Organizers

Lutz Geelhaar (Paul-Drude-Institut für Festkörperlektronik)
Brian A. Korgel (The University of Texas at Austin)
Maurizia Palumbo (Università di Roma “Tor Vergata”)
Riccardo Ruralli (Institut de Ciència de Materials de Barcelona, CSIC)
PROGRAM

Wednesday, September 19

09:00 Registration

09:30 Opening

Photovoltaics

09:45 Silvija Gradecak (MIT, Boston)
Nanowire-based hybrid organic/inorganic bulk heterojunction solar cells

10:15 Silke Christiansen (MPI for the Science of Light, Erlangen)
Nanowire device concepts for thin film photovoltaics

10:45 Chennupati Jagadish (Australian National University, Canberra)
III-V Compound Semiconductor Nanowires for Optoelectronic Devices

11:15 Coffee Break

Optoelectronics and optical properties

11:45 Hanwei Gao (UC Berkeley)
Cleaved-Coupled Nanowire Lasers

12:15 Matthew McDonald (University of Notre Dame)
Direct measurement of single CdSe nanowire absorption polarization anisotropies

12:30 Alf Mews (University of Hamburg)
Optical and electrical properties of individual CdSe nanowires

12:45 Junichi Motohisa (Hokkaido University)
Selective-area growth and optical properties of InP-based nanowires

13:15 Individual Lunch
**Majorana fermions**

14:45  **Vincent Mourik** (Delft University of Technology)
*Signatures of Majorana fermions in InSb nanowires with proximity induced superconductivity*

15:15  **Sébastien Plissard** (Eindhoven University of Technology)
*InSb nanowire structures for Majorana fermion manipulations*

15:30  **Hadas Shtrikman** (Weizmann Institute of Science)
*InAs nanowires – from growth aspects through splitting of cooper pairs to the search for Majorana fermions*

15:45  *Poster Session A & Coffee Break*

**Large-scale assembly**

17:15  **Zhiyong Fan** (Hong Kong University of Science and Technology)
*2-D and 3-D Integration of Nanowires for Electronics*

17:45  **Paola Prete** (Istituto per la Microelettronica e Microsistemi, CNR, Lecce)
*Au-catalyzed MOVPE of GaAs-based nanowires for photonic and photovoltaic applications: materials assessment and process scale-up*
Thursday, September 20

**Growth I**

09:00  **Vincent Consonni** (CNRS Grenoble)
*Nucleation and growth mechanisms of self-induced GaN nanowires grown by molecular beam epitaxy*

09:30  **Frank Glas** (CNRS - Laboratoire de Photonique et de Nanostructures, Marcoussis)
*Stress-driven quantum dot formation on top of nanowires*

09:45  **Martin Wölz** (PDI Berlin)
*Strain-engineering of nanowire multi-quantum wells demonstrated by phonon frequency shift*

10:00  **Jonas Johansson** (Lund University)
*Polytypism and heterostructure formation in III-V nanowires*

10:30  *Coffee Break*

**Doping I**

11:00  **Yossi Rosenwaks** (Tel-Aviv University)
*Dopant distribution in in-situ and ex-situ doped nanowires*

11:30  **Michele Amato** (École Polytechnique and Université Paris Sud)
*Engineering light absorption by switching co-doping in SiGe core-shell nanowires*

11:45  **Ádám Gali** (Hungarian Academy of Sciences)
*Ab Initio Study of Phosphorus Donors Acting as Quantum Bits in Silicon Nanowires*

12:00  **Naoki Fukata** (National Institute for Materials Science, Tsukuba)
*Recrystallization and Reactivation of Dopant Atoms in Ion- Implanted Silicon Nanowires*

12:30  *individual Lunch*
Optoelectronics and optical properties II

14:00  Moon-Ho Jo (Yonsei University)
Integrated Nano Optoelectronics

14:30  Michael Filler (Georgia Institute of Technology)
Tunable Localized Surface Plasmon Resonances in Silicon

14:45  Jonas Lähnemann (PDI Berlin)
Luminescence of GaAs nanowires consisting of wurtzite and zincblende segments

15:00  Gregor Koblmüller (Walter-Schottky-Institut, Munich)
Growth and Optical properties of (In,Ga)As Nanowire arrays on Silicon

15:30  Poster Session B & Coffee Break

Electron-based devices and properties

17:00  Walter Weber (Namlab Dresden)
Reconfigurable Nanowire Electronics

17:30  Jim Greer (Tyndall National Institute, Cork)
Bandgap engineering of a semi-metal to form a nanowire transistor

17:45  Alistair Rowe (Ecole Polytechnique, CNRS, Palaiseau)
Giant piezoresistance in silicon nanowires

18:00  Ricardo García (Instituto de Microelectrónica de Madrid)
Detection of the Early Stage of Recombinational DNA Repair by Silicon Nanowire Transistors

18:15  Brian Korgel (University of Texas at Austin)
Silicon and Germanium Nanowires for Next Generation High Capacity Lithium Ion Batteries
Friday, September 21

Growth II

09:00 Emmanuel Tutuc (University of Texas at Austin)
Band engineered, epitaxial Ge$_x$Ge$_{1-x}$ core-shell nanowires: growth, electron transport, and device applications

09:30 Simas Rackauskas (Aalto University)
In situ TEM observation of nanowire growth

09:45 Monica Cotta (UNICAMP)
Periodical diameter oscillations and mechanical stability of the nanoparticle during InP nanowire growth

10:00 Pere Roca i Cabarrocas (École Polytechnique, Palaiseau)
Plasma Assisted Silicon Nanowire Growth: a versatile process for Vertical and Horizontal Wires based on Low Melting Temperature Metal Catalysts

10:30 Coffee Break

Theory and Doping II

11:00 Alex Zunger (University of Colorado)
Electronic structure of Semiconductor Quantum wires: Energy levels spin splitting, and the core-multi shell design problem

11:30 Marta Galicka (Institute of Physics PAS, Warsaw)
First-Principles Study of Doped III-V nanowires

11:45 Emmanouil Dimakis (PDI Berlin)
Shell-doping of GaAs nanowires with Si for n-type conductivity

12:00 Xavier Cartoixà (Universitat Autònoma de Barcelona)
Molecular attachment and alkyl passivation in Silicon Nanowires

12:30 Closing
POSTER PRESENTATIONS

Session A

A01 Anttu (Lund Univ)
Absorption of light in InP nanowire arrays

A02 Dalmau (EPFL)
Characterization of the radial p-n junction on Si micropillar-array solar cells

A03 Schmitt (MPI light)
Nanowire arrays in multi-crystalline silicon thin films on glass: a highly flexible absorber material for third generation photovoltaics

A04 Kaynan (Hebrew U Jerusalem)
Hybrid Nanometric Structures with High Photocatalytic Activity obtained by Molecular Layer Deposition and Nanowire Scaffolds

A05 Musolino (PDI Berlin)
Towards light-emitting diodes based on the selective-area growth of III-N nanowires on Si substrates

A06 Zettler (PDI Berlin)
Toward inorganic/organic GaN-based nanowire light-emitting diodes based on Förster resonant energy transfer

A07 Vietmeyer (U Notre Dame)
Electric field-induced emission enhancement and modulation in CdSe nanowires

A08 Ryu (IMM Madrid)
Silicon nanowire transistors fabricated by AFM oxidation and Electron beam nanolithographies: Output and transfer characteristics

A09 Schoeters (Antwerp Univ)
Stability of Si epoxide defects in Silicon Nanowires

A10 Givan (Northwestern Univ)
Growth Environment and Incorporation Mechanism Impact on Dopant Distribution and Activity of VLS Grown Nanowires

A11 Casadei (EPFL)
Doping incorporation and acceptor deactivation in Be-doped GaAs nanowires

A12 Cirlin (Ioffe Inst)
Self-catalysed MBE grown GaAs nanowires with predictable Γ-shape

A13 Ermez (MIT)
Nucleation of self-assisted GaAs nanowires grown by MOCVD: Effect of Group-III precursor pre-deposition and substrate orientation
A14 Hestroffer (CEA Grenoble)  
In situ study of self-assembled GaN nanowire nucleation on silicon

A15 Fernández-Garrido (PDI Berlin)  
Role of crystal polarity and substrate defects in the spontaneous formation of GaN nanowires

A16 Yang (Freiburg Univ)  
ZnO Nanowires Derived from Seeded Solution Growth Based on the Dissolution-Reprecipitation Mechanism

A17 Dhanabalan (Parma)  
Optimization of the growth parameters for SiC/SiO2 core-shell NWs

A18 Liu (FHI Berlin)  
The effect of van der Waals forces on the structure and energy of nanowires on solid substrates

Session B

B01 Kusch (FU Berlin)  
A Resonant Raman study on wurtzite GaAs nanowires

B02 Hauswald (PDI Berlin)  
Recombination dynamics of free and bound excitons in GaN nanowires with different diameters grown by selective-area epitaxy on Si substrates

B03 Nasibulin (Aalto Univ)  
Gas phase synthesis of ZnO tetrapods for flexible and transparent UV sensor application

B04 Kamimura (PDI Berlin)  
(In,Ga)N nanowires for photoelectrochemical water splitting

B05 Wallentin (Lund Univ)  
Single GaInP nanowire p-i-n junctions

B06 Ruiz (FHI Berlin)  
Density-Functional Theory with Screened van der Waals Interactions for the Modeling of Hybrid Inorganic/Organic Systems

B07 Dhanabalan (Parma)  
Ternary InZnO nanowires by liquid metal seeded growth of ZnO nanostructures

B08 Schmidtbauer (IKZ Berlin)  
In-plane germanium nanowires grown by MBE on germanium substrates

B09 Kang (Yonsei Univ)  
Unconventional Roles of Metal Catalysts in Chemical-Vapor Syntheses of Nanowires
B10 Somaschini (PDI Berlin)
Au-assisted growth of Al$_x$Ga$_{1-x}$As nanowires on Si(111) by molecular beam epitaxy

B11 Hilse (PDI Berlin)
Growth of GaAs-Fe$_3$ Si core-shell nanowires with an out-of-plane magnetization by molecular beam epitaxy

B12 Hsiao (Linköping U)
Magnetron Sputter Epitaxy of Core-Shell AlInN Nanorods and Nanohelixes

B13 Kesaria (Bangalor)
GaN Nanostructures

B14 Novikov (Nottingham Univ)
Coalescence of In$_x$Ga$_{1-x}$N nanorods in molecular beam epitaxy

B15 Latzel (MPI light)
Fabrication of GaN-based nanorods using nanosphere lithography and RIE for nanodevice applications

B16 Fanetti (Trieste)
Contactless monitoring of doping with spatial resolution along single GaAs nanowires

B17 Amit (Tel Aviv University)
Dopant distribution measurements of ex situ doped silicon nanowires
ORAL PRESENTATIONS

Nanowire-based hybrid organic/inorganic bulk heterojunction solar cells

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Despite the fact that solar radiation accounts for most of the available renewable energy, only a small portion of it is currently being harnessed, mostly due to the production and installation costs of commercial photovoltaic (PV) devices. Emerging PV devices based on solution-processable conjugated polymers offer opportunities for the production of low-cost solar cells. To obtain high efficiencies of exciton dissociation and high photocurrent, it is desirable to have an interpenetrating network of electron-donor and electron-acceptor components within the device, referred to as a bulk heterojunction (BHJ). However, current limitations of the all-organic PV devices are inefficient hopping charge transport through the discontinuous percolation pathways in the BHJ films, and therefore modest power conversion efficiencies or non-competitive cost in the case of devices based on C60 derivatives.

We have developed an alternative type of nanowire-based solar cells that are based on organic/inorganic hybrid device structures and demonstrated two distinct hybrid BHJ architectures with enhanced power conversion efficiencies. The first device structure was composed of GaAs nanowires blended with a conjugated polymer poly(3-hexylthiophene) (P3HT) to form a uniform film consisting of dispersed nanowires in a polymer matrix. We observed that above a certain nanowire loading threshold, the nanowires facilitate P3HT molecular ordering, which leads to improved charge transport and yields devices with >2.3% power conversion efficiency. In the second device structure, CdS quantum dots were bound onto crystalline P3HT nanowires through solvent-assisted grafting and ligand exchange, leading to controlled organic-inorganic phase separation and an improved maximum power conversion efficiency of 4.1%.

In both cases, our results clearly demonstrate some of the benefits of organic-inorganic BHJ devices, mostly through enhanced absorption and improved carrier transport in the active region of the
device. We have also identified several critical parameters to further boost the device efficiency and enable scalable, cost-efficient production, and these will be discussed.

**Nanowire device concepts for thin film photovoltaics**

Silke Christiansen\(^1,2\), S. Schmitt\(^1\), B. Hoffmann\(^1\), G. Brönstrup\(^1\), M. Pietsch\(^1\), G. Sarau\(^1\), F. Schechtli\(^1\), M. Kiometzis\(^1\), D. Amkreutz\(^3\), B. Rech\(^3\)

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\(^2\) Institut of Photonic Technology, Jena, Germany
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The controlled synthesis of one-dimensional (1D) nanostructures, e.g. silicon nanowires (SiNWs) has opened up new areas for device applications in electronics, optoelectronics, thermoelectrics, photocatalysis, photovoltaics and sensing. For all device concepts based on SiNWs, the crystal structure, geometry (alignment of SiNW e.g. with respect to the substrate, pitch, shape etc.), interfacial properties between the SiNW and the substrate as well as the Si core and a potential oxide shell of the SiNWs, dopant concentrations and impurity levels are of key importance for best output characteristics of the devices.

Large areas of aligned SiNW arrays are fabricated on Si wafers and glass substrates via a metal-catalyzed wet chemical etching (WCE) or a dry, reactive ion etching (RIE) process with or without the use of densely packed diameter-reduced polystyrene (PS) spheres as a mask. The diameter, length, packing density, and even the shape of SiNWs can precisely be controlled and tuned by adjusting either plasma etching duration or chemical etching conditions and the nominal diameters of the PS spheres. The antireflective properties of SiNWs and thus the extremely high absorption in thin SiNW layers are essential for NW based next generation solar cells. Several cell concepts with SiNWs are realized including most interesting ones:

(i) a hybrid organic/inorganic solar cell using SiNWs as absorbers and conducting or semiconducting polymers for current extraction in different cell concepts.

(ii) a semiconductor-insulator-semiconductor (SIS) cell concept with SiNWs as absorbers and a tunneling barrier for charge carrier separation. The thin tunneling oxide, e.g. $\text{Al}_2\text{O}_3$ with a thickness of only a few Å and a transparent conductive oxide (TCO – here: $\text{Al}:\text{ZnO}$) are both grown
conformally around the SiNWs using atomic layer deposition (ALD).

The first solar cell prototypes of 1cm$^2$ area on glass substrates reached (i) open-circuit voltage of 620 mV, a short-circuit current density of 22 mA/cm$^2$ and efficiencies of >5% and (ii) an open-circuit voltage of 550 mV, a short-circuit current density of 33 mA/cm$^2$ and efficiencies of >9%.

The influence of the thickness, chemical nature of the tunneling oxide and back and front contact’s structure in the SIS cell will be discussed in detail.

Advanced analytical techniques will be applied to materials and device improvements: (i) the proper charge carrier separation is studied by electron beam induced current (EBIC); (ii) Glow discharge optical emission spectrometry (GDOES) permits to determine the free surface area of the SiNWs that strongly influences the open circuit voltage. All elements from hydrogen to uranium can easily be detected simultaneously, and GDOES offers limits-of-detection down to the ppm range.

Further optimization of the cells are realized (i) by using alternatives to TCOs to form electrodes such as graphene or silver nanowire webs. Preliminary electrical measurements will be shown. (ii) by modelling using numerical simulations and realization of enhanced absorption at reduced SiNW surface areas.

We see a real potential of the SIS SiNW based thin film cell for further improvement of cell parameters such as $V_{oc}$ to 600-700 mV and a power conversation efficiency of >15%.

### III-V Compound Semiconductor Nanowires for Optoelectronic Devices

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Abstract: We review various III-V compound semiconductor nanowires grown by metalorganic chemical vapor deposition, mainly focusing on phase control of InP nanowires, optical and structural properties of GaAs/AlGaAs core shell nanowires and their applications in solar cells.

Semiconductor nanowires have attracted intensive interest due to their novel physical properties and unique growth mechanisms and.
These quasi-one dimensional structures are great candidates for future nanoscale semiconductor electronic and optoelectronic devices. III-V compound semiconductor nanowires are of particular interest for optoelectronic devices due to their high optical emission efficiency and carrier mobility. Various III-V compound semiconductor nanowire-based optoelectronic devices, including solar cells, photodetectors and light emitting diodes have already been demonstrated.

