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DFG

International Workshop
on
Semiconducting
Nanoparticles

Duisburg, Germany

December 7th & 8th 2006

Venue: Tectrum Tower
Bismarckstr. 142, Duisburg



Program

date	time	topic	speaker	title	chair
Thursday, 7.12.					
	09:00	Welcome	Prorektor Eckart Hasselbrink	<i>Welcome</i>	Winterer
	09:15	invited lecture	Kevin Hennessy (ETH Zürich)	<i>Quantum nature of a single quantum dot coupled to a photonic nanocavity</i>	Wolf
	10:00	coffee break / poster session			
	10:30	invited lecture	Cedrik Meier (U Duisburg-Essen)	<i>Thermal switching between bright and dark excitons in silicon nanoparticles</i>	Wolf
	11:15	invited lecture	Marius Grundmann (U Leipzig)	<i>Structural and optical properties of linear ZnO nanostructures</i>	Wolf
	12:00	lunch break			
	13:00	invited lecture	Jose Ulloa (TU Eindhoven)	<i>Quantum dot formation studied at the atomic scale by cross-sectional scanning tunneling microscopy</i>	Lorke
	13:45	coffee break / poster session			
	14:45	invited lecture	Daniel Haegele (U Bochum)	<i>Spin noise spectroscopy in semiconductors</i>	Lorke
	15:30	invited lecture	Andreas Wieck (U Bochum)	<i>InAs Quantum dots and their electronic structure</i>	Lorke
	16:15	coffee break / poster session			
	16:45	invited lecture	Victor Klimov (LANL)	<i>Seven Excitons at a Cost of One Using Semiconductor Nanocrystals</i>	Bacher
	17:30	invited lecture	Carola Kryschi (U Erlangen-Nürnberg)	<i>Femtosecond spectroscopy study of the exciton relaxation dynamics in silicon quantum dots</i>	Bacher
	18:15	informal labtours to be arranged individually			

date	time	topic	speaker	title	chair
Friday, 8.12.					
	09:00	invited lecture	Thomas Ihn (ETH Zürich)	<i>Measuring current and noise by Wiggers counting single electrons</i>	
	09:45	coffee break / poster session			
	10:15	invited lecture	Margit Zacharias (U. Paderborn)	<i>Si Nanocrystals: New ways for an old material</i>	Wiggers
	11:00	invited lecture	Peter Klar (U Giessen)	<i>Mechanisms of energy and excitation transfer in Mn-doped II-VI nanostructures</i>	Wiggers
	11:45	lunch break			
	12:45	invited lecture	Hisazumi Akai (U Osaka)	<i>Large MR caused by an anti-phase boundary in half-metallic antiferromagnetic semiconductors</i>	Entel
	13:30	coffee break / poster session			
	14:30	invited lecture	Myrtil Kahn (CNRS Toulouse)	<i>Optical Properties of Zinc Oxide Nanoparticles</i>	Entel
	15:15	invited lecture	Andreas Waag (TU Braunschweig)		Entel
	16:00	coffee break / poster session			
	16:30	invited lecture	Masako Ogura (U Osaka)	<i>KKR CPA calculations and Neel temperatures of half-metallic antiferromagnetic semiconductors</i>	Winterer
	17:15	invited lecture	Karsten Albe (TU Darmstadt)	<i>Thermodynamics and Kinetics of Intrinsic Point Defects in ZnO</i>	Winterer
	18:00	invited lecture	Daniel Gamelin (U Washington)	<i>Dopant-Carrier Exchange Interactions in Colloidal Doped Semiconductor Nanocrystals</i>	Winterer
	18:45	transfer to restaurant			
	19:00	dinner at Schifferbörse Duisburg (open end)			

Oral / Invited Presentations

Quantum nature of a single quantum dot coupled to a photonic nanocavity

K. Hennessy

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Coupling semiconductor quantum dots to photonic cavities is a promising route for realizing quantum information tasks in the solid state. However, validating the efficacy of quantum dots for these applications requires confirmation of the quantum nature of the quantum-dot-cavity system. In this work we find a confirmation by observing quantum correlations in photoluminescence from a photonic crystal nanocavity interacting with one, and only one, quantum dot precisely aligned at the cavity center. The high quality factor and very small volume of the nanocavity allows us to realize the regime of strong coupling between the quantum dot and cavity mode. In this regime, we find that the photon stream from the cavity is anti-bunched, indicative of coupling between two discrete quantum states. These results show that quantum dots, although comprised of thousands of atoms, can be considered "artificial atoms" for quantum information applications.

