappa insulators with semiconductors and metals
V. V. Afanas'ev and A. Stesmans
J. Appl. Phys. 102, #081301 (p. 1-28)(2007)
35. Mechanism of O₂-anneal induced V_{fb} shifts of Ru gated stacks
Z. Li, T. Schram, L. Pantisano, A. Stesmans, T. Conard, S. Shamuilia, V. V. Afanasiev, A. Akheyar, S. Van Elschocht, D. P. Brunco, W. Deweerdt, Y. Naoki, P. Lehnen, S. De Gendt, and K. De Meyer,
Microelectron. Reliab. 47, 518-20 (2007)
36. Probing defects at interfaces and interlayers of low-dimensional Si/insulator (HfO₂; LaAlO₃) structures by electron spin resonance
A. Stesmans and V. V. Afanas'ev
Physica B 401-402, 550-5 (2007)

Jos Vanderleyden

Centre for Microbial and Plant Genetics

9.1. Composition of the team

Staff

Vanderleyden Jozef
Michiels Jan
De Mot René

Post-doc

Braeken Kristien
De Keersmaecker Sigrid
Moreels David

Ph.D. students

Spaepen Stijn
Li Wen
Hermans Kim
Janssens Joost
Kint Gwendoline
Lebeer Sarah
Sonck Kathleen
Steenackers Hans
Zhou Kai
Thijs Inge
Debkumari Bachaspatimayum
De Groote Valerie
Fauvart Maarten
Torres Gutierrez Roldan
Vercruysse Maarten
Verstraeten Nathalie
Vos Karen
Claes Ingmar
Demuyne Anneleen

9.2. Ph.D. students

Current (Ph.D. in progress)

Thijs, I., started 2003. Analysis of DNA-protein complexes in *Salmonella typhimurium* using immunoprecipitation and microarrays of intergenic DNA. Co-promoter with Kathleen Marchal.

Fadda, A., started 2004. Assessing different tools for the discovery of cis-regulatory elements in prokaryotes. Co-promoter with Kathleen Marchal.

Lebeer, S., started 2004. Molecular mechanisms of bacterial interactions in the gastrointestinal tract: chronic inflammatory bowel disease as a case study. Co-promoter with Sigrid De Keersmaecker.

Spaepen, S., started 2004. Genetic and biochemical analysis of the synthesis of secondary metabolites, indole-3-acetic acid and phenyl acetic acid in *Azospirillum brasilense*.

Sonck, K., started 2004. Genome wide proteomics analysis of quorum sensing signal in *Salmonella typhimurium*. Co-promoter with Sigrid De Keersmaecker.

Janssens, J., started 2005. Synthesis and biological screening of halogenated furanones and analogs aiming to interfere with bacterial cell-cell communication. Co-promoter with Dirk De Vos.

Torres-Gutierrez, R., started 2005. Analysis of the stimulatory effect of Plant Growth Promoting Rhizobacteria (PGPR) on the Rhizobium-bean symbiosis under containment and field conditions. Co-promoter with Jan Michiels.

Demuyne, A., started 2006. Catalysis with natural and modified cell wall compounds. Co-promoter with Sigrid De Keersmaecker and Bert Sels

Kint, G., started 2006. Protein tyrosine phosphorylation in *Salmonella enterica* serovar Typhimurium. Co-promoter with Sigrid De Keersmaecker.

Hermans, K., started 2006. Regulation of *Salmonella typhimurium* gene expression by small, non-coding RNAs. Co-promoter with Sigrid De Keersmaecker.

Steenackers, H., started 2006. Synthesis and biological screening of halogenated furanones and AI-2-derivatives for interference with bacterial cell-cell communication and virulence. Co-promoter with Dirk De Vos and Sigrid De Keersmaecker.