All the nanowires were grown on GaAs or InP (111)B substrates by Metalorganic Chemical Vapor Deposition (MOCVD) using Au nanoparticles as catalyst. InP nanowires were grown at temperatures from 400 to 500 °C with V/III ratios from 44 to 700. For GaAs/AlGaAs core-shell nanowires, GaAs core was grown by using a two-temperature growth procedure [1], AlGaAs shell was subsequently deposited at 650°C followed by GaAs capping layer to prevent oxidation of the AlGaAs shell. For solar cell structure, the nanowires were grown on p-doped substrates and the AlGaAs shell and GaAs cap were n-type doped. Electron microscopy, microphotoluminescence (PL), time-resolved PL, I-V characteristics and spectral response measurement were performed to characterize the nanowires and solar cell devices.

Results have shown the growth temperature together with V/III ratio and nanowire diameter are determining factors to obtain InP nanowires in ZB crystal or WZ crystal phase [2,3]. Mixed phases of ZB/WZ structures with a type II band alignment were also obtained in a single InP nanowire. Time resolved photoluminescence measurements have shown extremely long carrier lifetime (up to 8400 ps) in these structures [4]. Pure WZ and ZB InP nanowires also show distinctive polarization properties [5].

AlGaAs shell layer was found to be able to passivate the GaAs nanowire surface successfully and improve the PL emission efficiency significantly [6]. At the meanwhile, nearly intrinsic exciton lifetimes (~1 ns) were obtained which are comparable to high quality two-dimensional GaAs/AlGaAs double heterostructures [7]. Prototype nanowire solar cell devices were fabricated by planarizing the GaAs/AlGaAs/GaAs nanowire structures. The devices exhibit a spectrally broad photo-response and the conversion efficiency can be over 4%.

Acknowledgements
This work is financially supported by Australian Research Council (ARC). Australian National Fabrication Facility (ANFF) ACT node is acknowledged for the facilities used in this work.

Semiconductor nanowires with high optical gain offer promising solutions for lasers with small footprints and low power consumption. Although much effort has been directed towards controlling their size, shape, and composition, most nanowire lasers currently suffer from emitting at multiple frequencies, arising from the longitudinal modes native to simple Fabry-Pérot cavities. Here we demonstrate spectral manipulation of lasing modes by axially coupling two nanowire cavities through a nanoscale gap. Lasing operation at a single ultraviolet wavelength at room temperature was achieved in cleaved-coupled GaN nanowires with a lower threshold gain than that of the individual component nanowires. Good agreement was found between the measured lasing spectra and the predicted spectral modes obtained from simulated optical coupling properties, which presents design principles for rational control over the lasing modes in cleaved-coupled nanowire lasers. The highly monochromatic light from coupled nanowire lasers is anticipated to provide ultra-compact photon sources for laser-based...
remote sensing, high-density optical data storage, and long-distance optical communication.

Direct measurement of single CdSe nanowire absorption polarization anisotropies

Matthew P. McDonald, Felix Vietmeyer, Masaru Kuno*

Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, Indiana

Semiconductor nanowires (NWs) possess intrinsic polarization sensitivities, making them ideal candidates for a multitude of applications. However, to fully utilize this property, the absorption polarization dependence of individual NWs must be sufficiently understood. Towards this end, excitation polarization anisotropies ($\rho_{\text{exc}}$) have previously been observed in single NWs, where the photoluminescence is monitored as a function of excitation polarization. However, $\rho_{\text{exc}}$ measurements only indirectly measure the NW’s absorption polarization dependence and often lack the ability to probe band edge sensitivities.

In this work, we directly probe the extinction polarization anisotropy ($\rho_{\text{ext}}$) of individual CdSe NWs throughout the visible (480-750 nm) using single particle extinction spectroscopy. Here, $\rho_{\text{ext}} = \left(\sigma_{\text{ext}}^{||} - \sigma_{\text{ext}}^{\perp}\right) / \left(\sigma_{\text{ext}}^{||} + \sigma_{\text{ext}}^{\perp}\right)$, where $\sigma_{\text{ext}}^{||}$ ($\sigma_{\text{ext}}^{\perp}$) is the NW’s extinction cross section under parallel (perpendicularly) polarized illumination. Typical NW cross sections are $\sigma_{\text{ext}}^{||} \approx 10^{-11}$ and $\sigma_{\text{ext}}^{\perp} \approx 10^{-12}$ cm$^2$µm$^{-1}$.

In contrast with $\rho_{\text{exc}}$ spectra, observed $\rho_{\text{ext}}$ spectra have distinct spectral features that correlate well with theoretical transition rules derived from a 6-band $k \cdot p$ theory. This is the first time the absorption polarization sensitivities of an individual NW’s electronic transitions have been resolved at room temperature. The spectral features, along with magnitudes, suggest that the absorption polarization anisotropy of individual CdSe NWs originates from both confinement induced valance band mixing and dielectric contrast effects. This provides insight into the electronic transitions that dominate the optical properties of single CdSe nanowires and further elucidates their absorption polarization sensitivities.
Optical and electrical properties of individual CdSe nanowires

Alf Mews, Sebastian Schäfer, Zhe Wang, Anton Myalitsin, Dennis Franz, Tobias Kipp,

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Semiconductor nanowires (NWs) can be prepared by wet chemical methods using the so called SLS method where the Soluble precursors dissolve in the Liquid Bismuth catalyst to form Solid nanowires upon over saturation. Under different reaction conditions, nanowires with diameters of less than 5 nm, and also core-shell and block NWs are prepared [1]. In this contribution we will focus on the optical and electrical properties of individual CdSe-NWs. By employing single NW PL measurements and also TEM studies on the same individual NWs we establish a detailed structure property relationship. [2] Moreover we present a novel method combining Electrostatic Force Microscopy (EFM) including tip charging, with simultaneous PL measurements on individual semiconductor nanowires. We show that the initially homogeneously distributed charge is separated upon local illumination where the positive charges accumulate in the range of the Laser spot, whereas the negative charges migrate to the distant end of the NW. [3] Further, we actively charged isolated CdSe nanowires with a biased AFM tip to investigate the PL behavior in dependence of excess charges. Here we found that different voltage regimes can be identified which lead to PL enhancement but also to reversible and irreversible PL quenching [4]. Finally, we investigated axial type-II NW hetero structures from CdSe and CdTe to demonstrate charge separation across the interface [5].

Selective-area growth and optical properties of InP-based nanowires

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Semiconductor nanowires (NWs) are a new type of one-dimensional nanomaterials with diameter around few to few hundred nanometers, and have stimulated extensive interest in recent years because of their unique properties and potential applications as building blocks for nanoscale electronic and photonic devices. We have been reporting on the systematically controlled growth of III-V compound semiconductor NWs by catalyst-free selective area metalorganic vapor phase epitaxy (SA-MOVPE) on partially masked substrates. In this talk, I will review our study on the growth of InP NWs by SA-MOVPE [1-3]. Optical properties of NWs, which contains lateral [4] or vertical heterostructures [5], and application to light-emitting diodes [6] using InP NWs will also be given.

The work is mainly done in collaboration with Prof. Takashi Fukui, Prof. Kenji Hiruma, Prof. Shinjiro Hara, and Dr. Katsuhiro Tomioka.

References
Signatures of Majorana fermions in InSb nanowires with proximity induced superconductivity

Vincent Mourik

Kavli Institute of NanoScience, Delft University of Technology, The Netherlands

Majorana fermions are particles identical to their own antiparticles. Predicted a long time ago they have never been shown to exist as elementary particles. However, they have been theoretically predicted to exist as quasiparticle excitations in topological superconductors. Such a realization of Majorana fermions could be a good candidate to build a robust, decoherence protected qubit from. A particularly practical system to realize a topological superconductor is a nanowire with strong spin orbit coupling in which s-wave superconductivity is induced by the proximity effect [1,2]. We report electrical measurements on InSb nanowires contacted with one normal (Au) and one superconducting (NbTiN) electrode. Gate voltages vary the electron density in the nanowire and define a tunnel barrier between the normal and superconducting contacts. In the presence of magnetic fields of order 100 mT we observe bound, mid-gap states at zero bias voltage. These bound states stick to zero-energy while changing the magnetic field and gate voltages over large ranges, thus providing evidence for the existence of Majorana fermions in our system [3]. We report on the progress to find further evidence to the existence of Majorana fermions and their controlled creation in our system.

[3] Mourik et al., science.1222360
InSb nanowire structures for Majorana fermion manipulations


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III-V nanowires have shown great promises in the recent years thanks to the ability to control their dimensions, position, doping and to design heterostructures, both axially and laterally. This makes them ideally suited for fundamental transport physics studies and future electronic nanodevices. Over all the III-V semiconductors, InSb is the one having the highest electron mobility, the highest G-factor and the lowest band gap. These unique properties made them ideal material for detection of Majorana quasiparticles [1].

However, due to the growth conditions, InSb nanowire growth mechanism remains mainly unknown. Here we propose a study of gold-nucleated InSb nanowire arrays grown by MOVPE on (111) InP substrates. The influence of the growth conditions and of the array parameters on the nanowire shapes is discussed and global trends are given. A shape evolution from long and thin nanowires to nanocubes is reported [2]. Electrical measurements prove the high quality of these structures and mobilities up to 35000 cm²V⁻¹s⁻¹ are observed. Finally advanced structures based of InSb nanowires are studied for Majorana fermion manipulations.

InAs nanowires – from growth aspects through splitting of cooper pairs to the search for Majorana fermions

Anindya Das, Yuval Ronen, Moty Heiblum, Andrey V. Kretinin and Hadas Shtrikman

Braun Center for Submicron Research, Dept. of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel

InAs, a narrow gap semiconductor, when grown in the form of high aspect ratio nanowires, turns out to be one of the most attractive III-V materials for 1D physics studies. This is thanks to its small band gap, which facilitates the formation of non-alloyed Ohmic contacts, the strong spin-orbit coupling and the large Zeeman splitting associated with the typically large g-factor. The crystalline quality and purity of such nanowires are key issues when adopting them in mesoscopic systems such as nanowire superconductor hybrid devices. Stacking faults are suspected to have a deleterious effect on the transport properties of InAs nanowires and thus the importance of eliminating them. In addition, the purity of the nanowires is of utmost importance and therefore MBE growth is favorable over other pursued growth techniques.

We carried out a comprehensive study of the Kondo effect in an InAs nanowire based device where we observed Kondo valleys reaching conductance of nearly $2e^2/h$. This high conductance, combined with temperature far below the Kondo temperature, allows quantitative measurements of conductance scaling as a function of temperature, bias and magnetic field [1]. An important example for the utilization of high quality InAs nanowires is splitting of cooper pairs demonstrated in InAs nanowire/Al superconductor hybrid devices [2], where noise measurements were used to suggest possible entanglement of the split electrons [3]. Lately, InAs nanowires have joined InSb based structures in the search for Majorana fermions in a hybrid device which allows an intimate contact to a superconductor metal [4, 5]. Indeed we see evidence of Majorana fermions in an Al - InAs nanowire topological superconductor in the form of a distinct zero energy conductance peak appearing with an applied small magnetic field perpendicular to the spin-orbit effective field, fading away at higher magnetic fields as well as when the magnetic field is perpendicular to the nanowire.

In this work we will describe the Au-assisted VLS-MBE growth of InAs nanowires which made them suitable for the measurements described above. In order to obtain pure Wurtzite wires free of stacking faults we found the (011) InAs surface to be preferable compared to the (311)B and the (111)B surfaces. We attribute our
results to the lower and more stable supersaturation associated with the growth on the (011) surface.

SEM image of InAs nanowires grown on (011) InAs by Au-assisted VLS-MBE.


2-D and 3-D Integration of Nanowires for Electronics

Zhiyong Fan

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Semiconductor nanowires have been extensively explored as the building blocks for a variety of electronic and optoelectronic devices, including transistors, diodes, solar cells, etc. One of the major advantages of the synthetic nanomaterials rests in the low cost “bottom-up” growth methods. However, controlled assembly/integration of these materials in large scale normally remains as a challenge, whereas crucial for practical applications. Here we will introduce two approaches assembling crystalline semiconductor nanowires into ordered arrays. In the first approach, ordered arrays of NWs have been assembled by a simple contact printing method, which utilizes van de Waals interaction between nanowires and substrates. By tuning receiver substrate surface chemistry, density and alignment of nanowires can be readily modulated. With this generic approach, a wide range of
Au-catalyzed MOVPE of GaAs-based nanowires for photonic and photovoltaic applications: materials assessment and process scale-up

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$^2$Dept. of Engineering for Innovation, University of Salento, Lecce, Italy

Free-standing nanowires (NWs) based on III-V semiconductors are being considered ideal building blocks offering fascinating potential for future technological applications such as the realization of novel and efficient nanophotonic devices and photovoltaic cells. Self-assembly of III-V NWs by metalorganic vapor phase epitaxy (MOVPE) through the Au-catalyzed mechanism, is a most promising technology for the synthesis of NW-based devices, but it still requires demonstrating its entire potentials in terms of materials/device performances and industrial scalability. Here, we report on the self-assembly by MOVPE and properties of core-shell GaAs-AlGaAs NWs, as a case study.

In the first part of the talk, the morphology, size, inner composition, structure (defect content, lattice strain) and luminescence of as-grown GaAs and GaAs-AlGaAs NWs and their dependence of MOVPE conditions will be reported [1,2] The fabrication of photodetectors based on Schottky-contacted single core-shell GaAs-AlGaAs NWs will be then described. Noteworthy, as-fabricated detectors exhibit relatively strong polarization anisotropy of their spectral
photocurrent, and record high external quantum efficiencies (≈10% at 600 nm) [3]. Also, core-shell devices exhibit significantly improved dc and high-speed performances over bare GaAs NWs, and comparable to planar MSM photodetectors. Picosecond temporal response coupled with picoampere dark currents [4] demonstrates the device potential for high-speed imaging arrays and on-chip optical interconnects. The dynamic control of hot electron transfer rates in nanoscale heterojunctions is relevant for novel photovoltaic devices: the hot photoexcited electron transfer across the coaxial interface of a single GaAs/AlGaAs core-shell nanowire device will be reported [5].

The exploitation of GaAs-based NWs for photovoltaics requires the growth of uniform NWs arrays over large areas of relatively low cost substrates. In the second part of the talk we will report on a new approach for the controlled VLS growth of uniform dense arrays of well-aligned GaAs NWs over large substrate areas (over 2” dia. wafers and beyond). The growth of GaAs and GaAs-AlGaAs NWs on GaAs and Si using this new technology will be then demonstrated. The complex interplay between the NW size and height, and their array density in determining the radial (vapor-solid) growth rate of a shell material during the MOVPE process will be finally reported and assessed by validation of a shell vapour growth model.

Nucleation and growth mechanisms of self-induced GaN nanowires grown by molecular beam epitaxy

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The self-induced growth of GaN nanowires by molecular beam epitaxy is a promising approach for the fabrication of low-cost light-emitting diodes on silicon. In contrast to the catalyst-induced growth, the self-induced approach has the great advantage to avoid the use of any foreign material in the form of collectors or masks that could result in the GaN nanowire contamination, but involves complex nucleation and growth mechanisms. Typically, a highly nitrogen-rich vapour phase is required and often combined with a high substrate temperature for the nanowire self-induced formation. In this paper, the nucleation and growth mechanisms are discussed in details from theoretical and experimental results. A special emphasis is made on the underlying physical processes governing the successive steps of the self-induced growth from the very onset of the nucleation stage to the nanowire elongation.

Stress-driven quantum dot formation on top of nanowires

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On a bulk substrate, a misfitting deposit may grow as 3D islands because the lateral free surfaces of such islands permit efficient strain relaxation [1]. Conversely, when misfitting material is grown on top of a nanowire (NW), it usually adopts the diameter of the latter. Indeed, since elastic relaxation at the NW sidewalls is very effective [2], there seems to be little driving force for forming an island narrower than the NW. Hence, at least in VLS growth, to form a quantum dot (QD) in a NW, one first deposits a layer that adopts the NW radius, subsequent shell growth providing lateral confinement. Here, we explore the possibility of another mode of QD formation, whereby the layer adopts a diameter smaller than that of the NW. We model the energetics of the problem, not its
kinetics. We consider a cylindrically symmetric system consisting of a NW foot of radius $R_{NW}$ topped by an axial island with misfit $\varepsilon_0$, radius $R \leq R_{NW}$ and height $H$. By minimizing the total energy (taken as the sum of the elastic energy due to the coherent relaxation of the system and of the surface energy of the island sidewalls), we find the optimal deposit geometry $(R,H)$ at constant volume $\pi R^2 H$. We find that, somewhat surprisingly, at given deposit volume, there may be a large gain in energy in forming an island rather than a disk of radius $R_{NW}$. The preference for islands increases with $\varepsilon_0$ and $R_{NW}$. For instance, in the (In,Ga)N system, the total energy may be more than halved for perfectly realistic misfits of a few % and NW radii of a few tens of nm (Fig. 1). The predicted optimal islands differ markedly from disks, being much taller and narrower. There is a critical NW radius for islanding, which decreases when misfit increases but depends little on deposited volume (Fig. 1). However, at very low deposited volume (typically less than one monolayer), islanding is inhibited (e.g. up to C in Fig. 1), which is reminiscent of SK growth. The present effect is expected to occur primarily for catalyst-free growth. Actually, the spontaneous formation of core-shell structures [3] or insertions narrower than the NW foot [4,5] observed for misfitting growth on top of a NW in III-nitrides systems, might be a manifestation of this effect. Although islanding introduces a non deterministic aspect in heterostructure formation, the spontaneous formation of a shell following islanding seems beneficial.