Thermal switching between bright and dark excitons in silicon nanoparticles

C. Meier

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Silicon nanoparticles are attractive candidates for photovoltaic and optoelectronics applications, as they allow to combine the advantages of a semiconducting material with the ease of handling of dispersed particles. Moreover, the availability of silicon and the scalability of heterogenous gas-phase synthesis routes allows for potential low-cost devices.

However, to understand the intrinsic optical properties of this material system, it is necessary to perform detailed spectroscopic studies. Especially the excitonic properties of this indirect bandgap semiconductor nanoparticle material are extremely interesting.

The excitonic fine structure of silicon nanoparticles is investigated by time-resolved and magnetic-field dependent photoluminescence. The results are analyzed using the common model of an excitonic fine structure consisting of a bright and a dark exciton. We find that the radiative recombination rates of both excitons differ only by a factor of eight. This makes it possible to thermally switch the nature of the recombination from bright-exciton-like to dark-exciton-like. The validity of our model is further supported by magnetic-field dependent measurements, in which effects of state mixing are observed.

We will show that silicon nanoparticles offer a unique possibility to directly assess dark exciton photoluminescence.

Structural and optical properties of linear ZnO nanostructures

M. Grundmann

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ZnO nanorods have been grown with pulsed laser deposition on various substrates. The wire direction is along the c-axis. With the intent to use such structures as nano light-emitters the optical properties have been optimized and investigated in detail. The optical modes are dominantly whispering gallery modes in the hexagonal cross-section of the wire. A discussion of and results on low-threshold, optically pumped lasing in ZnO wires will be presented.

Quantum dot formation studied at the atomic scale by cross-sectional scanning tunneling microscopy

J. M.Ulloa and P. M.Koenraad

COBRA-Department of Applied Physics, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

Cross-sectional scanning-tunneling microscopy (X-STM) is used for an atomic scale analysis of the formation of self-assembled quantum dots (QD) under a range of growth conditions and various material combinations. This technique allows determining the size, shape and composition of the buried nanostructures. This is of crucial importance, because QDs have to be capped for any application, and the capping process can drastically modify the QD structure. The composition of the strained QDs was determined by fitting the measured outward relaxation of the cleaved surface to the one calculated by a three-dimensional finite element model based on elasticity theory. The composition of the wetting layer and the capping layer was also determined in the same way, and the effect of the segregation was included in the calculation. This result was compared to the one obtained directly by counting the individual In, As or Sb atoms as a function of the distance along the growth direction. X-STM measurements show that the size and composition profile of InAs self-assembled quantum dots depend strongly on the substrate on which the dots are formed but also on the capping material and procedure. The role of critical issues like dot decomposition, intermixing, As/P exchange and phase separation in the capping layer will be analyzed at the atomic scale.

Spin noise spectroscopy in semiconductors

D. Hägele

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The characterization of nanoscopic and mesoscopic solid state quantum systems is a fundamental precondition for future applications in quantum information processing.

Optical spin noise spectroscopy, which for the first time was successfully demonstrated in semiconductors by our group, offers new possibilities for the investigation of such systems. In contrast to traditional optical excitation spectroscopy, noise spectroscopy does not require an external perturbation of the system, but yields information by detecting fluctuations of the quantum system in thermal equilibrium [1]. Using spin noise spectroscopy, we were able to find the longest spin lifetimes of donor bound electrons in bulk GaAs ever measured. We estimate that the method is suitable also for observing spin dynamics of a single electron in a quantum dot.

[1] M. Oestreich, M. Römer, R. J. Haug, and D. Hägele, Phys. Rev. Lett. 95, 216603 (2005).