Claes, I., started 2007. Immunomodulation by *Lactobacillus rhamnosus* GG: study of extracellular polysaccharides and proteins. Co-promoter with Sigrid De Keersmaecker

Zhou, K., started 2007. The *Lactobacillus rhamnosus* GG Embp adhesion as a gateway for new formulations in the probiotic market. Co-promoter with Sigrid De Keersmaecker.

Ph.D. attained

Braeken, K., 2006. Molecular analysis of the RelA/SpoT-mediated response and of quorum sensing-regulated genes in the symbiotic bacterium *Rhizobium etli* CNPAF512. Promoters: Jos Vanderleyden and Jan Michiels

Rediers, H., 2006. Study of the interaction of the plant growth-promoting bacterium *Pseudomonas stutzeri* A15 with its plant host using in vivo expression technology (IVET). Promoters: René De Mot and Jos Vanderleyden

Benhassine-Hamadouche, T., 2007. Régulation de l'expression du gene *nifA* chez *Rhizobium etli*. Implication de protéines "histone-like". Soutenance à l'Université des Sciences et de Technologie Houari Boumediene, Juillet 1, 2007, Algiers; Co-directeur : Jos Vanderleyden.

Ndayizeye, M., 2007. Functional analysis of the *Rhizobium etli* CNPAF512 oligopeptide permease genes and linked D-2-hydroxyacid dehydrogenase gene in free-living growth and during symbiosis with *Phaseolus vulgaris*. Promoters: Jan Michiels and Jos Vanderleyden.

Perea Vélez, M., 2007. Functional analysis of probiotic characteristics of *Lactobacillus rhamnosus* GG. Promoter: Jos Vanderleyden

Remans, R., 2007. Searching for nitrogen under phosphorus deficiency: the interplay between common bean (*Phaseolus vulgaris* L.), *Rhizobium* and plant growth-promoting rhizobacteria. Promoters: Jos Vanderleyden and Jan Michiels

9.3. Main achievements

- The **ipdC gene product**, a key enzyme in the production of auxins by *Azospirillum brasilense*, was **characterized via a biochemical analysis**. Therefore, the recombinant enzyme was expressed and purified via heterologous overexpression in *Escherichia coli* and subsequent affinity chromatography. The molecular mass of the holoenzyme was determined by size-exclusion chromatography, suggesting a tetrameric structure, which is typical for 2-keto acid decarboxylases. The enzyme shows the highest *k_{cat}* value for phenylpyruvate. Comparing values for the specificity constant *k_{cat}/K_m*, indole-3-pyruvate is converted 10-fold less efficiently, while no activity could be detected with benzoylformate. The enzyme shows pronounced substrate activation with indole-3-pyruvate and some other aromatic substrates, while for phenylpyruvate it appears to obey classical Michaelis-Menten kinetics. Based on these data, a reclassification of the ipdC gene product of *A. brasilense* as a phenylpyruvate decarboxylase (EC 4.1.1.43) was proposed.
- Phenylpyruvate decarboxylase (PPDC) of *Azospirillum brasilense* is a thiamine diphosphate-dependent enzyme that catalyses the nonoxidative decarboxylation of indole- and phenylpyruvate. Analogous to yeast pyruvate decarboxylases, PPDC is subject to allosteric substrate activation, showing sigmoidal *v* versus *[S]* plots. The crystal structure of this enzyme was determined at 1.5 Å resolution. The subunit architecture of PPDC is characteristic for other members of the pyruvate oxidase family, with each subunit consisting of three domains with an open *a/b* topology. An active site loop, bearing the catalytic residues His112 and His113, could not be modelled due to flexibility. The biological tetramer is best described as an asymmetric dimer of dimers. A cysteine residue that has been suggested as the site for regulatory substrate binding in yeast pyruvate decarboxylase is not conserved, requiring a different mechanism for allosteric substrate activation in PPDC. Only minor changes occur in the interactions with the cofactors, thiamine diphosphate and Mg²⁺, compared to pyruvate decarboxylase. A greater diversity is observed in the substrate binding pocket accounting for the difference in substrate specificity. Moreover, a **catalytically important glutamate residue conserved in nearly all decarboxylases is replaced by a leucine in PPDC**.
- Thiamine diphosphate-dependent enzymes are involved in a wide variety of metabolic pathways. The molecular mechanism behind active site communication and substrate activation, observed in some of these enzymes, has since long been an area of debate. We reported the **crystal structures of a phenylpyruvate decarboxylase in complex with its substrates and a covalent reaction intermediate analogue**. These structures reveal the regulatory site and unveil the mechanism of allosteric substrate activation. This signal transduction relies on quaternary structure reorganizations, domain rotations and a pathway of local conformational changes that are relayed from the regulatory site to the active site. The current findings thus uncover the molecular mechanism by which the binding of a substrate in the regulatory site is linked to the mounting of the catalytic machinery in the active site in this ThDP-dependent enzyme.
- Under certain environmental and soil conditions, the bacterium *Azospirillum brasilense* can promote plant growth, crop yields and N-content of plants. It has been demonstrated that the observed increases in plant growth can probably be explained in large part by the enhanced root proliferation, which in its turn is related to bacterial indole-3 acetic acid (IAA) biosynthesis. Evidence has been accumulating that some microorganisms, make use of indole as a signalling molecule, steering microbial behaviour, such as biofilm formation. The findings on indole signalling and the similarity with IAA signalling in *Azospirillum* pose questions regarding targets of this signalling. As yet, no receptor nor a membrane transport system for IAA have been described in *A. brasilense*. This project therefore proposes the **isolation and characterization of IAA binding proteins in *A. brasilense* following the 3 objective strategy**. (1) The first objective is to verify whether *A.*