Figure 1: Map of the variations with NW radius and deposit volume, of the ratio of the minimal energy of the system (at given deposit volume) to its energy in the disk configuration. The deposit volume is expressed in monolayers with NW radius. $\varepsilon_0 = 4\%$. The grey zones at left and bottom are where the disk is favored, whereas island formation is preferred in the colored areas. Horizontal arrow illustrates that, at fixed deposit volume, a critical radius is reached (point A) upon NW radius increase. Vertical arrow illustrates that, at fixed NW radius, a critical deposit thickness is reached (point C).

Technologically relevant epitaxial semiconductor films are biaxially strained if the substrate has a different lattice constant. This strain significantly modifies many material properties like carrier mobility and band gap. In planar layers, strain is maximum for coherent growth and can relax only through the formation of crystal defects. In contrast, axial nanowire (NW) heterostructures allow for the elastic strain relaxation at the free sidewalls. Here, we demonstrate that the strain state of such NW heterostructures can be engineered by choosing appropriate heights of the NW segments. We grew self-induced GaN nanowires (NWs) containing axial In$_x$Ga$_{1-x}$N heterostructures by plasma-assisted molecular beam epitaxy and varied the height of the GaN barriers from sample to sample. In order to probe the strain state of the In$_x$Ga$_{1-x}$N insertions, we measured the E1 LO phonon frequency by Raman spectroscopy under resonant excitation, as seen in Fig. 1. This phonon frequency shifts linearly with the ratio dbarrier/dSL between barrier height and the height of the entire superlattice. Thus, the degree of strain in the In$_x$Ga$_{1-x}$N insertions has been adjusted simply by tuning the barrier height and without changing the composition or height of the insertions themselves. The origin for this additional degree of freedom in the engineering of materials properties is that in NW heterostructures both the insertion and the barrier are strained and relax elastically at the free sidewalls. The barrier height affects the degree of relaxation in the barriers, which in turn influences the strain state of the insertions [Wölz et al., APL 100, 179902 (2012)]. With the aim to understand not only the Raman line position but also its linewidth, we calculated the strain distribution in NW heterostructures, and the result is presented in Fig. 2. Linear elastic theory reveals a progressive relaxation from the center of the NW to the sidewall, and the resulting broadening of phonon spectra is quantified based on published deformation potentials. We find that the expected broadening is much smaller than the experimental broadening. Hence, the latter has to be caused by another factor,
and the only viable origin is a significant fluctuation in In content within the probed NW ensemble. Taking into account this effect in the simulations of the Raman spectra allows us to assess the compositional fluctuations of the $\text{In}_x\text{Ga}_{1-x}\text{N}$ NW segments in the NW ensemble. Since the analysis of the In content in a statistically relevant number of NWs by local methods like transmission electron microscopy would be a very tedious task, the combination of strain simulations with an ensemble technique such as Raman spectroscopy is a powerful tool for the determination of the compositional distribution in the NW ensemble.

Fig. 1. Resonant Raman spectra for $\text{In}_x\text{Ga}_{1-x}\text{N}$ samples with different degrees of relaxation but constant $x$. $\delta_{\text{barrier}}/\delta_{\text{SL}}$ quantifies the strain relative to the pseudomorphic (fully strained) case. The $E_1$ $\text{In}_x\text{Ga}_{1-x}\text{N}$ phonon mode shifts to higher frequencies with increasing strain.

Fig. 2. Strain states in axial NW heterostructure: atomic displacement (left) and out-of-plane strain $e_{zz}$ (right). The non-uniform strain profile was calculated with the cylindrical model from Kaganer and Belov [PRB 85, 125402 (2012)]. The red, green and blue curves represent the displacement and strain at the radial positions indicated by the arrows (NW center, 80% and 95% of NW radius).

**Polytypism and heterostructure formation in III-V nanowires**

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Metal particle seeded III–V semiconductor nanowires are currently being investigated for a wide range of applications in electronics, photonics, and life sciences. Many of these applications require well-defined crystal structure and also heterostructures with well-controlled junctions. However, growth under arbitrary conditions often results in nanowires with a poorly controlled crystal structure. Switching material under similar, arbitrary conditions will most likely result in axial nanowire heterostructures with compositionally uncontrolled heterojunctions and significant amount of lateral overgrowth, or in the worst case – kinked nanowires, which means that the wires do not continue to grow straight and vertical to the substrate. In the first part of the presentation, I will start by explaining the occurrence of wurtzite (2H) in materials that
have zinc blende (3C) as the bulk stable crystal structure. However, several observations of higher polytypes, such as 4H and 6H, motivates the consideration of more polytypes than just 2H and 3C when predicting the influence of experimental and materials parameters on the crystal structure of III–V nanowires. Using combinatorics and an Ising model, I will discuss how to include these higher polytypes into an established nucleation modeling framework. I will compare the model predictions with experiments, both in nanowire systems with and without long range crystalline order. In the second part of the presentation, I will derive a general mass transport model for the compositional grading along the axial heterojunction in metal particle seeded III–V nanowires. According to this model and for abrupt precursor switching, the length of the graded region at the heterojunction is proportional to the axial growth rate and to the square of the nanowire radius. It is inversely proportional to the diffusivity of precursor material through the metal particle. As an example, I will discuss the model in view of gold particle seeded GaAs-on-InAs nanowire heterostructures grown with metal organic vapor phase epitaxy. This materials combination has a challenging interface, which is difficult to get abrupt. Based on an idea from the model, a precursor pulsing method was tested and by this the sharpness of the heterojunctions was increased by at least a factor of two. Finally, I will merge the two themes, polytypism and axial heterostructures. Here, I will discuss the growth of straight, axial heterostructures with compositionally abrupt heterojunction in the materials combination InAs-on-GaAs. This is something that has never been managed before, although several attempts have been made. However, by choosing optimum nanowire diameter and by controlling the crystal structure of both materials during growth of the heterojunction, the yield of straight nanowire could be optimized.

**Dopant distribution in in-situ and ex-situ doped nanowires**

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The incorporation of electrically active dopants in semiconductor nanowires (NWs) is crucial to the development of electronic and optoelectronic devices. However, the conventional doping mechanism, where dopants are introduced in-situ during growth, results in both axial and radial inhomogeneous doping profiles as a result of both the growth and doping processes [1-3].
We use quantitative Kelvin probe force microscopy (KPFM) and nano-probe scanning Auger spectroscopy to measure both the longitudinal and radial dopant distribution in doped Si nanowires. The longitudinal doping profile of phosphorus doped, untapered SiNWs shows an order of magnitude enhancement of the dopant concentration toward the NW's base, and this is explained due to vapor-solid surface doping during their growth inside the reactor. This process also induces very inhomogeneous radial doping profile which was observed via successive chemical etching of a single NW and measuring its surface potential using KPFM. These results are compared to measurements conducted on monolayer doped NWs [4]. This process makes an advantage of the precision of electron beam lithography as well as the selectivity and controllability of chemical monolayer formation to produce tailor-made dopant profiles.


**Engineering light absorption by switching codoping in SiGe coreshell nanowires**

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Tuning the electronic and optical features of materials through size reduction [1], alloying [2, 3] and doping [4] can pave the way to very exciting device applications, in particular in the field of photovoltaics [5]. By means of *ab-initio* calculations in the framework of Density Functional Theory we investigate the structural, electronic and optical properties of codoped SiGe coreshell nanowires [6]. We show how the simultaneous addition of impurities can result in a gain of energy with respect to the single-doping cases. Moreover we demonstrate how the Si/Ge band offset and the impurity position into the wire can strongly modify the energetic levels of dopants into the bandgap. This electronic tenability reflects into a strong modulation of the optical absorption spectra when positions of dopants are switched, suggesting a promising way to engineering light absorption in nanostructures.

References:

*Ab Initio* Study of Phosphorus Donors Acting as Quantum Bits in Silicon Nanowires

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A phosphorus (P) donor has been extensively studied in bulk Si to realize the concept of Kane quantum computers. In most cases the quantum bit was realized as an entanglement between the donor electron spin and the nonzero nuclei spin of the donor impurity mediated by the hyperfine coupling between them. The donor ionization energies and the spin–lattice relaxation time limited the temperatures to a few kelvin in these experiments. Here, we demonstrate by means of ab-initio density functional theory calculations that quantum confinement in thin Si nanowires (SiNWs) results in (i) larger excitation energies of donor impurity and (ii) a sensitive manipulation of the hyperfine coupling by external electric field. We propose that these features may allow to realize the quantum bit (qubit) experiments at elevated temperatures with a strength of electric fields applicable in current field-effect transistor technology. We also show that the strength of quantum confinement and the presence of strain induced by the surface termination may significantly affect the ground and excited states of the donors in thin SiNWs, possibly allowing an optical read-out of the electron spin [1].


**Recrystallization and Reactivation of Dopant Atoms in Ion-Implanted Silicon Nanowires**

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Silicon and germanium nanowires (SiNWs and GeNWs) are anticipated for the realization of next-generation metal-oxide-semiconductor field-effect transistors (MOSFETs) and solar cells. Impurity doping is one of the key techniques for the NWs devices. Ion implantation is now commonly used in semiconductor manufacturing. This technique allows the precise control of dopant concentration and provides uniformity in the growth direction. In bulk Si, the introducing of dopant impurities and defects, their interaction, the recrystallization process with defect annihilation in
implanted regions, and the subsequent reactivation process of dopant impurities have been extensively investigated. The recrystallization process with defect annihilation is a key point for controlling the reactivation and distribution of dopant atoms. In order to clarify them, we applied Raman and electron spin resonance methods, which we established to characterize the status of dopant atoms in SiNWs [1-3]. Recrystallization of SiNWs after ion implantation strongly depends on the ion doses and species. Full amorphization by high-dose implantation induces polycrystal structures in SiNWs even after high-temperature annealing, with this tendency more pronounced for heavy ions. Hot-implantation techniques dramatically suppress polycrystallization in SiNWs, resulting in reversion to the original single-crystal structures and consequently high reactivation rate of dopant atoms. The chemical bonding states and electrical activities of implanted boron (B) and phosphorus (P) atoms were evaluated by Raman scattering and electron spin resonance (ESR), demonstrating the formation of p- and n-type SiNWs [4].


**Integrated Nano Optoelectronics**

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Si:Ge alloy semiconductor nanocrystals (NCs) offer challenging opportunities for integrated optoelectronics/optoplasmics, since they potentially allow unprecedentedly strong light-matter interaction in the wavelength range of the optical communication. In this talk, we discuss the recent research efforts of my laboratory to develop optoelectronic components based on individual group IV NCs. We present experimental demonstration of the individual NC optoelectronic devices, including broadband Si:Ge nanowire (NW) photodetectors, intra NW $p$-$n$ diodes, Ge NC electrooptical modulators and near-field plasmonic NW detectors, where the unique size effects at the nanometer scales commonly manifest themselves. In particular, we demonstrated a scanning photocurrent imaging technique to investigate dynamics of photocarriers in individual Si:Ge NWs, which provides spatially and spectrally resolved local information without ensemble average. Our
observations represent inherent size-effects of internal gain in semiconductor NCs, thereby provide a new insight into nano-optoplasmonics.

Related recent publications:

Tunable Localized Surface Plasmon Resonances in Silicon

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Localized surface plasmon resonances (LSPRs) in semiconductors offer new opportunities to engineer the interaction of electromagnetic radiation with solid-state materials. Importantly, the carrier density of semiconductors, and thus LSPR frequency, can be modulated via chemical doping and/or electric field. This capability is a significant departure from the fixed carrier densities of traditional plasmonic metals (e.g. Ag and Au) and promises novel active devices. In addition, the direct integration of plasmonic and excitonic behavior opens the door to fundamentally distinct functionality. Here, we demonstrate and systematically control LSPRs in nanoscale Si for the first time. Highly aligned Si nanowires are synthesized via the vapor-liquid-solid (VLS) technique with a combination of Si2H6 and PCl3 precursors (Figure 1A). PCl3 simultaneously delivers P atoms to the nanowire core and Cl atoms to the sidewall. Adsorbed Cl atoms limit radial dopant incorporation and help maintain a uniform dopant profile as the nanowire
Elongates. Electron microscopy shows that the nanowires are single crystalline and <111> oriented with very few lattice defects. In-situ infrared spectroscopy measurements reveal intense polarization dependent mid-IR absorption bands only for the P-doped nanowires, which we assign to longitudinal LSPRs. A significantly weaker transverse mode is occasionally observed as well. The LSPR frequency can be readily tuned by varying nanowire length (Figure 1B). Mie-Gans theory supports our experimental results and indicates that electrically active dopant concentrations exceed 1020 cm⁻³ for all nanowire lengths (Figure 1C). A series of control experiments confirm that the observed modes result from P doping rather than the Au catalyst droplet and/or Cl surface termination. Our findings open a new route to engineer the properties of this ubiquitous semiconductor and highlight the importance of understanding the chemical phenomena that govern bottom-up nanostructure synthesis.

**Figure 1** (A) Cross-sectional SEM images of undoped (top) and P-doped (bottom) Si nanowire arrays. Scale bars, 400 nm. (B) Dependence of LSPR frequency on Si nanowire length. (C) Comparison of observed frequencies with Mie-Gans theory.
Luminescence of GaAs nanowires consisting of wurtzite and zincblende segments

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The equilibrium modification of bulk III-As semiconductors is the zincblende (ZB) phase. However, these materials crystallize partially or even predominantly in the wurtzite (WZ) structure when grown in the nanowire form. In particular, GaAs nanowires often exhibit a mixed crystal structure with ZB and WZ segments alternating along the nanowire axis. Since these two phases differ from each other in their energy gap, GaAs nanowires represent quantum structures with complex optical properties, the interpretation of which is currently discussed controversially. In particular, the value of the energy gap of WZ GaAs ($E^\text{WZ}_{\text{gap}}$) is under debate.

We have investigated single GaAs NWs by micro-photoluminescence and spatially resolved cathodoluminescence (CL) spectroscopy. The luminescence spectrum of GaAs NWs consisting of WZ and ZB segments is spread over a wide spectral range, where the optical emission occurs either predominantly above or below the energy gap of ZB GaAs ($E^\text{ZB}_{\text{gap}}$) depending on the growth conditions. These results are explained by means of a qualitative model assuming that $E^\text{WZ}_{\text{gap}}$ is larger than $E^\text{ZB}_{\text{gap}}$ and that GaAs NWs with alternating ZB and WZ segments along the wire axis establish a type-II band alignment, where electrons captured within the ZB segments recombine with holes of the neighboring WZ segments. Thus, the corresponding transition energy depends on the degree of confinement of the electrons, i.e., on the thickness of the ZB segments and exceeds $E^\text{ZB}_{\text{gap}}$ only for very thin ZB insertions. At low temperatures, the incorporation of carbon acceptors plays a major role in determining the spectral profile, as these can effectively bind holes in the ZB segments. Our results clarify why in some previous investigations a luminescence signal was only observed for energies below $E^\text{ZB}_{\text{gap}}$, while in other studies a luminescence signal was also observed above the energy gap of ZB GaAs. From the CL measurements of single GaAs NWs performed at room temperature, we deduce a lower bound of 55 meV for the difference between the corresponding energy gaps, i.e. $E^\text{WZ}_{\text{gap}} - E^\text{ZB}_{\text{gap}}$.

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Growth and Optical properties of (In,Ga)As Nanowire arrays on Silicon

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Group-III arsenide nanowires (NW) exhibit significant potential to drive new applications in nano-electronic and photonic devices especially when integrated on low-cost silicon (Si) platform. In particular, (In,Ga)As-based NWs and their heterostructures are of great interest due to their wide functionalities in NW field effect transistors, light absorbers and emitters covering a large spectral region.

Here, recent insights on the growth and optical properties of self-induced, catalyst-free (In,Ga)As NW arrays on Si (111) substrate are reported. Using a combination of nanoimprint lithography (NIL) for large-scale pre-patterned Si (111) templates and subsequent high-purity molecular beam epitaxy (MBE), spontaneous non-catalytic growth of well-aligned (In,Ga)As NWs [1,2] can be realized with very high-yield (> 90%) and pristine non-tapered morphological homogeneity. Details on the rate-limiting mechanisms will be given for the underlying selective area epitaxy (SAE) growth process, as investigated by: e.g. (i) tuning of the interwire distance (i.e., via self-limited growth) [3,4], (ii) modification of growth parameters [5], or (iii) variation of composition (i.e., In$_{1-x}$Ga$_x$As) [6].

Based on the finely tuned aspect ratios, further insights into the largely unexplored optical properties of these NWs will be presented using low-T photoluminescence (PL) spectroscopy. First, for binary, unpassivated InAs NWs the main emission characteristics are determined, revealing a wurtzite-dominated band edge emission with peak position very similar to bulk zinc-blende InAs. Furthermore, direct effects of NW aspect ratio tuning on radial quantum confinement are observed and confirmed by model calculations [7].