InAs Quantum dots and their electronic structure

A. Wieck

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In strained InAs layers, grown on GaAs by molecular beam epitaxy, quantum dots (QDs) are formed in a self-organizing manner. This so-called Stranski-Krastanov growth mode leads to disc-shaped InAs quantum dots with typical diameters of a few 10nm and a few nm height. These dots are distributed randomly in one layer with typical densities of 10^{10} - 10^{11} cm⁻². By focussed ion beam decoration, we achieve preferential growth at intentional sites of single quantum dots. In covering these dots of small bandgap with GaAs of a larger bandgap, a DC voltage applied to a metallic Schottky-gate on the surface tunes the carrier occupation of the dots. By a small AC voltage modulation and charge current recording, the capacitance of a quantum dot ensemble (typ. 10^6 QDs) is measured at low temperatures. If additional carriers enter in the dots, the effective dielectric width of the capacitor gate-QDs is decreased, leading to an increase of its capacitance. The size homogeneity of our QDs is so high that every additional charge carrier per QD leads to a well resolved capacitance peak. In this way, the electron and hole occupancy of the QDs are spectroscopically investigated.

Seven Excitons at a Cost of One Using Semiconductor Nanocrystals

V. Klimov

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A usual assumption is that absorption of a single photon by a material produces a single electron-hole pair (exciton), while the photon energy in excess of the energy gap is dissipated as heat. In 2004, we reported for the first time that nanocrystals of PbSe could respond to absorption of a single photon by producing two or more excitons with the unity probability (Phys. Rev. Lett. 92, 186601, 2004). More recently, we observed generation of up to seven excitons per absorbed photon (Nano Lett. 6, 424, 2006), which corresponds to the ultimate limit allowed by energy conservation for the excitation energy used in these measurements. This presentation discusses such aspects of multiexciton generation in nanocrystals as characteristic time scales of this process, statistics of photogenerated multiexciton populations, the limits on photon-to-exciton conversion efficiencies, and implications of multiexciton generation in photovoltaics and photocatalysis.

Femtosecond Spectroscopy Study of the Exciton Relaxation Dynamics in Silicon Quantum Dots

C. Kryschi

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Silicon nanoparticles (SiNP) with sizes smaller than the Wannier exciton radius have been observed to exhibit visible photoluminescence with quantum yields up to 37% which is understood to arise from quantum confined excitonic levels. In addition to the quantum-confined exciton luminescence (i.e. core luminescence) radiative deactivation also may take place from localized states in the SiNP surface which are assigned to defects in the native oxide shell (i.e. surface-state luminescence). The intensity of the core luminescence is observed to be highly sensitive to various polar compounds physisorbed at the surface. Using stationary fluorescence and femtosecond-resolved transient absorption spectroscopy we have studied the relaxation dynamics of excited surface states and confined excitons of distinctly surface-treated SiNP with mean sizes of 4 nm.

Measuring current and noise by counting single electrons

T. Ihn, S. Gustavsson, R. Leturcq, R. Schleser, T. Müller, K. Ensslin

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Fluctuations of the electrical current in time are called noise. The measurement of shot noise provides information beyond that contained in the average current. In semiconductor quantum dots, measurements of the shot noise with conventional techniques are difficult due to the very low current levels. We will present measurements of the current fluctuations in a quantum dot performed by counting electrons one by one using a quantum point contact as a charge detector. In this way we are able to measure currents down to the sub attoampere regime, as well as shot noise levels that are 5-6 orders of magnitude lower than in conventional experimental setups. In addition, these measurements give access to the full distribution of the current fluctuations, known as full counting statistics.

We find a reduction of the shot noise below its classical value if the dot is symmetrically coupled to its leads. This reduction can be understood as a direct consequence of the Coulomb blockade effect leading to increased electronic correlations. The third moment of the noise shows a similar reduction.

While these measurements are so far limited to low currents, and therefore to long time scales, we will discuss prospects of this measurement technique to access even smaller time scales down to nanoseconds.

Si Nanocrystals: New ways for an old material

M. Zacharias

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First experimental results more than one decade ago demonstrating the visible room temperature luminescence of Si nanocrystals in implanted SiO₂ or porous Si triggered the strong interest in the fabrication of Si nanocrystals and their properties. Basic fundamental questions concerning quantum confinement effects in indirect semiconductors, potential applications such as light emission from electrically excited Si nanocrystals, energy transfer to Er³⁺ ions, and non volatile Si NC based memories also stimulated the broad interest in this material system. For clarifying the origin of the observed luminescence signal as well as for applications, tight control over the size of the nanocrystals is essential. The talk will give an overview about ways for size controlled Si nanocrystals. Basic properties as well as different applications including memory applications will be discussed in details.