brasilensis can produce biofilms on abiotic (polystyrene) surfaces, and we will address this point by developing and optimizing a reproducible *A. brasiliensis* associated biofilm model, defining environmental factors crucial to the biofilm formation process. (2) The second objective of the project is to determine differences between gene or expressed protein profiles of *A. brasiliensis* biofilms (wild type or mutant) compared to planktonic cells using DNA-microarray analyses or 2D proteome analyses respectively. (3) In a later stage, extraction and purification of IAA-binding proteins from well-established and characterized single species biofilms of *A. brasiliensis* will be performed using biochemical methods such as affinity chromatography.

- ChIP-chip technology, which is Chromatin Immuno Precipitation combined with microarrays, allowed us to directly **visualize the interaction of regulatory proteins with their DNA targets relevant under in vivo conditions**. In this way, we were able to extend the HilA virulence regulon in *Salmonella Typhimurium*.

- Atomic Force Microscopy is being used to study **the surfaces of lactic acid bacteria**. At this stage we have completed the structural analysis of the cell surface. Presently, functionalized AFM tips are being used to unravel the properties, e.g. lectin binding capacity, of the polysaccharides at the surface of the cell.

9.4. Publications

1. Braeken, K., Moris, M., Daniels, R., Vanderleyden, J., and Michiels, J. (2006)
New horizons for (p)ppGpp in bacterial and plant physiology.
Trends in Microbiology 14 (1), 45-54.
2. Daniels, R., Reynaert, S., Hoekstra, H., Verreth, C., Janssens, J., Braeken, K., Fauvart, M., Beullens, S., Heusdens, C., Lambrichts, I., De Vos, D., Vanderleyden, J., Vermant, J., and Michiels, J. (2006)
Quorum signal molecules as biosurfactants affecting swarming in *Rhizobium etli*.
Proceedings of the National Academy of Sciences of the United States of America 103 (40), 14965-14970.
3. De Keersmaecker, S.C.J., Braeken, K., Verhoeven, T.L.A., Perea Vélez, M., Lebeer, S., Vanderleyden, J., and Hols, P. (2006)
Flow cytometric testing of green fluorescent protein-tagged *Lactobacillus rhamnosus* GG for response to defensins.
Appl. Environ. Microbiol. 72 (7), 4923-4930.
4. De Keersmaecker, S.C.J., Thijs, I.M.V., Vanderleyden, J., and Marchal, K. (2006)
Integration of omics data: how well does it work for bacteria?
Mol. Microbiol. 62 (5), 1239-1250.
5. De Keersmaecker, S.C., Sonck, K., and Vanderleyden, J. (2006)
Let LuxS speak up in AI-2 signaling.
Trends in Microbiology 14 (3), 114-119.
6. De Keersmaecker, S.C.J., Verhoeven, T.L.A., Desair, J., Marchal, K., Vanderleyden, J., and Nagy, I. (2006)
Strong antimicrobial activity of *Lactobacillus rhamnosus* GG against *Salmonella typhimurium* is due to accumulation of lactic acid.