In addition, I will report on the emission properties of composition-tuned In$_{1-x}$Ga$_x$As NWs and show how through careful growth optimization the Ga content can be varied over a large band gap region while PL linewidths remain largely unmodified. This remarkable finding points to the superiority of SAE growth on NIL-Si (111) substrates giving very low degree of phase separation. In contrast, self-assembled, spatially uncorrelated In$_{1-x}$Ga$_x$As NW arrays show larger compositional inhomogeneity with increased peakwidths in 2θ–ω high-resolution x-ray diffraction scans as well as broadened Raman modes [6].
Finally, since many physical properties in these very high aspect ratio NWs are governed by surface effects, I will introduce several in situ surface passivation schemes based on radial pseudomorphic core-shell NW heterostructures and demonstrate their effectiveness on light emission enhancement.


Reconfigurable Nanowire Electronics

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Silicon nanowires (NW) are considered possible candidates for future electronic applications, as they hold the promise of combining one-dimensional transport with state-of-the-art silicon technology. Therein nanometer-scale silicon to metal junctions play a fundamental role. In this talk, the synthesis and electronic transport properties of Si and metallic NiSi\textsubscript{2} NWs as well as NiSi\textsubscript{2}/Si/NiSi\textsubscript{2} longitudinal NW heterostructures will be shown. A special emphasis will be given on the implementation of the properties of such nanowire heterostructures to conceive novel transistor and circuit architectures. Silicon-NWs are grown by Au-catalyzed chemical vapor deposition following the vapor-liquid-solid growth mechanism. Segments of these Si-NWs are transformed into metallic ones by a longitudinal volume diffusion process. Single-crystalline NiSi\textsubscript{2} NW segments are formed along the Ni diffusion path by an epitaxy limited solid-state reaction. The resulting interfaces have a sharpness of at most a couple of nanometers [1]. Schottky barrier field effect transistors (SBFET) were fabricated by a NiSi\textsubscript{2} encroachment from both NW ends, confining a pristine Si segment, which constitutes the active region, in between. The intruded metallic NiSi\textsubscript{2} segments act as extended source and drain regions providing nanometer scale Schottky contacts. Initially, a common back-gate steers the FET. The NiSi\textsubscript{2} NW electrodes strongly enhance the gate field at the Schottky junction, efficiently adjusting the width of the Schottky barriers and tuning the current injection. The transistor operation is controlled by switching between thermionic...
emission and tunneling through the Schottky contacts as proven by scanning gate microscopy [2]. To boost device functionality, this transport mechanism is used to independently control the charge carrier injection through each Schottky junction. With a multiple gate structure the Si energy bands are bent locally at the S/D-junctions in such a way that either electron or hole injection dominates. Simultaneously, the other type of carriers can be blocked effectively. By applying this method the control over polarity of the transistors was achieved [3]. The same devices can be programmed to operate either as a p- or n-type FETs depending on the biasing of the individual top-gates. Future computing circuits can make use of this reconfiguration method to perform different logic operations with the same hardware.


**Bandgap engineering of a semi-metal to form a nanowire transistor**

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Energy bandgaps are observed to increase with decreasing diameter due to quantum confinement in quasi-one-dimensional semiconductor nanostructures or nanowires. A similar effect is observed in semimetal nanowires for sufficiently small wire diameters: a band-gap is induced, and the semimetal nanowire becomes a semiconductor. We demonstrate that on the length scale on which the semimetal–semiconductor transition occurs, enables the use of bandgap engineering to form a field-effect transistor near atomic dimensions and eliminates the need for doping in the transistor’s source, channel, or drain. By removing the requirement to supply free carriers by introducing dopant impurities, quantum confinement allows for a materials engineering to overcome the primary obstacle to fabricating sub-5 nm transistors, enabling aggressive scaling to near atomic limits.
Electronic transmission and current are calculated from a first-principles Hamiltonian using density functional theory within a non-equilibrium Green’s function (NEGF) implementation. The transistor structure consists of a SnNW with varying cross section. In the central region, the cross section is small enough for the tin to become semiconducting and defines a channel region. The cross section is then increased on either side of the channel to form a metallic source and drain resulting. The channel region is surrounded by a gate stack, as in a gate all-around MOSFET. The design of a dopant-free, monomaterial field effect transistor is demonstrated. The drain–source current voltage characteristic of the confinement modulated gap transistor shows that the sub-threshold slope and the on/off ratio are 72.6 mV/dec and up to 104, respectively. That such figures can be achieved at essentially molecular length scales in a conceivably manufacturable design bodes well for continued nanoelectronic miniaturization.

Piezoresistance is the change in electrical resistivity of a solid with an applied mechanical stress. In crystalline semiconductors such as silicon, an applied stress changes the electronic band structure principally modifying the transport effective mass of the charge carriers [1, 2]. In 2006 a giant piezoresistance, up to 100 times larger than that observed in bulk silicon, was reported in bottom-up grown silicon nanowires [3] with diameters ranging up to 100 nm. It was later noted that the apparently giant effect occurred in nanowires that were partially depleted of charge carriers and an electrostatic description of the effect was developed [4]. In parallel with this, ab-initio calculations have suggested that a potentially similar effect may exist in nanowires with diameters in the range of 10 monolayers [5]. Given that the initial and subsequent reports of giant piezoresistance concern much larger diameter wires, attention has focused on experimental investigations of the electrostatic (or “piezopinch”) model. In a recent work [6], we investigated the piezoresistance of a large number of top-down fabricated silicon nanowires, nanoribbons and microwires, all of which were partially depleted of charge carriers. Both nominally n-doped, p-doped and unintentionally doped samples were studied. In all cases without exception the measured piezoresistance is that of bulk silicon. Moreover, these nano- and micro-structures exhibit a stress-independent dielectric relaxation in which the application of a voltage across the sample results in the significant bi-exponential drift of the resulting current. In effect, the act of measuring the resistance changes its value, reminiscent of so-called “memristance”. The resulting drift in the measured resistance is much larger than the true piezoresistance. Moreover, it results in signals that strongly resemble those initially claimed as being due to the application of an external mechanical stress [3]. I will present an overview of the current state-of-affairs concerning the giant piezoresistance, including reference to our own new efforts on bottom-up grown silicon nanowires as well as the rapidly growing literature on the subject.

Detection of the Early Stage of Recombinational DNA Repair by Silicon Nanowire Transistors

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Keywords: Silicon nanowire transistors, AFM oxidation nanolithography, protein-DNA, RecA, presynapsis

A silicon nanowire-based biosensor has been designed and applied for label-free and ultrasensitive detection of the early stage of recombinational DNA repair by RecA protein [1]. Silicon nanowires transistors were fabricated by atomic force microscopy nanolithography and integrated into a microfluidic environment (see Fig. 1) [2]. The sensor operates by measuring the changes in the resistance of the nanowire as the biomolecular reactions proceed. We show that the nanoelectronic sensor can detect and differentiate several steps in the binding of RecA to a single stranded DNA filament taking place on the nanowire-aqueous interface (see Fig. 2). We report relative changes in the resistance of 3.5% which are related to the interaction of 250 RecA•single stranded DNA complexes.[3] This change is not observed when a competing protein, SsbA, is present. Spectroscopy data confirm the presence of the protein-DNA complexes on the functionalized silicon surfaces.
Silicon and Germanium Nanowires for Next Generation High Capacity Lithium Ion Batteries

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Lithium (Li)-ion batteries have the highest energy and power density of any available rechargeable battery technology and they are widely used to power portable electronics. Still, Li-ion batteries are needed with lower cost, lighter weight, higher energy density, and better performance at fast charge/discharge rates. The most demanding Li-ion batteries applications of in battery-powered electric vehicles and large-scale (or grid) energy storage require unprecedented enhancements in energy and power density. One way to increase the energy density of a Li-ion battery is to replace the graphite anode with silicon (Si) or germanium (Ge). Si and Ge have significantly higher lithium storage capacities than graphite (3,579 mA h g⁻¹ and 1,384 mA h g⁻¹ compared to 373 mA h g⁻¹). Si and Ge, however, undergo massive volume expansions when lithiated—by about 280%. Nanowires are being explored for Li-ion batteries because they can more or less tolerate these volume changes without degradation. Battery performance, however, relies on all of the constituents of the anode, including electrolyte and binder formulations. Seeds used to grow the nanowires can also influence the battery performance. Here, we present the latest battery results from our laboratory using large quantities of Si and Ge nanowires grown by solution-based methods. The highest performance Si nanowires have been grown using tin seeds, which...
is also electrochemically active, and Ge nanowires have exhibited the best rate capability with capacities near the theoretical capacity due to its reasonably high electrical conductivity and fast Li diffusion.

**Band engineered, epitaxial Ge-Si$_x$Ge$_{1-x}$ core-shell nanowires: growth, electron transport, and device applications**

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The combination of vapor-liquid-solid growth mechanism with epitaxial film growth allows the realization of (Ge) – silicon-germanium (Si$_x$Ge$_{1-x}$) band-engineered core-shell nanowire heterostructures, where the shell content and thickness can be accurately controlled. Understanding the electronic and structural properties of such heterostructures is not only of fundamental importance, but can have direct implications for aggressively scaled, non-planar complementary metal-oxide-semiconductor devices. In this presentation we will discuss the growth and characterization of epitaxial Ge-Si$_x$Ge$_{1-x}$ core-shell nanowires, carrier mobility and strain measurements in such heterostructures, as well as the realization of field-effect transistors and tunneling field-effect transistors.


**In situ TEM observation of nanowire growth**

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Non-catalytic growth methods offer facile fabrication of pure nanowires without the need for catalyst preparation. Unfortunately, the mechanism of nanowire formation during metal oxidation is not
known. There are also fundamental questions related to the material transport and crystal formation mechanisms during nanowire growth. We observed for the first time nanowire during the catalyst free growth. Our results present solid evidence for the questions related to the nanowire growth mechanism during metal oxidation: are there any particles involved in the growth, and does the nanowire formation occur by addition of material at the top or bottom of the growing nanowire (i.e., a tip or a root growth mechanism).

This work substantiates non-catalytic tip growth of nanowires, obtained by in situ environmental TEM studies of nanowire growth during Cu and Fe oxidation. Based on the results, we propose a mechanism for nanowire growth by preferential metal ion diffusion in planar defects (twin boundaries and stacking faults), and subsequent layer-by-layer arrangement at the tip of the nanowire. One can hope that in the future, defects can be used to drive and even control the process of growth and the geometry of nanowires in a similar manner to what can be done with the help of catalyst particles. Although we have investigated only CuO and Fe₂O₃ nanowire formation, the growth mechanism is not limited to the formation of metal oxide nanowires. Similar mechanisms could also be applied to the non-catalytic growth of other nanowires or of ionic crystals by oxidation-reduction reactions.

**Periodical diameter oscillations and mechanical stability of the nanoparticle during InP nanowire growth**

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Semiconductor nanowires (NWs) have shown promising applications to new generations of devices due to their electronic properties and geometric configurations. Despite the huge advance in NW science in the past decade, new structures and aspects of NW growth dynamics can still be obtained. In this work we show InP nanowires
with an axial structure different from what is commonly reported in literature. The nanowires present periodical variations in diameter without any changes in growth parameters during the run and were obtained using very small (~5nm in size) catalytic Au nanoparticles (NPs). Statistical analysis of their morphology from scanning electron microscopy images has shown that the axial distance between the maximum diameter scales inversely with the Indium precursor flow provided during growth. Using transmission electron microscopy, the periodic oscillations in diameter are associated with a very large increase of stacking fault densities and crystallographic phase changes, from wurtzite to zinc blend. We have modeled the formation of this morphology as resulting from the NP partly wetting the NW sidewalls periodically during growth. The competition between different precursor incorporation routes leads to a geometrical deformation on the triple-phase line (TPL)[1], increasing the interface free energy and locally changing the contact angle between the catalyst NP and the top of the NW. Depending on the magnitude of this change, the mechanical equilibrium of the NP can be altered [2]. This instability of the NP on the NW leads to crystallographic phase changes [3] and causes the NP to wet the nanowire sidewall [4]. In this condition, however, catalytic growth on this lateral region is favored, leading to an increase in the diameter of the nanowire if we assume a constant NP volume. This hypothesis is supported by Energy-dispersive X-ray spectroscopy ex-situ measurements. Therefore, this increase in diameter leads to further changes in the contact angle in order to restore the equilibrium position of the NP on top of the NW.

Keywords: Nanowires, polytypism, III-V semiconductors, triple phase line.
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Plasma Assisted Silicon Nanowire Growth: a versatile process for Vertical and Horizontal Wires based on Low Melting Temperature Metal Catalysts

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Vapour-Liquid-Solid has been established as a powerful way to produce nanowires of various materials. While gold is the most widely used catalyst, it has a serious drawback when applied to the production of silicon nanowires. Indeed, Au is known to introduce deep defect levels in the gap of crystalline silicon. Over the past five years we have been developing a plasma assisted silicon nanowire growth process, where low temperature melting metals such as In, Sn and Bi are used as catalysts [1]. Liquid metal drops are simply obtained in a plasma reactor by a hydrogen plasma reduction of thin metal or metal-oxide layers at ~ 250 °C. Once the catalyst is formed, one has the choice between i) to maintain the temperature and switch to a silane plasma to produce vertical SiNWs [2] or ii) to decrease the temperature in order to cover the solid metal drops by a thin hydrogenated amorphous silicon layer. After this, a simple annealing will activate the growth of in-plane SiNWs [3]. The research performed so far has allowed us to demonstrate the potential of this approach for the production of radial junction solar cells [4] and thin film transistors [5]. In this presentation we review these results and discuss remaining challenges. In particular 1) the control of the density and size of catalyst drops and their dependence on the nature of the substrate; 2) the effects of the size of the catalyst drops and growth temperature on the crystallinity of the SiNWs; 3) the removal of the residual metal on top of the silicon nanowires.

Electronic structure of Semiconductor Quantum wires: Energy levels spin splitting, and the core-multi shell design problem

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We will show how atomistic pseudopotential theory of nanowires is able to build a bridge between the structure and the function. Structural degrees of freedom include diameter, identity of various core and shells, as well as polytypes (WZ, ZB). Function includes wavefunction localization; Direct-indirect band gaps; type I vs Type II and spin splitting. Recent relevant papers include Refs (1)-(4) below.

This work was done in collaboration with L.Zhang and J.W.Luo and was funded by the Department of Energy, Office of Science.


First-Principles Study of Doped III-V nanowires

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The potential application of GaAs and InAs nanowires in novel electronic devices requires controllable p-type and n-type conductivity. The problem of doping of nanowires has become now
a major challenge to the growers of one-dimensional III-V semiconductor structures. It occurs that specific growth conditions for nanowires, their crystal structure and orientation of their side facets may lead to different incorporation behavior than known for planar layers [1]. To explain the observed phenomena we study theoretically the properties of GaAs and InAs nanowires, in which one cation/anion is substituted by a dopant. Since the III-V semiconductor nanowires can grow in both, zinc-blende (ZB) and wurtzite (WZ) structures, we check whether the crystal structure of the wire has an impact on the doping level and the distribution of impurities in III-V nanowires and, most important, on the electronic properties of the doped nanowires. We consider ZB nanowires oriented along (111) axis and WZ nanowires along (0001) axis. Using \textit{ab initio} methods we have calculated the formation and segregation energies of III-V nanowires, in which Be atom substitutes cation and Si substitutes either anion or cation atom. To study the electronic properties we have calculated the density of states of the doped nanowires. The calculations have shown that the distribution of impurities in GaAs and InAs wires as well as their conductivity depend crucially on the crystal structure. Similar results have been recently obtained for GaAs nanowires doped with Mn, where a structure-dependent ferromagnetism was predicted [2].

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\textbf{Shell-doping of GaAs nanowires with Si for n-type conductivity}

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Semiconductor nanowires have been envisioned as a pathway to the monolithic integration of semiconducting materials with very different properties, as well as a functional interface with soft matter. A wide research field focusing on nanowire device applications has emerged over the last decade proving the
tremendous potential of this type of nanostructure. In our work we focus on the integration of group-III arsenides (III-As) with silicon, two semiconductors that paved the way in the era of (opto-)electronics covering different areas of the field according to their properties. The monolithic bridging of the two has been long awaited, and nanowires are the most promising way to realize that goal.

We demonstrate the potential of using Si as n-type dopant in GaAs nanowires grown epitaxially on Si substrates by molecular beam epitaxy. The achievement of n-type conductivity for nanowires is essential for the realization of functional devices, and is particularly significant when a dopant as well understood and advantageous as Si is employed.