Mechanisms of energy and excitation transfer in Mn-doped II-VI nanostructures

P. J. Klar

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In wide-gap II-VI semiconductors doped with Mn such as ZnS:Mn or ZnSe:Mn the Mn^{2+} ions are incorporated on cation sites. The tetrahedral crystal field shifts and splits the 3d states in energy compared to the free Mn^{2+} ion. The 6S ground state of the free Mn^{2+} ion (which according to Hund's rule has all five electron spins aligned parallel giving rise to a total spin $S = 5/2$) is shifted down in energy by the crystal field and is referred to as 6A_1 . The first excited quartet state 4G of the free ion is split into four states which with increasing energy are labeled according to the irreducible representation of T_d symmetry by 4T_1 , 4T_2 , 4A_1 and 4E (all having a total spin of $S = 3/2$). The transitions between the excited states ($S = 3/2$) and the ground state ($S = 5/2$) are spin forbidden. Nevertheless, the luminescence of wide-gap II-VI materials the so called yellow emission band due to the 4T_1 to 6A_1 transition which is observed in addition to, or even instead of the excitonic emission. For smallest Mn concentrations and dominantly isolated Mn-ion centres the decay time of the ${}^4T_1 \rightarrow {}^6A_1$ transition was found to be about 1.8 ms and reduces into the μs range with increasing Mn concentration, mainly caused by the so called "concentration quenching". On the one hand, this manifests that an energy transfer from the band states into the Mn system takes place and, on the other hand, it demonstrates that the excitation also travels within the Mn system. The underlying mechanisms of energy transfer are also important for other systems like Er doped Si or SiO_2 where dipole forbidden internal transitions can be effectively excited via band states. It will be discussed how time-resolved PL studies on II-Mn-VI quantum disc and quantum dot structures can reveal more information about the transfer processes taking place in these systems.

Large MR caused by an anti-phase boundary in half-metallic antiferromagnetic semiconductors

H. Akai and M. Ogura

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Due to strong electron scattering caused by the existence of anti-phase boundaries in the half-metallic antiferromagnetic semiconductors, these materials might show a significant magnetoresistance. The quantitative analysis of this phenomena is discussed on the basis of first-principles calculation using KKR-CPA-LDA combined with the Kubo-Greenwood formula.

Optical Properties of Zinc Oxide Nanoparticles

M. Kahn and B. Chaudret

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Recently, we developed an organometallic approach for the preparation of ZnO nanoparticles of controlled size and shape [1-4]. This method consists of the exothermic hydrolysis reaction of the organometallic precursor, $[\text{Zn}(\text{c-C}_6\text{H}_{11})_2]$, toward water in order to access to well crystalline ZnO nanoparticles. The kinetic of the reaction and therefore the size and shape of these particles are well controlled by the organic ligands introduced in the reaction medium.

The emission properties of nanocrystalline ZnO particles prepared following this method have been investigated.[5] Spherical particles and nanorods have been studied. The influence of the shape of the particles and of the ligands used for their elaboration on the luminescence properties in the visible domain will be presented. Interestingly, two different emissions are observed at 440 nm (≈ 2.82 eV) and at 580 nm (≈ 2.14 eV) that are associated with the presence of surface defects on the particles. The origin of such emissions will be discussed.

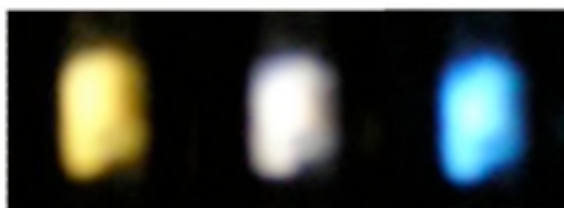


Figure 1: Emission colors of ZnO nanoparticles as a function of the excitation wavelength.

More recently, the effects of the addition of organolithium precursor during the synthesis of ZnO nanoparticles have been studied.[6] The particular role of lithium ions for the control of the particles growth and its consequences for the photoluminescence properties will be presented (Figure 2).