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Auxin signaling in plant defense.
Science Letter, 313 (5784) 171.
8. Benhassine, T., Fauvart, M., Vanderleyden, J., and Michiels, J. (2007)
Interaction of an IHF-like protein with the *Rhizobium etli* nifA promoter.
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9. Braeken,K., Daniels,R., Vos,K., Fauvart,M., Bachaspatimayum,D., Vanderleyden,J., and Michiels,J. (2007)
Genetic determinants of swarming in *Rhizobium etli*. *Microb.Ecol.*
Epub ahead of publication.
10. Cappuyns,A.M., Bernaerts,K., Smet,I.Y., Ona,O., Vanderleyden,J., Prinsen,E., and Van Impe,J.F. (2007)
Optimal fed batch experiment design for estimation of monod kinetics of *Azospirillum brasilense*: from theory to practice.
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11. De Mot,R. (2007)
Actinomycete-like proteasomes in a Gram-negative bacterium.
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12. De Mot,R., Schoofs,G., and Nagy,I. (2007)
Proteome analysis of *Streptomyces coelicolor* mutants affected in the proteasome system reveals changes in stress-responsive proteins.
Arch.Microbiol. 188 257-271.
13. Fauvart,M., Braeken,K., Daniels,R., Vos,K., Ndayizeye,M., Noben,J.-P., Robben,J., Vanderleyden,J., and Michiels,J. (2007)
Identification of a novel glyoxylate reductase supports phylogeny-based enzymatic substrate specificity prediction.
Biochim.Biophys.Acta 1774 (9), 1092-1098.
14. Janssens,J., Metzger,K., Daniels,R., Ptacek,D., Verhoeven,T., Habel,L.W., Vanderleyden,J., De Vos,D., and De Keersmaecker,S. (2007)
Synthesis of N-acyl homoserine lactone analogues reveals strong activators of SdiA, the *Salmonella enterica* serovar Typhimurium LuxR homologue.
Appl Environ Microbiol 73 (2), 535-544.
15. Janssens,J.C., Steenackers,H., Metzger,K., Daniels,R., Ptacek,D., Verhoeven,T., Hermans,K., Vanderleyden,J., De Vos,D.E., and De Keersmaecker,S.C. (2007)
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Communications in Agricultural and Applied Biological Sciences 72 (1), 41-45.
17. Lebeer,S., Verhoeven,T.L.A., Perea Vélez,M., Vanderleyden,J., and De Keersmaecker,S.C.J. (2007)
Impact of environmental and genetic factors on biofilm formation by the probiotic strain *Lactobacillus rhamnosus* GG.
Appl Environ Microbiol 73 (21), 6768-6775.
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Functional analysis of *luxS* in the probiotic strain *Lactobacillus rhamnosus* GG reveals a central metabolic role important for growth and biofilm formation.
J.Bacteriol. 189 (3), 860-871..
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Identification of salt stress inducible genes that control cell envelope related functions in *Azospirillum brasilense* Sp7.
Mol.Genet.Genomics 278 (1), 43-51.