We show that the amphoteric behavior of Si that typically accompanies the vapor-liquid-solid growth mode is adequately controlled when a shell doping scheme is utilized instead, i.e. when a Si-doped GaAs shell layer is grown conformally around the undoped GaAs nanowire core in the vapor-solid mode. The incorporation site of Si was evaluated by Raman spectroscopy, and correlated with the growth conditions of the doped shell. In that way, we identified a growth window that ensures the incorporation of Si as donor, and obtained donor concentrations up to $1 \times 10^{19} \text{ cm}^{-3}$, with the compensation level by Si acceptors remaining below 10%. Finally, charge transport measurements on planarized shell-doped nanowire ensembles were employed to probe the doping efficiency and the surface depletion of free-carriers.

Molecular attachment and alkyl passivation in Silicon Nanowires

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As traditional substitutional dopants are ineffective in thin silicon nanowires (SiNWs) due to dielectric and quantum confinement effects, we must look for alternative avenues. Surface adsorption by select molecular species can provide the necessary charge transfer, as we have recently shown [1]. This will also be used to explain the observed gas sensing properties of porous Si [2]. In other cases molecular absorption is an unwelcome effect, and surface passivation is used to protect SiNWs from exposure to, for example,
oxygen, or other performance-degrading agents. To this end, there has been a recent proposal to use alkyl groups (methyl, ethyl, propyl, etc.) rather than hydrogen to passivate SiNWs [3]. We will present calculations studying the energetics of alkyl passivation on different reconstructed Si surfaces, and discuss the implications for SiNWs.

 References:
POSTER PRESENTATIONS
Absorption of light in InP nanowire arrays

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Abstract
We study by electrodynamic modeling the interaction of light with an array of InP nanowires and find general design principles for efficient light-management in vertical nanowire arrays for next-generation photovoltaics. First, InP nanowires with diameters of less than 100 nm are not a recommended design due to poor absorption of light of long wavelengths. In contrast, we discover two specific diameters, the first of 170 nm and the second of 410 nm, that give a maximum of the absorption efficiency of solar energy, irrespective of the nanowire length. For wavelengths close to the band gap wavelength, these diameters give rise to strongly absorbing nanophotonic resonances in the individual nanowires. This shows up for the nanowire array as an absorption peak enabling the maximum of the absorption efficiency. This mechanism of enhancing the absorption close to the band gap wavelength by a suitable choice of the nanowire diameter is applicable also for nanowires of other semiconductor materials. The optimized diameters for other direct band gap semiconductor nanowires can be obtained easily from the results found here for InP by rescaling with the band gap wavelength and refractive index of the new nanowire material. We find also that with increasing length of the nanowires, the optimized value of the period of the array increases. Such optimized absorption efficiency of the nanowire array is considerably higher than that of a thin film of InP.
Characterization of the radial $p$-$n$ junction on Si micropillar-array solar cells

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Semiconductor nanowires are considered good candidates to be integrated as active photovoltaic components thanks to the many advantages that they bring to the devices. By exploiting core-shell radial $p$-$n$ junction designs carrier extraction can be achieved efficiently thanks to the short collection lengths while simultaneously obtaining high optical absorption.

Si microwire arrays were fabricated by a top-down method based on a combination of optical lithography and deep reactive ion etching on a $p$-doped Si wafer. A radial $p$-$n$ junction was obtained by POCl$_3$ diffusion. Efficiencies up to 9.7% under AM 1.5G solar illumination were obtained. In order to study the influence of the $pn$ junction design on the overall performance of the device, different $p$- and $n$-doping profiles and thicknesses were evaluated. It was showed that the minimum wire diameter is limited by the depletion width resulting from the $p$- and $n$- concentrations. In addition, the radius of the not depleted core should be of the same range but not bigger than the diffusion length of the minority carriers. It was also demonstrated that, by decreasing the doping concentration of the $p$-core by two orders of magnitude (from $\sim10^{16}$ to $\sim10^{14}$ cm$^{-3}$), a higher external quantum efficiency was obtained, especially at the infrared regime, where photons are mainly absorbed in the bulk and, hence, they are farther from the junction. Finally, a variation on the diffusion conditions was performed, in order to change the doping profile, as well as the shell thickness and the junction depth. It was concluded that having the junction closer to the surface reduces losses within the emitter region. By reducing the shell thickness from 635 nm to 270nm, a 4.6% increase of the short-circuit current density was obtained, as well as a higher external quantum efficiency in the visible regime (from 400 to 850 nm).

Finally, in order to calculate recombination rates both in the bulk and at the surface, impedance spectroscopy measurements were carried out. This is a technique largely used on electrochemical systems but not fully exploited on solid-state devices. The impedance of the system was measured for a wide range of frequencies and voltages. The spectra obtained were fitted by an equivalent circuit and, consequently, important parameters such as junction and diffusion capacitances, parallel resistance and effective lifetime could be extracted. As well, a physical model of the system was obtained.
Nanowire arrays in multi-crystalline silicon thin films on glass: a highly flexible absorber material for third generation photovoltaics

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Abstract: Controlled patterning of large grained multi-crystalline silicon (Si) thin films of only ~6µm thickness on glass could be realized using nanosphere lithography (NSL) in combination with reactive ion etching (RIE). Thereby, silicon nanowires (SiNWs) formed perpendicular to the film surface, independently of the crystal orientation of the underlying grains and with entirely pre-determined geometrical properties such as lengths and diameters (Figure 1). The SiNW-patterned thin films show properties, which ideally qualify them as absorber material for photovoltaics (PV). X-ray photoelectron spectroscopy (XPS) studies showed an electronic grade surface quality of the SiNWs. Integrating sphere measurements could prove that patterning of Si thin films with SiNWs permits an enhancement of the spectral absorption of visible light of up to 50% and results in resonant absorption peaks depending on the geometry of the highly ordered SiNW arrays. In the SiNWs, radial and axial p-n junctions were formed by phosphorous diffusion and charge separation in the junctions of single wires could be proven by electron beam induced current (EBIC) measurements. Based on this, the absorptivity of single SiNWs, as the constituting unit of the resonantly absorbing arrays, could be further investigated. In the EBIC setup under the SEM, the external quantum efficiency of the now contacted single wires could be determined, by irradiating them with monochromatic light through an optical fiber. The measured current from single wires showed resonances for certain spectral lines, which could be correlated to resonances in the spectral absorption cross-section from first principle Mie calculations on cylindrical Si structures of the same diameter. These findings pave the way for tailoring the absorption in third generation thin film PV devices. Together with the high structural and electrical quality of the newly created absorber materials they open up a new research field of glass-based SiNW thin film PV.

Figure 1 Left: SE and EBSD images in an SEM of a mcSi thin film on glass with a surface area partially covered with SiNWs. The EBSD image shows a variety of different grains. Along trajectories A / B the grain misorientation (a measure for dislocation densities) was measured. EBSD detail: SiNWs on five different grains with different crystal orientations along the wire axis. SE detail (45° tilt): Grain boundary at the transition of SiNWs and unpatterned mcSi layer. RIE permits SiNW formation perpendicular to the surface irrespectively of the grain orientation (scale bars left: 50µm / right: 3µm).
Hybrid Nanometric Structures with High Photocatalytic Activity obtained by Molecular Layer Deposition and Nanowire Scaffolds

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Molecular Layer Deposition (MLD) provides a promising path for overcoming some of the limitations encountered using conventional methods for the formation of catalytic metal oxide films at the nanometric scale for high aspect ratio structures by combining the highly controlled, self-limiting characteristics of the Atomic Layer Deposition (ALD) approach with the flexibility introduced by the organic molecular constituent. Here we present the use of Chemical Vapor Deposition (CVD) and MLD for the formation of well controlled metal oxide-nanowire (NW) hybrid structures with high photocatalytic activity. The formation of nanotubes (NTs), with controllable wall thickness and enhanced surface area, is demonstrated using NW scaffolds. The molecular permeability of organic-inorganic metal oxide hybrid allow soft etch of Germanium NW to yield NTs in minutes. In sharp contrast, TiO$_2$ NTs prepared under similar conditions required several hours of etch to remove the Germanium core. The photocatalytic activity of the films and NT structures were investigated using hydroxyl-functionalized porphyrin and Methylene blue as spectroscopic markers. TEM imaging and electron diffraction, XPS, UV-Vis spectroscopy and Spectroscopic Ellipsometry were employed for structural and composition analyses of the films and NTs. Overall, our results indicate that thermally annealed Ti-EG film photocatalytic activity is about 5-fold increased compared to TiO$_2$ film prepared by ALD for optimal process conditions. Comparison of Ti-EG films and NTs morphologies demonstrated increased dye loading capacity with linear dye loading increase with wall thickness and similar photocatalytic degradation rates.
Towards light-emitting diodes based on the selective-area growth of III-N nanowires on Si substrates

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Light-emitting diodes (LEDs) based on III-N nanowires (NWs) are an attractive alternative to conventional planar layers, since the NW geometry enables the elastic relaxation of strain at the free sidewalls. Thus, NWs with (In,Ga)N/GaN heterostructures can be grown in high structural quality on cost-effective Si substrates and are able to emit light in the entire visible spectral range from blue to red. However, (In,Ga)N/GaN NW ensembles grown by self-assembly processes suffer from a variation in the In incorporation and exhibit the former goal requires the AlN buffer to be of high structural quality and to allow LED operation. The former goal requires the AlN buffer to be of high structural quality and to exhibit a smooth and defect-free surface. To this end, the formation of both SiN and Al droplets has to be avoided, and the growth temperature should be sufficiently high. Since all these requirements cannot be achieved under the same growth conditions, we developed a procedure involving the deposition of a very thin (1 nm) AlN nucleation layer at low temperature (50 °C) before continuing the growth at higher temperature (680 °C). We varied the total thickness of the AlN buffer layer between 2 and 14 nm and investigated the resulting incubation times for the self-induced growth of GaN NWs. In particular, we monitored by line-of-sight quadrupole mass spectrometry when the amount of Ga atoms desorbing from the sample surface started to decrease, thus indicating the onset of NW nucleation. A sufficiently short incubation time was found for a minimum AlN buffer layer thickness of 4 nm.

In order to prove the feasibility of operating LEDs on such an AlN buffer layer on n-type Si(111), we grew Si-doped GaN NWs on the buffer layer. The NW ensembles were vertically contacted by our NW LED process, i.e. the space between the NWs was filled up by spin-on glass, and the top of the NWs and the backside of the substrate were metallized. Preliminary electrical measurements showed an ohmic behavior, and further measurements are in progress.

Finally, NW LED structures consisting of a Si-doped GaN base and a Mg-doped GaN cap with an axial (In,Ga)N/GaN heterostructure embedded as active region were grown on the AlN buffer layer. Both the morphology and the photoluminescence of the sample are similar to analogous ones grown directly on Si that have been successfully fabricated into NW LEDs exhibiting electroluminescence. Further investigations are in progress to elucidate the operation of the LED on the AlN buffer layer.

Toward inorganic/organic GaN-based nanowire light-emitting diodes based on Förster resonant energy transfer

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GaN is the state-of-the-art material for the fabrication of blue light emitting diodes but, in terms of internal quantum efficiency, GaN-based LEDs cannot compete with organic light emitting diodes (OLEDs). However, OLEDs exhibit poor electrical properties that hindered them from seriously rivaling GaN-based LEDs. The fabrication of hybrid GaN/organic semiconductor heterostructures may allow for combining the individual material’s strength while compensating for their deficits. In this context, Förster resonant energy transfer (FRET) can be utilized to transfer electrically injected carriers from GaN to an organic semiconductor overlayer, where electrons and holes can recombine radiatively in a more efficient way [1-4]. Since FRET relies on dipole-dipole interaction coupling, the separation between the GaN active region and the organic semiconductor cannot be higher than a few nm. Thus, it cannot be used in conventional planar LEDs because the required thickness for the top contact layer is typically more than 100 nm. This problem can be circumvented using GaN nanowires (NWs), where the GaN active region at the side facets can be covered with an organic semiconductor.

In this work, GaN-based structures were grown by plasma-assisted molecular beam epitaxy to study the FRET process in hybrid GaN/organic semiconductor systems. In a first stage, planar InGaN single quantum wells with different GaN cap thicknesses were prepared on both polar and non-polar GaN surfaces (c-plane and m-plane, respectively) to analyse how the efficiency of the FRET process is affected by the interlayer thickness and the orientation of the GaN layer. In a second stage, GaN multiple quantum disks embedded in self-induced AlGaN NWs were prepared to investigate the FRET process in such nanostructures.


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Electric field-induced emission enhancement and modulation in CdSe nanowires

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Semiconductor nanowires (NWs) are an ideal platform for optoelectronic applications with minimal space requirements. Their unique properties are readily exploited to create single NW chemical/biosensors, LEDs, lasers, and photodetectors. These technologies can be used as building blocks to create nanoscale assemblies with an extremely wide range of functionalities. In recent years, significant progress has been made towards a microscopic picture of phenomena that give NWs their unique properties. NW optical properties, particularly absorption of light and its polarization sensitivity to light polarization are well understood. At the same time, processes that occur after photoexcitation and define photoluminescence quantum yields as well as carrier lifetimes are still challenging to understand.

In particular, quantum yields on the order of 1% suggest that defects play a key role in dictating the NWs’ optical and electrical response. This connection between a system’s optical/electrical properties and defects was established more than 50 years ago. In today’s nanomaterials, defect investigations are even more relevant due to the large fraction of atoms that reside at the surface of nanostructures given their enhanced surface-to-volume ratios. The advent of heterostructures such as core/shell species and mixed metal/semiconductor hybrid systems means the existence of additional interfaces, possessing large surface areas.

In all cases, little is known about the nature of associated defects since limited means exist for probing them. In this study, we monitor individual NW emission intensities in parallel plate capacitor-like structure. CdSe nanowires show reversible emission intensity enhancements of ~14±7% when subjected to electric field strengths ranging from 5 MV/m to 22 MV/m. As a consequence, alternating positive and negative biases yield emission intensity modulation depths of ~15%. These emission sensitivities are rationalized by the field-induced modulation of carrier detrapping rates from NW defect sites responsible for nonradiative relaxation processes. The exclusion of these states from subsequent photophysics leads to observed photoluminescence quantum yield enhancements. We explain the phenomenon by developing a kinetic model to account for field-induced variations of carrier detrapping rates through a nanoscale Poole-Frenkel effect. The observed effect allows direct visualization of trap state behavior in individual CdSe nanowires and represents a first step towards developing new optical techniques that can probe defects in low dimensional materials.
Silicon nanowire transistors fabricated by AFM oxidation and Electron beam nanolithographies: Output and transfer characteristics

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Abstract

We have fabricated silicon nanowire field effect transistors (SiNWs) by using two top-down nanolithographies: AFM local oxidation nanolithography (LON) and electron beam lithography (EBL). The top-down nanolithographies define a mask that upon exposure to a reactive ion etching generates the silicon nanowire. In AFM the mask is made of silicon dioxide, while in electron beam is a cross-linked negative resist. We have measured and compared the electrical characteristics of the SiNWs field-effect transistors fabricated by both methods. The output and transfer curves of the devices fabricated by the top-down lithographies are qualitatively similar. The $I_{on}/I_{off}$ ratio, subthreshold slope and electron mobilities of the fabricated transistor are more dependent on the geometry of the device than on the method to fabricate it. For SiNWs of 50-100 nm in width we have measured $I_{on}/I_{off}$ ratios of $10^5$, and mobilities of 1000 cm$^2$/V.s.

Figures. (a) AFM image of a Si nanowire bridging two gold electrodes. The SiNW has been fabricated by AFM oxidation. (b) Output characteristics of the device shown in (a). (c) AFM image of a Si nanowire bridging two gold electrodes. The SiNW has been fabricated by electron beam nanolithography. (d) Output characteristics of the device shown in (c). The insets in (a) and (c) show the respective SiNW cross-sections.
Stability of Si epoxide defects in Silicon Nanowires

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The last decades Moore’s law has been driving the semiconducting industry to decrease the dimensions of the transistors towards nano related dimensions. It has been demonstrated that Si nanowires can be an important building block in these nanotransistors¹. The increase in band gap as a result of quantum confinement² also makes it interesting for the use in optical applications. For most applications however these Si nanowires are surrounded by a (native) oxide. Understanding the defects that can arise at the Si/Si₅ₓ interface of these wires is thus of prime importance for understanding the properties of the resulting transistors.

Here we focus on one particular defect, the Si epoxide defect (a three membered Si-O-Si ring). This defect is known to be present at the Si/Si₅ₓ interface of oxidized Si surfaces³. To investigate if it is also present in oxidized wires the oxidation process has been modeled using Molecular Dynamics simulations. In the resulting models of the Si/Si₅ₓ core-shell wires the presence of Si epoxide is clearly visible. As expected the epoxide is present at the interface. A possible origin of the defect at the interface is the stress generated by the lattice mismatch. But remarkably the epoxide is also present at the surface of the wires, which is not observed for flat surfaces.

To investigate this defect in more detail we perform Density Functional Theory calculations on pristine wires with one epoxide defect at the surface. Investigating the formation energy as a function of the diameter shows that the stability of the defect depends strongly on the curvature of the wire. Large curvature appears to stabilize the defect. If we compare the the Density of States of the wires with and without the defect it is clear that the defect has a significant influence. The defect induces an electronic state within the band gap. The position of this state in the gap is also heavily dependent on the diameter. For smaller wires the defect level goes deeper within the band gap. This state within the band gap and its dependence on the diameter could be important for optical applications.