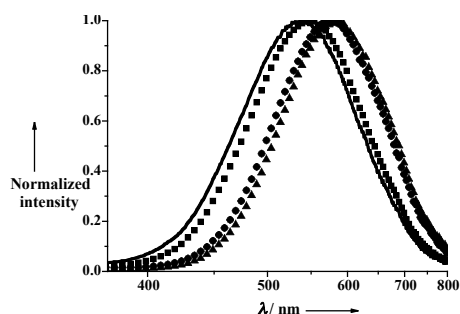


Figure 2: Normalized emission spectra of ZnO:Li nanoparticles for a Li/Zn molar ratio of 0.01, 0.02, 0.05 and 0.1. λ excitation = 320 nm.

- [1] M. L. Kahn, M. Monge, A. Maisonnat, B. Chaudret, in French Patent CNRS, Fr 03-042825, 2003.
- [2] M. Monge, M. L. Kahn, A. Maisonnat, B. Chaudret, *Angew. Chem. Int. Ed.* 2003, 42, 5321.
- [3] M. L. Kahn, M. Monge, V. Collière, F. Senocq, A. Maisonnat, B. Chaudret, *Adv. Funct. Mater.* 2005, 15, 458.
- [4] M. L. Kahn, M. Monge, E. Snoeck, A. Maisonnat, B. Chaudret, *Small* 2005, 1, 221.
- [5] M. L. Kahn, T. Cardinal, O. Bousquet, M. Monge, V. Jubera, B. Chaudret, *Chem. Phys. Chem.* 2006, 7, 2392.
- [6] A. Glaria, M. L. Kahn, T. Cardinal, F. Senocq, V. Jubera, B. Chaudret, Submitted.

Oxide Eletronics : Opto - Magneto – Nano

A. Waag

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ZnO is a semiconductor material, which exhibits a bandgap of 3.37 eV and a very large exciton binding energy of 60 meV. This makes the material interesting for optoelectronic applications in the blue and ultraviolet spectral range. In contrast to GaN, ZnO can be grown even at very low temperatures of below 100 °C. In addition, magnetic ions like Co, V or Mn can be incorporated into ZnO isoelectronically, in order to form a transparent ferromagnetic semiconductor with potential application in spinelectronics. Another interesting aspect of ZnO is that a variety of nanostructures can be grown showing unique physical properties and potential applications in nanoscale devices.

An overview of the state of the art concerning the development of a ZnO based technology for opto- mangeto- and nanoeletcronics will be given.

KKR CPA calculations and Neel temperatures of half-metallic antiferromagnetic semiconductors

M. Ogura

Department of Physics, Osaka University, 1-1 Machikaneyama, Toyonaka, 560-0043 Osaka, Japan

Half-metallic antiferromagnets are a new type of spintronics materials that are half-metallic and yet carry no magnetization. Such materials, however, have not been yet proven to exist experimentally. Recently, many diluted ferromagnetic semiconductors (DMSs) are designed theoretically. In these DMSs, local magnetic states are stabilized for the impurity bands formed in semiconductor gaps. In a similar way, half metallic antiferromagnetic DMSs may be realized for the impurity bands in the gaps. In the present study, we investigate the electronic and magnetic structure of the half-metallic antiferromagnetic DMSs on the basis of first principles electronic structure calculation. Furthermore, the magnetic transition temperature of these systems is calculated by use of the cluster-type approximation proposed by Mano many years ago. The exchange coupling constants used in the cluster approximation are obtained by the method of Liechtenstein.

We have calculated the electronic structure of several types of DMSs, II-VI, III-V, chalcopyrite and so on using the KKR-CPA-LDA method. To realize the antiferromagnetism, we have to introduce at least two kinds of transition metals into them. In DMSs containing two kinds of magnetic ions, one being more than half-filling and the other less than half-filling, the local magnetic moments of two ions can couple anti-parallel to each other due to the double-exchange interaction. Such antiferromagnetic states often turn out to be more stable than the ferromagnetic ones. As a result, many combinations show half-metallic antiferromagnetism. The electronic structures of these half-metallic antiferromagnetic DMSs are discussed.