20. Ormeño-Orrillo, E., Luyten, E., Vanderleyden, J., and Martinez-Romero, E. (2007) Three loci involved in lipopolysaccharide biosynthesis in *Rhizobium tropici* CIAT899. *Environ. Microbiol.* In press.
21. Pedreschi, R., Vanstreels, E., Carpentier, S., Hertog, M., Lammertyn, J., Robben, J., Noben, J.-P., Swennen, R., Vanderleyden, J., and Nicolai, B.M. (2007) Proteomic analysis of core breakdown disorder in Conference pears (*Pyrus communis* L.). *Proteomics* 7 2083-2099.
22. Perea Vélez, M., Verhoeven, T.L.A., Draing, C., Von Aulock, S., Pfitzenmaier, M., Geyer, A., Lambrichts, I., Pot, B., Vanderleyden, J., and De Keersmaecker, S.C.J. (2007) Functional analysis of D-alanylation of lipoteichoic acid in the probiotic strain *Lactobacillus rhamnosus* GG. *Appl Environ Microbiol* 73 (11), 3595-3604.
23. Perea Vélez, M., Hermans, K., Verhoeven, T.L.A., Lebeer, S.E., Vanderleyden, J., and De Keersmaecker, S.C.J. (2007) Identification and characterization of starter lactic acid bacteria and probiotics from Columbian dairy products. *J. Appl. Microbiol.* 103 666-674.
24. Rediers, H., Vanderleyden, J., and De Mot, R. (2007) Nitrate respiration in *Pseudomonas stutzeri* A15 and its involvement in rice and wheat root colonization. *Microbiol. Res.* Epub ahead of print.
25. Remans, R., Snoeck, C., Verreth, C., Croonenborghs, A., Luyten, E., Ndayizeye, M., Martinez-Romero, E., Michiels, J., and Vanderleyden, J. (2007) Inactivation of the nodH gene in *Sinorhizobium* sp. BR816 enhances symbiosis with *Phaseolus vulgaris* L. *FEMS Microbiol. Lett.* 266, 210-217.
26. Remans, R., Croonenborghs, A., Torres Gutierrez, R., Michiels, J., and Vanderleyden, J. (2007) Effects of plant growth-promoting rhizobacteria on nodulation of *Phaseolus vulgaris* L. are dependent on plant P nutrition. *Eur. J. Plant Pathol.* 119 341-351.
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28. Spaepen, S., Versées, W., Gocke, D., Pohl, M., Steyaert, J., and Vanderleyden, J. (2007) Characterization of phenylpyruvate decarboxylase, involved in auxin production of *Azospirillum brasilense*. *J. Bacteriol.* 189 (21), 7626-7633.
29. Spaepen, S., Vanderleyden, J., and Remans, R. (2007) Indole-3-acetic acid in microbial and microorganism-plant signaling. *FEMS Microbiol. Rev.* 31 425-448.
30. Thijs, I.M.V., De Keersmaecker, S.C.J., Fadda, A., Engelen, K., Zhao, H., McClelland, M., Marchal, K., and Vanderleyden, J. (2007) Delineation of the *Salmonella enterica* serovar typhimurium HilA regulon through genome-wide location and transcript analysis. *J. Bacteriol.* 189 (13), 4587-4596.
31. Triplett, E., Rolfe, B.G., Cocking, E.C., Kennedy, I., and Vanderleyden, J. (2007) A nitrogen story. *Microbe* 2 (8), 372-373.

32. Versées,W., Spaepen,S., Vanderleyden,J., and Steyaert,J. (2007)
The crystal structure of phenylpyruvate decarboxylase from *Azospirillum brasilense* at 1.5 Å resolution. Implications for its catalytic and regulatory mechanism.
FEBS J. 274 (91), 2363-2375.
33. Versées,W., Spaepen,S., Wood,M.D., Leeper,F.J., Vanderleyden,J., and Steyaert,J. (2007)
Molecular mechanism of allosteric substrate activation in a thiamine diphosphate-dependent decarboxylase.
J.Biol.Chem. 282(48), 35269-78.
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FEMS Microbiol.Lett. 276 (2), 140-148.