To evaluate the possibility of removing the defect we also investigate the hydrogenation of the defect. Here we find an enhanced endothermicity as a function of decreasing diameter. Nudged elastic band calculations indicate that before this reaction can occur a repulsive barrier of the order of 0.5 eV has to be overcome.

Growth Environment and Incorporation Mechanism Impact on Dopant Distribution and Activity of VLS Grown Nanowires.


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The incorporation of electrically active dopants into nanowires (NW) is essential to the development of semiconductor NWs based electronic devices. The ability to engineer the electrical properties of nanowires grown by the vapor liquid solid (VLS) process is currently limited by our incomplete understanding of the doping mechanism. During the recent years, several studies have shown evidence of inhomogeneous radial dopant distributions in SiNWs and the resulting effects on their electrical properties [1-2]. However, the longitudinal dopant profile has not been addressed to the same extent. Studies employing both indirect and direct measurement techniques (such as scanning photocurrent microscopy, Kelvin probe force microscopy and atom probe tomography) have addressed variations in longitudinal dopant profiles in SiNWs and related them to radial dopant variations induced by the growth process [3-4]. Nevertheless, a direct measurement (which is not restricted to a relatively small area of interest) of the dopant concentrations along entire VLS grown nanowire has not been demonstrated yet.

We have measured the longitudinal doping profile of phosphorus doped, untapered SiNWs using nanoprobe scanning Auger. First, we have found order of magnitude enhancements in the dopant concentration toward the NW's base as expected from previous indirect measurements. Importantly, the physical dopant profile is not identical to the active dopant profile, as shown by comparison with scanning photocurrent microscopy and Kelvin probe force microscopy measurements. In addition, high dopant concentrations were measured in the vicinity of the NWs' tip, which can be attributed to reservoir effect. Second, we measured intentional variations in doping concentration along the nanowire, the obtained results show that different dopant incorporation mechanisms could be distinguished. The resolution and sensitivity of scanning Auger microscopy as analytical tool for dopant concentration measurements will be compared to the other available techniques to indicate unique capabilities that can advance our understanding of nanowire doping.

Doping incorporation and acceptor deactivation in Be-doped GaAs nanowires

Achieving controlled doping in semiconductor nanowires is of fundamental importance for their future implementation in the next generation of electronic and optoeletronic devices. Due to the particular growth mechanisms of nanowires, controlled doping still remains a challenge. In this study we report on the doping of GaAs nanowires with Beryllium (Be). Be is a p-type dopant in GaAs, that enables the achievement of high carrier concentrations.

Nanowires are grown by Molecular Beam Epitaxy (MBE) via self-catalytic vapor-liquid-solid (VLS) process directly on a silicon substrate \(^1,2\). The clean conditions of MBE\(^3\) and the absence of using gold as catalytic seed give rise to high crystal quality nanowires \(^4,5\). We intentionally introduce Be atoms into extremely pure GaAs nanowires, which should lead to p-doping. We realize electrical transport experiments with multiple nanoscale contacts to determine the conductivity of the nanowires along the axis. By examining the dependence of the conductivity along the nanowire axis and as a function of the growth conditions, we derive a model for the doping mechanisms of GaAs nanowires with Be. In the model, we consider the two possible incorporation paths of Be: from the side facets (vapor-solid deposition) and from the gallium droplet (vapor-liquid-solid deposition). We believe this model corresponds to a more general behavior and that it could be extended to other similar dopants such as Tellurium.

References:

SELF-CATALYSED MBE GROWN GaAs NANOWIRES WITH PREDICTIBLE Γ – SHAPE

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Novel NW structures suitable for functionalization and interfacing like bridged NWs, arched NW, tilted or curved NWs are of particular interest in a view of new device applications. In this work, we describe the method allow us to predictably grow GaAs NWs consisting of two perpendicular segments.

We start with traditional growth of self-catalysed GaAs NWs on Si(111) substrate during 15 min at 610\textdegree C. The growth is terminated under Ga flux while As shutter is closed for 30 s. This stage is presented in Fig.1, a. Most of NWs has typical bending shape oriented in six equivalent $<110>$ directions. In the second stage, As flux is initiated again for next 5 min keeping Ga shutter open. Resulting structure is presented in Fig. 1, b. The NWs always have two perpendicular sections. In Fig. 1. c typical TEM image of the upper part of the NW is presented. In most cases, in the segment elongated in [110] direction a stacking fault along the segment is systematically observed. Probably, the formation of the stacking faults leads to the growth direction change.

![Fig. 1. a,b – SEM images taken after first and second stages of the NWs growth, c – TEM image of the resulting NW (upper part).](image)
Nucleation of self-assisted GaAs nanowires grown by MOCVD: Effect of Group-III precursor pre-deposition and substrate orientation

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Nanowires combine the intrinsic properties of semiconductors with low dimensionality, which makes them potential building blocks for optoelectronic applications. Nanowire growth generally involves metal seed particles; however, metal particles may introduce impurities to the nanowires and deteriorate their optoelectronic properties. Self-assisted growth method can eliminate contamination, since it does not utilize a foreign metal particle. Furthermore, for many applications a dense nanowire array is highly desirable. In literature, molecular beam epitaxy grown self-assisted GaAs nanowires have been reported, but metal-organic chemical vapor deposition (MOCVD) has not been explored so far despite the fact that MOCVD is an industrial-scale technique that can yield high growth rates and high nanowire throughput.

In this study, the effects of group-III precursor pre-deposition and substrate orientation on nucleation of self-assisted GaAs nanowires grown by MOCVD are explored. No mask layer or external seed particles are used to promote the nanowire growth. Instead, Ga droplet formation is initiated by engaging group-III precursor into the growth chamber before group-V precursor is introduced. This in situ pre-deposition duration, combined with substrate orientation has effects on areal nanowire density and nanowire morphology. For both substrate orientations (GaAs (111) and (110)), it is observed that in general, areal density increases with increasing group-III pre-deposition duration up to a certain limit. For the same durations of group-III pre-deposition, the density of nanowires grown on GaAs (111) substrate is higher than the nanowires grown on GaAs (110), which is attributed to different surface diffusion length of Ga adatoms. Interestingly, in the case of no pre-deposition of group-III material (when both precursors are engaged simultaneously for growth), nanowires are still observed in both substrate orientations. This indicates that either group-III droplets can still be formed in the presence of group-V material, or nucleation of nanowires can occur without the need of group-III droplets. This study shows the importance of parameters such as pre-deposition step and substrate orientation for achieving dense nanowire arrays with an epitaxial relationship with the substrate.
In situ study of self-assembled GaN nanowire nucleation on silicon

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ABSTRACT

In contrast to most columnar nanostructures fabricated by molecular beam epitaxy (MBE), GaN nanowires (NWs) have the advantage to grow without requiring the help of any external catalyst. Since the first reports on their elaboration by plasma-assisted MBE in the late 90s [1,2], the dependence of their morphology on the growth conditions has been widely investigated (see for instance Ref. [3]). Nevertheless, mechanisms beneath the very first stages of their emergence are still not fully apprehended [4,5].

In this context, with the aim of clarifying GaN NW nucleation in plasma-assisted MBE, in situ grazing incidence X-ray diffraction was performed at the BM32 beamline of the European Synchrotron Radiation Facility of Grenoble. The results are supported by reflection high energy electron diffraction observations. We show that nitridation of Si(111) - 7×7 reconstructed surface occurs during N - plasma ignition because of an unavoidable leakage of active nitrogen and despite the closed N shutter. This nitridation is detected by the apparition of a 8×8 surface reconstruction, consistent with the formation of crystalline β-Si₃N₄. When subsequently providing Ga and N atoms, we observe that Ga only starts to be incorporated after β-Si₃N₄ has been amorphized, which induces a delay in the beginning of the nucleation. Conversely, we show that this delay do not exist when using a thin AlN buffer: when exposing the Si(111) surface to Al and N, AlN forms at the expense of β-Si₃N₄, resulting in a reduced delay of the growth start. Based on these results, GaN NWs nucleation dynamics can now be thoroughly explained, both on bare silicon and on AlN/silicon, allowing a better mastering of their growth, understanding of their morphology and of their polarity.

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Role of crystal polarity and substrate defects in the spontaneous formation of GaN nanowires

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GaN nanowires (NWs) have attracted great interest for the fabrication of nanoscale devices such as light emitting diodes, bio-sensors, and photovoltaic cells because, independent of the substrate used for growth, they exhibit a high crystal quality. However, despite the potential of these nanostructures, and the fact that they have been grown by plasma-assisted molecular beam epitaxy (PA-MBE) since the late nineties [1,2], the physical mechanisms underlying the spontaneous formation of GaN NWs are not well understood.

Spontaneous GaN NWs grown by PA-MBE crystallize in the wurtzite structure with the polar <0001> axis parallel to the growth direction. The [0001] and [000\bar{1}] directions (known as Ga- and N-polar orientations, respectively) are thus non-equivalent. In the case of the growth of epitaxial films, it is well established that the polarity of the layer has a strong impact on their properties since it determines the direction of both spontaneous and piezoelectric polarization fields, affects the morphology, and influences the incorporation of dopants, impurities, and the formation of native point defects. Despite these facts, the role of the polarity in the spontaneous nucleation and growth of GaN NWs is unknown. Another important open question is whether or not defects are responsible for the nucleation of GaN NWs.

In this work, we investigate how a preset crystal polarity affects the spontaneous formation of GaN NWs in PA-MBE. The polarity is set by the use of 6H-SiC(0001) and 6H-SiC(000\bar{1}) substrates. The coherently strained AlN buffer layer grown on these substrates replicates the polarity of SiC and allow us to investigate how, in the absence of structural and morphological defects of the substrate, the crystal polarity influences the spontaneous formation of GaN NWs. The successful growth of homogeneous and dense NW arrays on N-polar AlN evidences that the spontaneous formation of GaN NWs does not require substrate defects. However, crystal polarity is found to play a major role since on Al-polar AlN we do not observe the formation of Ga-polar GaN NWs. Instead of that, a faceted Ga-polar GaN layer interspersed with a few N-polar GaN NWs is observed whose formation is likely to be induced by a parasitic effect. Thus, the present results demonstrate that, in the absence of substrate defects, spontaneous GaN NWs are always N-polar.

Independent of the fundamental reason behind the inherent tendency of GaN NWs to grow along the [000\bar{1}] direction, the present findings are essential for establishing an understanding of the spontaneous formation of GaN NWs, and of high technological relevance due to the major influence of the polarity on the properties of GaN-based devices.


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**ZnO Nanowires Derived from Seeded Solution Growth Based on the Dissolution-Reprecipitation Mechanism**

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ZnO nanowires have attracted considerable attention over the last decade due to their potential applications in optical, sensing, photovoltaic and catalytic fields. Wet chemical methods have been demonstrated as a very versatile technique for growing 1D ZnO nanostructures.1 Especially, a distinctive advantage emerging via this approach is the possibility of providing 1D ZnO nanostructures with specific morphology or arrangement, which are directly linked to the functional requirements of practical devices for optimal performance. This presentation will introduce a strategy for fabricating novel ZnO nanowires by seeded solution growth based on the dissolution-reprecipitation mechanism.2 The growth mode and different critical parameters on the morphological conversions of ZnO will be discussed.

We will first demonstrate the formation of single-crystalline ZnO branched nanowires (see the image) under the assistance of a polymer surfactant using this mechanism.3 This hexabranched polymorph has been long-time missing in the gallery of solution-grown ZnO nanostructures. We investigate the generality of this polymer-assisted growth process using different ZnO seed layers including continuous film, patterned dots and vertically aligned nanowire arrays. All the obtained branched nanostructures are of single crystallinity in nature which is methodologically determined by the homoepitaxial growth mode. We will also present how to use this strategy to grow very long ZnO nanowires with small diameters and 1D layered ZnO nanostructures with or without the addition of surfactants.

This dissolution-reprecipitation mechanism is fairly general for solution growth of ZnO and can be extended to design of diverse 1D ZnO nanostructures.

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References:
OPTIMIZATION OF THE GROWTH PARAMETERS FOR SiC/SiO$_2$ CORE-SHELL NWs

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Nanowires (NWs) open promising near-future perspectives for the design and fabrication of nanoscale devices. The main interests are in nanoelectronic devices (e.g. nano field-effect transistors), nano-electromechanical systems able to operate even in harsh environments, and nano-sensors exploiting the SiC NWs as biocompatible nano-probes for biological systems.

Core-shell nanowires (NW) structures of SiC/SiO$_2$ interesting for fundamental studies and technological applications: functionalized β-SiC nanowires with amorphous silicon dioxide wrapping layer have the potential to act as highly sensitive detector elements in bio-chemical field.

Many methods have been reported for the preparation of SiC NWs using a catalyst on silicon substrates: chemical vapour deposition (CVD), physical vapour deposition (PVD), direct synthesis at high-temperature by reaction of different powders such as SiO, C and oxides with carbothermal reduction.

Here we report the growth of the β-SiC/SiO$_2$ structure on Si (001) by using carbon monoxide as a precursor with different partial pressures in nitrogen as carrier gas. nickel nitrate and iron nitrate in 0.01 M ethanol solution were used as catalysts with different type and concentration of surfactants to obtain good distribution on substrate surface. Growth time and temperature were also investigated.

The morphology of nanowires was observed using a Field Emission Gun Scanning Electron Microscope (SEM FEG) while a Transmission Electron Microscopy (TEM) was used to detect the core-shell structure and their structural characterization.

The surfactant produces a better dispersion of the catalytic solution on the surface of the substrate allowing a more uniform coating of nanowires.

Smaller oxide clusters appear on the substrate surface after dewetting using more diluted catalyst solution with respect to 0.01M and this seems to affect the growth kinetics.

It has been identified a range of temperature which allows to obtain the core, out of this range the wires are not obtained or were only silica.

With a growth time of only 5 minutes no variations in the morphology were observed and the core was already present; long growth times increase the shell diameter while carbon oxide concentration in vapour phase can influence the core diameter.
The effect of van der Waals forces on the structure and energy of nanowires on solid substrates

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Self-assembly of organic nanowires is a promising approach to design electronic nanodevices [1]. Due to the delicate balance between the intermolecular and molecule–surface interactions, the accurate determination of the preferred growth direction and self-assembly of nanowires presents a great challenge for both theory and experiment [2]. Recently, we developed a method based on density-functional theory with van der Waals (vdW) interactions (PBE+vdWsurf [3]) to accurately model adsorbates on surfaces, by a synergetic linkage of the PBE+vdW method [4] for intermolecular interactions with the Lifshitz-Zaremba-Kohn theory [5] for the dielectric screening within the substrate surface.

Here, we apply the PBE+vdWsurf method to study the adsorption of benzene on transition-metal surfaces (Cu, Ag, Au, Pd, Pt, Rh, Ir): an important benchmark system for more complex interfaces. We demonstrate that the vdW forces dramatically modify the potential-energy surface and enhance the binding energy by more than 0.7 eV for all metals. The screening of the vdW energy plays a critical role in most metals, shortening the equilibrium adsorption distance by 0.25 Å for Cu, and lowering the binding energy by 0.27 eV for Rh. The calculated adsorption structure from the PBE+vdWsurf method agree to 0.1 Å with state-of-the-art experimental data, and the adsorption energies are in excellent agreement (~0.1 eV) with temperature-programmed desorption and microcalorimetry measurements [6-8]. Most notably in the case of benzene/Pt(111), the computed adsorption energies are in excellent agreement with the calorimetry data at all coverages [8], confirming the validity of our method in the description of intermolecular interactions for molecules adsorbed on surfaces.

A Resonant Raman study on wurtzite GaAs nanowires

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III-V semiconducting nanowires often crystallize in the wurtzite (WZ) structure, which is metastable in bulk material\textsuperscript{1,2}. Bulk GaAs has a zincblende (ZB) structure. Because of the lower surface energy of the WZ phase and the large surface-to-volume ratio of nanostructures, GaAs NW's can show a pure WZ, a pure ZB or a mixture of ZB and WZ phase\textsuperscript{2}. The properties, in particular, the band structure and fundamental gap $E_{\text{wz}}^0$ of WZ GaAs are controversially debated. The knowledge of the optical gap and the bandstructure of WZ GaAs allows to develop new NW-based devices in the field of optics, electronics and biological sensing\textsuperscript{3}. We perform resonant Raman experiments on ZB and WZ GaAs NWs with comparable diameters to determine the optical bandgap $E_{\text{wz}}^0$ of WZ GaAs. Our measurements show consistently $E_{\text{wz}}^0 = 1.460$ eV at room-temperature, 35 meV above the ZB gap, using TO, LO and 2LO resonance profiles. By comparing Raman resonances with incoming light polarized parallel and perpendicular to the wire c-axis we find a splitting of 65 meV between the heavy and light hole band at the Γ point of WZ GaAs.

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Recombination dynamics of free and bound excitons in GaN nanowires with different diameters grown by selective-area epitaxy on Si substrates

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Selective-area growth (SAG) of nanowires (NWs) by molecular beam epitaxy constitutes an important step towards uniform III-V NW arrays on Si[1]. Using this approach, the diameter and length distribution of self-induced GaN NWs can be reduced significantly compared to the growth on non-patterned substrates. We have recently found that certain properties such as the granular emission pattern of LEDs based on self-assembled NWs are closely related to these fluctuations in NW morphology. Therefore, a homogeneous NW size and a controlled position are desirable for future NW-based optoelectronic devices with predictable characteristics.

In this work, we study the influence of different diameters and pitches of selectively grown GaN NWs on their optical properties. The NWs grow with a very high yield in pre-patterned holes defined by electron beam lithography in a SiOₓ-mask with a very low rate of parasitic growth. The NWs have diameters and periods in the range of 70–260 nm and 0.3–1.0 µm, respectively. All investigated NW arrays have been grown side by side on the same sample to ensure similar growth conditions. Time-integrated μ-photoluminescence (μ-PL) spectra at 10 K are dominated by the donor-bound exciton transitions of unstrained GaN with a FWHM in the range of 1 meV and show basically no stacking fault-related luminescence. This indicates a very high crystal quality of SAG GaN NWs comparable with state-of-the art self-assembled GaN NW ensembles.

Furthermore, time-resolved PL is used to investigate the recombination dynamics of free and bound excitons in dependance of the average NW diameter. We compare the PL-lifetime, μ-PL spectra and integrated intensities of various NW diameter and pitch configurations and draw conclusions regarding a possible influence of coalescence due to multiple nucleation and non-radiative surface recombination in these ordered NW arrays.


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Gas phase synthesis of ZnO tetrapods for flexible and transparent UV sensor application

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Keywords: nanostructure, synthesis, tetrapod, ZnO, UV sensor.

Zinc oxide (ZnO) is a direct wide band gap (3.37 eV) semiconductor material with a large exciton binding energy (60 meV). It has gained significant attention because of the unique optical, piezoelectric and magnetic properties, as well as capability of band gap tuning (Rackauskas et al., 2009). Non-catalytically grown ZnO nanostructures can be observed in various morphologies such as nanowires, nanobelts, nanobridges and nanonails, nanoshells, tetrapods. The latter is one of the most gorgeous structures with many promising applications in solar cells, lasers, field emitters, UV and gas sensors.

Zinc oxide tetrapods (ZnO-Ts) were discovered in smoke from zinc-smelting plants and first studied in chemical vapor deposition systems. ZnO-Ts were produced in the lab scale through hydrothermal process, vapor synthesis from ZnO and Cu mixture, or directly from Zn powder, when tetrapods are collected on reactor walls or filtered at the outlet. Direct synthesis of ZnO-Ts from the metal vapor has obvious advantages of low temperature process and high yield, still the control of uniform concentration is rather difficult.

Figure 1. ZnO-T morphology at different temperatures and vapor pressures. Tetrapods shown are not in the scale.

In this work, we designed and constructed a vertical flow reactor for the controlled synthesis and collection of ZnO-Ts. In order to find favorable synthesis conditions, we varied the growth temperature and Zn vapor pressure. The overall trend of ZnO-T morphology change is summarized in Fig. 1. From our experimental data one can see that highly anisotropic structures were obtained above 650 °C (Rackauskas et al., 2012). In order to modify the band gap and transparency of ZnO-Ts, we introduced magnesium vapor during the tetrapod growth.

Applicability of the produced ZnO-T structures was examined by fabricating transparent and flexible UV sensors. Flexible transparent UV sensor (Fig. 2) was made by drying droplet of ZnO-T solution in ethanol between two transparent single-wall carbon nanotube (SWCNT) film contacts, on a polyethylene terephthalate (PET) substrate. SWCNT electrode fabrication is described elsewhere, shortly, a one step process was used, filtered SWCNTs without any post processing were transferred from a filter by pressing it onto PET substrate. To obtain high optical transparency, sample synthesized at $y_{Mg} = 2.3\%$ and SWCNT electrodes with 95% transparency were used. UV sensing experiments were made under UV intensity of 30 $\mu W/cm^2$ at the wavelength of 365 nm. Inset in Fig. 2 shows a UV sensor response to the illumination. Initial current 0.032 pA increased to 1.45 pA under the UV illumination, which is 45 fold change. Response time to 90% of current change was 0.9 s.

Figure 2. A photo of ZnO-T UV sensor. Inset shows the sensor response to excitation at 365 nm.

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(In,Ga)N nanowires for photoelectrochemical water splitting

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(In,Ga)N alloys are promising candidates for solar water splitting because their bandgap energy can be tuned from the ultraviolet to the near infrared region, thus covering the entire solar spectrum. In addition, their conduction and valence band edges can straddle the H\textsuperscript{+}/H\textsubscript{2} and O\textsubscript{2}/H\textsubscript{2}O redox potentials. However, it is difficult to grow (In,Ga)N bulk layers in high structural quality because of the lack of lattice-matched substrates. On the other hand, nanowires are known to accommodate lattice mismatch by lateral elastic relaxation without the formation of defects. Moreover, the nanowire geometry has many advantages such as enhanced light absorption, high surface area for electrochemical reactions, and improved carrier collection efficiency. So far, overall water splitting has been reported for GaN nanowire photocatalysts \cite{1}. However, GaN absorbs only the UV part of the solar spectrum, and there is still a problem with separating the evolving mixture of H\textsubscript{2} and O\textsubscript{2} gases. In this presentation, we report the growth and investigation of (In,Ga)N nanowires for water splitting using photoelectrochemical cells, which enable the separate production of H\textsubscript{2} and O\textsubscript{2}. Both n- and p-type (In,Ga)N nanowires with varying indium compositions up to 41\% were grown on n- and p-type Si(111) substrates by molecular beam epitaxy, respectively. We measured the photoelectrochemical properties by means of electrochemical mass spectrometry (EMS), which allows the online detection of volatile products like H\textsubscript{2} and O\textsubscript{2} generated from electrochemical reactions during cyclic voltammetry. Thus, we demonstrated photoelectrochemical hydrogen evolution by water splitting using p-(In,Ga)N nanowires. Details on the growth and photoelectrochemical measurements will be presented.

Single GaInP nanowire p-i-n junctions

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GaInP, P can theoretically reach a direct band gap of up to 2.2 eV at room temperature,[1] but at the corresponding composition there is no suitable substrate for thin-film growth. Axial nanowire (NW) heterostructures, however, can be grown with large lattice mismatch. Here we demonstrate doping of GaInP NWs with a bandgap close to the theoretical limit.

First, the growth of Au-seeded undoped GaInP NWs was investigated, using TMGa, TMIn and PH3 in a MOVPE system. The composition could be controlled throughout the GaInP range by tuning the TMGa and TMIn flows.[2] The radial growth was prevented by in situ use of HCl, as previously demonstrated for InP NWs.[3] The non-capped nanowires emitted room-temperature photoluminescence strongly in the energy range of 1.43 to 2.16 eV, correlated with the band gap expected from the materials composition.

Next, we investigated in situ doping of GaInP NWs using DEZn for p-doping and H2S for n-doping.[4] TEM revealed that both dopants affected the crystal structure, similar to InP NWs. Both dopants decreased the Ga fraction. Electrical measurements using NW-FETs demonstrated p- and n-type doping.

Finally, we made single NW p-i-n junctions. The devices showed typical diode behavior with an ideality factor of 2.1. Photocurrent spectroscopy indicated a bandgap of around 2.1 eV. In forward bias, the diodes showed room temperature electroluminescence at 2.18 eV (569 nm), in good agreement with photoluminescence and photocurrent spectroscopy measurements. There was also lower-energy emission, presumably due to recombination in the lower-bandgap p- and n-regions. Our results demonstrate that GaInP NWs are promising components for optoelectric devices such as light-emitting diodes and solar cells.

Density-Functional Theory with Screened van der Waals Interactions for the Modeling of Hybrid Inorganic/Organic Systems

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Molecule-surface and intermolecular interactions play an essential role in the structure and electronic properties of hybrid inorganic/organic interfaces. In particular, nonlocal van der Waals (vdW) interactions have been proved to be critical in the formation of the structure of long-range ordered phases of large aromatic molecules on metal surfaces \([\text{PRL} \ 100, \ 136103 \ (2008)]\) and the quantitative behaviour of self-assembly molecular wires on H-terminated semiconductor surfaces \([\text{PRB} \ 84, \ 241406 \ (R) \ (2011)]\). Conventional density-functional theory (DFT) and state-of-the-art theoretical methods fail to predict the behaviour of interfaces where intermolecular interactions are crucial, pointing to the need of including an accurate description of vdW interactions in state-of-the-art theoretical methods.

We propose a method (DFT+vdW\(_{\text{surf}}\)) that extends pairwise vdW corrections to the modeling of adsorbates on surfaces. By combining dispersion-corrected density-functional theory (the DFT+vdW method) \([\text{PRL} \ 102, \ 073005 \ (2009)]\) with the Lifshitz-Zaremba-Kohn adsorption theory \([\text{PRB} \ 13, \ 2270 \ (1976)]\), our method successfully includes: \(i)\) the many-body collective response of the substrate electrons and, \(ii)\) the interface polarization effects via the inclusion of semilocal hybridization.

We show that the DFT+vdW\(_{\text{surf}}\) method yields geometries in remarkable agreement (\(\approx 0.1 \text{ Å}\)) with normal incidence x-ray standing wave measurements for 3,4,9,10-perylene-tetracarboxylic acid dianhydride \((\text{C}_{24}\text{H}_{8}\text{O}_{6}, \text{PTCDA})\) on Cu(111), Ag(111), and Au(111). Similarly, we obtained accurate results in the energy and structure of additional inorganic/organic interfaces such as naphtalene and benzene on metal surfaces among other examples. The DFT+vdW\(_{\text{surf}}\) method is equally applicable to adsorbed molecules on metals, semiconductors, or insulator surfaces. It is regarded to be relevant in the accurate modeling of the structure and energetic processes found in the formation of molecular nanowires on inorganic surfaces.
Zinc oxide (ZnO) nanostructures are nowadays widely studied and also the interest in growing and characterizing nanostructured ternary M-Zn-O oxides is continuously growing. Especially, the add of trivalent atoms (e.g. Al, Ga or In) in high concentrations is important not only for band-gap engineering but also for creating nanostructured transparent conducting oxides (TCOs) for photovoltaic applications. InZnO films, for example, already demonstrated to have similar electrical conductivity and better transparency in both the visible and the IR regions compared to ITO.

Following the successful results in the self-catalysed vapour phase growth of ZnO nanostructures, starting from Zn at relatively low temperature (480°C), nanowires of the ternary In-Zn oxide have been obtained at the same temperature by seeding the growth with a molten In layer on the substrate. This approach has been followed to overcome the low vapour pressure of In, which makes co-evaporation and vapour transport impossible in this temperature range (below 500°C). Pure metallic Zn powder was used as source material and alumina as substrate for growth. Indium metal was deposited on the alumina substrate with a thickness of few microns. Source and substrate were kept one next to the other (with the substrate in downstream position) at the center of the furnace, while Ar and O₂ were used as inert transporting gas and reactive gas respectively. Experiments were carried out with different parameters in order to study their influence on the growth of InZnO nanowires.

Morphology of nanostructures were observed using Scanning Electron Microscope (SEM). It was clear that they grow selectively only where indium was present and that no growth of nanostructures was found directly on alumina substrates. The density, size and shape of the nanostructures depend on growth conditions and among the different observed morphologies sharp needle-shaped nanowires are the predominant one. The length and diameter of the InZnO nanowires ranges between 2 to 3 µm and 50 to 150 nm respectively.

The structural studies were carried out using High Resolution Transmission Electron Microscopy (HR-TEM). STEM-EDS mapping analysis confirmed the presence of In with a percentage of 0.8-2.0%. Photoluminescence studies showed that there was no evident band-edge shift respect to ZnO, while the typical defect band in the visible region is not present in the InZnO nanostructures.

The presented growth technique is, in principle, extendible to other ternary M-Zn-O oxides in which the added metal is molten in this temperature range (e.g. Al or Ga).
Abstract Nanowires 2012

Title: In-plane germanium nanowires grown by MBE on germanium substrates

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Germanium nanostructures in combination with silicon substrates are prospective elements for high-frequency circuits and infrared optoelectronics. As a preliminary approach in dealing with this topic, our actual work is focused on fundamental aspects of homoepitaxial Ge nanowire (NW) formation.

The experiments were carried out in a MBE chamber equipped with effusion cells for germanium and gold. Ge NW are grown by means of the vapor-liquid-solid (VLS) process at 450 °C using gold as liquid catalyst. (111), (001), and (011) oriented substrates were applied to study their influence on the NW growth directions. Inhomogeneous areal density of NW was the reason to take a closer look on the substrate preparation. The last surface preparation step before transferring the substrate into vacuum was modified by etching with different chemical agents. Various surface terminations can be obtained by aqueous HF, HCl, HBr, or (NH₄)₂S solutions. Comparative studies were made on (011) oriented substrates. This orientation is advantageous among all the considered surfaces for three reasons. First, the total number of <110> directions that can emerge during growth is the lowest. Second, there are merely two <110> in-plane directions that are arranged in line. Third, exclusively this orientation enables <110> directed growth perpendicular to the surface.

Independent from the substrate orientation the growth direction of Ge NW is along <110>. The wires are laterally bounded by flat {111} facets and exhibit two inclined {111} top facets resulting in a V-shaped tip pointing towards the growth direction. The side facets show only single atomic steps, no tapering has been found. Furthermore, inclined nanowires are significantly longer than their vertical counterparts, which may be due to the direct impingement of material onto the NW sidewalls. The preferential <110> directed growth is subject to current research and has been recently attributed to low supersaturation inside the gold droplet as it is the case in MBE growth. However, increasing the deposition rate did not lead to a change of the growth direction in our experiments.

Similarly to the previously described NW, in-plane NW (sometimes also called lateral NW) grow preferentially along <110> too. These in-plane nanowires consist of two inclined top-facets and four {111} side-facets that are aligned perpendicular to the substrate surface. The gold droplet that is attached to two {111} side facets is laterally pushed ahead during growth along <110> direction. If such movement is hindered by an obstacle the growth direction changes to <100>, hereby forming {111} micro-facets. This tendency can obviously be influenced by the type of applied wet-chemical pre-treatment in a way that the fraction of <110> in-plane NW increases with the stability of the respective surface termination. Change in growth direction is completely avoided by etching with (NH₄)₂S solution. However, exposing surfaces etched in such a manner to ambient air for 24 hours before transfer to vacuum, <100> in-plane NW occur again. We conclude that the loss of surface termination leads to partial oxidation. When desorbing such an inhomogeneous oxide before growth minor morphological peculiarities can arise. These may influence the movement of gold droplets.
Unconventional Roles of Metal Catalysts in Chemical-Vapor Syntheses of Nanowires

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Metal catalysts are prerequisites in many synthetic routes of one-dimensional nanocrystals and their growth patterns are largely dictated by the choice of catalytic nanoparticles. Here we report two unconventional synthetic methods, solid catalytic nanowire growth and non-catalytic spontaneous nanowire growth, in direct comparison to the conventional liquid catalytic growth. First, we present unprecedentedly low-temperature growth of Ge nanowires with the uniform diameter distribution at sub-10 nm, employing solid Cu-catalysts. Based on the parallel comparison to the growth from the eutectic liquid catalysts (Au), we attribute the attainable low-temperature growth of the uniformly thick Ge nanowires to the fact that the growth involves the Cu catalysts in solid-phases during the selective decomposition of GeH₄. Second, we present the spontaneous growth of NiSiₓ nanowires in a self-organized fashion without employing the metal catalytic nanoparticles. We discuss this spontaneous growth of NiSiₓ NWs within the frame of the nucleation kinetics in the low supersaturation limit in analogous with the earlier examples of the vapor-condensation at the low vapor pressures. Finally, we discuss the contrast in thermodynamic limit of each catalytic nanowire growth.
Au-assisted growth of Al$_x$Ga$_{1-x}$As nanowires on Si(111) by molecular beam epitaxy

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Semiconductor nanowires (NWs) are promising candidates for a future generation of nanoelectronic devices[1]. In this field, arsenide NWs have been deeply investigated, because they may pave the way for the monolithic integration of III-V materials on silicon substrates. Many groups have already reported the growth of GaAs and GaAs/Al$_x$Ga$_{1-x}$As core-shell NWs, and devices based on these materials have been successfully realized[2]. On the contrary, ternary Al$_x$Ga$_{1-x}$As NWs grown on Si(111) have been less extensively addressed and a systematic study on their fabrication is not present in the literature. However, the controlled synthesis of ternary NWs would be important for the realization of a GaAs/Al$_x$Ga$_{1-x}$As quantum well system, which is prototypical of III-V semiconductors.

Here we describe the growth by molecular beam epitaxy (MBE) and the properties of Al$_x$Ga$_{1-x}$As NWs on bare Si(111), using gold as catalyst. Au droplets were prepared in situ by depositing around 1.2 nm Au at 500°C and annealed in arsenic at the same temperature for 10 min. To promote the NW growth, the group-III element shutters were opened for a total growth time of 30 minutes. A V/III flux ratio equal to 2 was kept constant for all the experiments and the nominal Al content was varied between 0 % and 50 %. After growth the sample morphology was investigated by scanning electron microscopy (SEM) and the aluminum content was measured by energy dispersive X-Ray spectroscopy (EDX) in a SEM. Comparing with pure GaAs NWs, we found that adding an aluminum flux deeply changed the sample morphology, causing a strong reduction in the NW number density. For the highest Al composition ($x = 0.5$) no NWs were obtained, indicating that the presence of Al atoms made the NW growth more difficult. We believe this effect to be caused by an increase of the eutectic temperature of the Au-Ga catalyst particle, when also Al is present in the droplet. The single NW geometrical features were also altered, as pure GaAs measured around 3 μm in length and possessed a diameter of around 50 nm, while Al$_x$Ga$_{1-x}$As NWs became significantly shorter and thinner, as the Al content was increased. The NW composition, measured by EDX, was found to be in fairly good agreement with the incoming beam fluxes, being around 80% of the nominal values. Along a single NW the composition was constant, suggesting a homogeneous incorporation of Al throughout the growth. We also fabricated GaAs/Al$_x$Ga$_{1-x}$As NW heterostructures and we found that GaAs tended to grow axially on the top of Al$_x$Ga$_{1-x}$As segments, while Al$_x$Ga$_{1-x}$As mainly formed a core-shell structure around GaAs bases.

We believe that our results could lead to the realization of GaAs quantum dots embedded in Al$_x$Ga$_{1-x}$As NWs for single photon emission and for transport measurements based on surface acoustic waves, as we recently demonstrated in In$_x$Ga$_{1-x}$As/GaAs NW heterostructures[3].

REFERENCES

Growth of GaAs-Fe$_3$Si core-shell nanowires with an out-of-plane magnetization by molecular beam epitaxy

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The shape anisotropy of thin magnetic films causes difficulties for the fabrication of high quality spintronic devices. A very promising way to overcome these difficulties is the use of the unique geometry of nanowires. The high aspect ratio and the perpendicular alignment of nanowires to the substrate allow for an out-of-plane magnetization in the magnetic thin film for ferromagnet-semiconductor core-shell nanowire heterostructures.

In this work, we investigate the growth of GaAs-Fe$_3$Si core-shell nanowires by molecular beam epitaxy (MBE). In a first growth step, GaAs nanowires were fabricated on a clean Si(111) substrate covered with a thin Si-oxide layer in the III-V chamber of the MBE system. The GaAs nanowire cores were grown at a substrate temperature of 580 °C, a V/III-flux-ratio of 1.0 and an equivalent two-dimensional GaAs growth rate of 100 nm/h. Throughout the present work, these growth parameters were not varied.

After transferring the samples under ultra high vacuum conditions to the metal growth chamber of the same MBE system, a second and final growth step was carried out. Now, the GaAs nanowires were coated with a thin Fe$_3$Si layer grown at different substrate temperatures between 100 °C and 350 °C. The same fluxes of Fe and Si were used as those needed to obtain smooth stoichiometric planar Fe$_3$Si layers.

Scanning electron microscopy (SEM) shows nanowires with smooth side walls for growth temperatures of the Fe$_3$Si shell below 250 °C, whereas nanowires with significantly rough side walls are obtained for higher growth temperatures. As it is known from planar Fe$_3$Si layers on GaAs substrates, all engaged elements very eagerly tend to react with each other at high growth temperatures resulting in the formation of precipitates at the interface and rough surfaces. Thus, SEM already indicates that there is not any more a clear-cut core-shell structure present in the nanowires for Fe$_3$Si growth temperatures above 250 °C.

The magnetic texture of the Fe$_3$Si shell was investigated by magnetic force microscopy (MFM) on nanowires that were transferred to a clean Si substrate. With the MFM method, magnetic stray fields perpendicular to the substrate plane are measured by a phase shift. MFM images obtained from nanowires with a shell growth temperature of 100 °C show a clear bright and dark contrast (magnetic stray fields coming out and pointing into the substrate plane) on the ends of every nanowire which indicates that the magnetic moment of the Fe$_3$Si shell is oriented along the nanowire. Thus, an out-of-plane orientation of the magnetization of the thin Fe$_3$Si layer is present in these GaAs-Fe$_3$Si core-shell nanowire heterostructures.

In contrast, no stray field was measured for core-shell nanowires with Fe$_3$Si growth temperatures above 100 °C. As the above mentioned interdiffusion of Fe and Ga at high temperatures destroys the magnetic properties of Fe$_3$Si, the MFM investigation reveals a more precise value for the maximum shell growth temperature of about 100 °C.

In summary, this work demonstrates that the growth of GaAs-Fe$_3$Si core-shell nanowires with the desired out-of-plane magnetization for high quality spintronic applications is successful by a simple two-step MBE growth approach, whereas it turned out that the temperature of the Fe$_3$Si shell growth should not be higher than 100 °C.
Magnetron Sputter Epitaxy of Core-Shell AlInN Nanorods and Nanohelixes

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Core-shell nanorods and related nanomaterials have attracted much attention because such nanorods have large junction areas surrounding the rod core, which can significantly enhance the quantum efficiency of devices. Development of Al$_{1-x}$In$_x$N core-shell nanorods is potentially a great benefit for fabricating semiconductor nanoscale optoelectronics, utilizing a broad-bandgap range of 0.7-6.2 eV [1]. Moreover, chiral metamaterials, often fabricated by lithography and glancing angle deposition, have received much attention thanks their great potential for applications such as highly sensitive mechanical resonantors, broadband circular polarizer, etc. Here we demonstrate how a controlled curved-lattice epitaxial growth [2] (CLEG) of AlInN nanorods [3] can be exploited as a new route for tailoring helical nano-metamaterials.

Well separated AlInN nanorods, exhibiting clear hexagonal cross sections were nucleated on the Ti$_{0.21}$Zr$_{0.79}$N seed layers, which were epitaxially grown in-situ onto sapphire substrates by ultrahigh-vacuum (UHV) magnetron sputter epitaxy (MSE). By temporal control of the azimuthal orientation of the deposition fluxes, right-handed and left-handed AlInN nanohelixes, comprising 5 turns at 200 nm pitch, were obtained. Both nanorods and nanohelixes were grown rather homogenously in both length and diameter. The crystal structure of the nanorods determined by X-ray diffraction and selected-area electron diffraction showed a wurtzite structure with preferential $c$-axis orientation along the growth direction. Core-shell straight nanorod and curved nanorod structures were observed with a higher In (Al) concentration in the cores (shells) by mass-contrast (scanning) transmission electron microscopy [(S)TEM] in combination with energy dispersive X-ray spectroscopy (EDX). Curved lattices, showing a centered symmetrical curve in the nanorod and an asymmetrical curve in the nanohelixes, were clearly resolved by high-resolution TEM. Low-loss electron energy loss spectroscopy (LLEELS) [5] in a nano-probe line scan across a nanohelix showed an asymmetrical composition distribution confirming the CLEG. The handedness of reflected circular polarized light is governed by the helix chirality, as determined by spectroscopic Müller-matrix ellipsometry (SE). The formation of core-shell structure may be associated with a spinodal decomposition of the Al$_{1-x}$In$_x$N alloy due to the wide-range immiscibility of AlN and InN.[4] An uneven mass contrast observed at the interface reveals that regions of different composition were formed at the initial nucleation process. By tracing the initial growth of nanorods, we find that the nanorods were grown at In-rich domains and there initiated the formation of core-shell nanorods with In-rich cores.

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References:
GaN Nanostructures

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Abstract:

Recent approaches to mitigate deleterious effect of lattice mismatch between III-nitrides and substrates such as Al₂O₃ (0001) and Si (111), (100), include the use of buffer layers, Lateral over layer growth and nanostructure formation. In our recent work in this direction, where we form GaN nanostructures on c-plane sapphire, Si(001) and Si (111) surfaces, by choosing high nitrogen rich growth by Molecular Beam Epitaxy. The conditions provide highly crystalline wurzite GaN nanostructure formation of different morphologies depending on the kinetics of growth. We also use substrate temperature (450°C to 880°C), gallium flux and nitrogen flow rate (2 to 8 sccm) control to tune GaN properties. We form wedge shaped GaN nanowalls at low temperatures, and dislocation ridden but faceted 2D-films at high temperatures. In a critical growth parametric window, we form hexagonal shaped, self organized epitaxial GaN nanorods. The single crystal nanowalls and columns show high structural, optical and electrical properties. We show that the misfit-dislocations (edge and screw) formed at this lattice mismatched interface, induce the growth of self-assembled nanowall and nanorod formation, respectively. The nanostructures show broad band edge emission but no defect emission.

The nanowall network formed at the edge dislocations promotes 1-D nanocolumn formations in the void between walls in a Frank type spiral growth of m-faceted GaN. These highly dense m-faceted nanocolumns are hexagonally shaped wurzite, c-oriented structures and are defect controlled. We show that depending on the kinetics of the growth, we can control the twist parameters of the Burger’s vector leading to compact and defected rods, Frank-Read growth and nanotubes formation. By FFT image analysis we compute nanocolumn size, shape density and supra-structural arrangement, and used XRD and PL to their structural and optical emission properties. We propose a model that shows our speculated growth mechanisms for the shapes of nano-column formation.

References:

Coalescence of In$_x$Ga$_{1-x}$N nanorods in molecular beam epitaxy.

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In order to effectively convert solar energy into electric power or any other form of usable energy we need to develop novel semiconductor materials, which will absorb photons over the full solar energy spectrum. In$_x$Ga$_{1-x}$N alloys have a direct band gap of from 0.7 to 3.4 eV, which covers most of the visible spectrum. These alloys are now actively studied worldwide for solar cell applications. However, the material quality of the In$_x$Ga$_{1-x}$N alloys with intermediate composition remains poor. The growth of nanorods promises a possible solution to the In$_x$Ga$_{1-x}$N material problems.

The growth of In$_x$Ga$_{1-x}$N nanorods by MBE has been investigated for over a decade. It is now well-established that 3-D growth leading to nanorods can be achieved over the full composition range by a low III:N ratio (so called N-rich conditions). The growth of discrete nanorods, which have been found to be mostly free of threading defects, is a catalyst-free process, thus promising good control over material quality and doping. As well as high structural perfection, there is good evidence that MBE-grown nitride nanorods are of high optical and optoelectronic quality.

Together with the other groups we have demonstrated the growth of GaN nanorods by MBE on (0001) sapphire surfaces under N-rich conditions. We have also shown that, by changing from N-rich to Ga-rich conditions, the growth mode can be changed from vertical to lateral, leading to growth of a continuous overlayer. As a result of growing the nanorod layer, many of the threading defects present in the intermediate layer are eliminated, leading to coalesced GaN overlayers with average threading defect densities down to $10^8$ cm$^{-2}$, up to two orders of magnitude lower than in continuous epilayers.

Our current studies aim to establish In$_x$Ga$_{1-x}$N as a basis for high efficiency solar cells, by using nanorod geometry to overcome materials limitations associated with high densities of threading defects and layer strains that affect continuous In$_x$Ga$_{1-x}$N epilayers. We have studied MBE growth of In$_x$Ga$_{1-x}$N on Si (111) substrates. We have established the MBE growth conditions required for the growth of InN and In$_x$Ga$_{1-x}$N nanorods. We have investigated the MBE growth conditions required for efficient coalescence of In$_x$Ga$_{1-x}$N nanorods over a wide composition range. In the current presentation we will discuss differences and similarities in the coalescence processes of GaN, InN and In$_x$Ga$_{1-x}$N nanorods by plasma-assisted MBE.
Fabrication of GaN-based nanorods using nanosphere lithography and RIE for nanodevice applications

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Abstract
Recently there has been an upsurge of interest in making GaN-based vertically standing nanorods and nanowires using masking and etching techniques. For InGaN/GaN multiple quantum well-based LEDs, the nanopillar structures may relieve strain and accommodate the large lattice mismatch at the interface. This leads to the increase of radiative recombination efficiency and thus to improved LED performance. Moreover, using these nanorods and nanowires created by the top-down approach, one can fabricate many novel nanodevices such as nano-PN junctions, nano-photovoltaic devices and nano-photodetectors based on GaN. In this work we will report about the fabrication of GaN-based nanorods using a combination of nanosphere lithography (NSL) and reactive ion etching (RIE).

Using NSL involving silica nanospheres, we defined the mask on c-plane GaN epilayer and then fabricated an array of GaN nanorods using RIE with chlorine based chemistry. The diameter and spacing of the nanorods can precisely be controlled by choosing spheres of appropriate diameter and subsequently shrinking them to the desired size. For the example of about 600 nm wide and 1000 nm long nanorods, an interesting feature was, that although we used circular masks, hexagonal faceting turned out. Various characterization methods such as X-ray diffraction, μ-Raman and cathodoluminescence (CL) have been performed.

We propose that GaN-nanorod-based LEDs could benefit from relieved strain resulting in reduction of the quantum confined Stark effect eventually giving higher light output. By carefully choosing the geometrical parameters, the nanorod diameter and spacing, a strongly enhanced directed emission of photons parallel to the rods’ long axis might be possible due to a photonic band gap for the lateral directions.
Contactless monitoring of doping with spatial resolution along single GaAs nanowires.

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Local probing of doping level along the axis of a single semiconductor nanowire (NW) opens an opportunity to characterize engineered NWs, such as axial hetero-junctions and p-n- junctions, and to compare the effective doping of NWs grown simultaneously on the same substrate. In the absence of a Fermi-level pinning, the doping level in semiconductors is reflected by the Fermi Energy (FE) position within the semiconductor bandgap.

Si in GaAs is an amphoteric impurity, behaving as a donor when incorporated in Ga sites, and as an acceptor if incorporated in As sites. The available growth models associate p-doping to vapor-liquid-solid growth and n-doping to vapor-solid growth on the NW walls [1]. The dependence of Si incorporation on the growth conditions has allowed engineering of inhomogeneous doped NWs (e.g. radial p-i-n junctions with photovoltaic properties [2]).

We studied the local effective doping in individual MBE grown, Si-doped, self-catalyzed GaAs NWs by means of scanning photoemission spectroscopy (SPEM). This technique allows the acquisition of photoemission (PE) spectra at selected points of the sample using a micro-probe of around 100 nm. The changes in Binding Energy (BE) position of the PE spectra taken along the NWs can be used as fingerprints for the variations in the FE position within the bandgap. In the present study information about variations in the local effective doping of the GaAs NWs was obtained from the Ga 3d core level spectra, measured along several individual NWs from two samples.

Our results confirm that the Si doped, self-catalyzed NWs are typically p-type, where different doping levels can be obtained by varying the Si flux. Nevertheless, NWs belonging to the same sample are not always homogeneously doped and in some cases they can even show different polarities (p or n). We have observed strong correlation between the morphology of the NWs and their doping level; key parameters, such as the NW orientation, the diameter and the presence of catalyst particle on top are found to play important role in the definition of the NW electronic properties. The analysis of the results allows to make some considerations about the mechanism of Si incorporation during the growth, which likely depends on the local effective As/Ga ratio.

(Left) Three representative Ga 3d spectra of NWs from two samples, measured in the indicated points (Middle) SEM pictures of the NWs. (Right) Ga 3d BE positions for different NWs in the same two samples. Enclosed in the same circle are the NWs of the same morphology.

Dopant distribution measurements of ex situ doped silicon nanowires

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Semiconductor nanowires show tremendous promise in the areas of advanced optoelectronic, electronic, and mechanical devices. For such applications to become commercially viable, large-scale integration of nanowires into devices is required, and uniformity in electrical properties is of critical importance. In particular, it is desirable to maintain controlled and uniform dopant distribution in the growth process. The conventional doping mechanism, where dopants are introduced \textit{in situ} during growth, results in both axial and radial inhomogeneous doping profiles as a result of the combined nanowire synthesis and doping process. The conventional approach of nanowire synthesis and \textit{in-situ} doping also suffer from limited ability to form well defined and abrupt chemical composition gradient (junctions) required for advanced applications.

In this presentation, we describe the use and extension of the recently described monolayer doping method\textsuperscript{1} utilizing the precision of electron beam lithography as well as the selectivity and controllability of chemical monolayer formation to produce tailor-made doping profiles in VLS grown silicon nanowires.

We apply Kelvin Probe Force Microscopy and current-voltage measurements together with TCAD simulation, to measure the radial and axial distribution of \textit{electrically active} dopants in \textit{ex situ} doped wires. Our measurements show phosphorus concentrations raging from intrinsic to more than $10^{18}cm^{-3}$, for different fabrication recipes. The results also show some significant contribution of surface states to the electrical characteristics of the nanowires.

\textsuperscript{1}J. Ho \textit{et al.}, \textit{Nature Materials} 7, 62-67 (2008)