Thermodynamics and Kinetics of Intrinsic Point Defects in ZnO

K. Albe

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Understanding the thermodynamics and kinetics of intrinsic point defects in ZnO is of key importance for controlling the properties and processing conditions of nanodevices.

Unfortunately, there exist so far not even a concise picture about intrinsic point defects in bulk ZnO.

We have therefore carried out density-functional theory calculations in order to obtain a more profound understanding of defect populations and self-diffusion coefficients.

It is shown that the oxygen interstitial in a dumbbell-like configuration is the key for understanding oxygen self-diffusion. The migration enthalpies are strongly dependent on the charge state ranging between 0.3 and 1.0 eV. The barriers for vacancy migration on the other hand are only weakly dependent on the charge state and somewhat higher. In case of zinc, interstitials are moving via a second neighbor interstitialcy mechanism. They become mobile at temperatures between 80 and 130 K, which coincides with the range of experimentally determined onset temperatures for annealing due to intrinsic defects. The influence of the Fermi level and chemical environment on the self-diffusion coefficients is discussed. Finally, some outlook is given on the implication of these findings for understanding intrinsic defects in nanoparticles.

Dopant-Carrier Exchange Interactions in Colloidal Doped Semiconductor Nanocrystals

D. Gamelin

University of Washington, Seattle, Box 351700, 98115-1700 Seattle, U.S.A.

The generation and manipulation of electron spins in magnetic semiconductor nanostructures is a central theme of the emerging field of spintronics. Carrier-dopant magnetic exchange interactions in diluted magnetic semiconductors provide the basis for many important magneto-electronic phenomena, including carrier-mediated ferromagnetism, magnetic polaron nucleation, and proposed spin-based quantum information processing schemes. This talk will describe our group's recent investigations into the use of photochemical carrier generation and magneto-optical spectroscopies to probe carrier-dopant interactions in colloidal diluted magnetic semiconductor quantum dots.

- [1] Norberg, N. S.; Parks, G. L.; Salley, G. M.; Gamelin, D. R. "Giant Excitonic Zeeman Splittings in Co²⁺-doped ZnSe Quantum Dots." *J. Am. Chem. Soc.*, 2006, 128, 13195-13203.
- [2] Liu, W. K.; Whitaker, K. M.; Kittilstved, K. R.; Gamelin, D. R. "Stable Photogenerated Carriers in Magnetic Semiconductor Nanocrystals." *J. Am. Chem. Soc.*, 2006, 128, 3910-3911.
- [3] Norberg, N. S.; Kittilstved, K. R.; Amonette, J. E.; Kukkadapu, R. K.; Schwartz, D. A.; Gamelin, D. R. "Synthesis of Colloidal Mn²⁺:ZnO Quantum Dots and High-TC Ferromagnetic Nanocrystalline Thin Films." *J. Am. Chem. Soc.*, 2004, 126, 9387-9398.
- [4] Schwartz, D. A.; Norberg, N. S.; Nguyen, Q. P.; Parker, J. M.; Gamelin, D. R. "Magnetic Quantum Dots: Synthesis, Spectroscopy, and Magnetism of Co²⁺- and Ni²⁺-Doped ZnO Nanocrystals." *J. Am. Chem. Soc.*, 2003, 125, 13205-13218.
- [5] Norberg, N. S.; Dalpian, G. M.; Chelikowsky, J. R.; Gamelin, D. R. "Energetic Pinning of Magnetic Impurity Levels in Quantum Confined Semiconductor Nanocrystals." *Nano Letters*, in press.

Poster Presentations

Chemical Vapor Synthesis and Structural Characterization of Doped and Undoped ZnO Nanocrystals

M. Ali

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ZnO is an interesting material because of its wide range of applications. It has applications in photonic devices, sensors, transparent and conducting film etc. Doped and undoped ZnO nanocrystals have been synthesized by chemical vapor synthesis method. We have used metalorganic precursors. Characterizations of nanoparticles have been performed by XRD, TEM and EXAFS methods.

Theoretical studies on doped, semiconducting nanoparticles

S. Buschmann, S. K. Nayak and P. Entel

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We study the properties of nanoparticles using first-principles methods based on density functional theory and norm-conserving pseudopotentials. The Kohn-Sham equations are sampled and solved self-consistently on a real space grid using high order finite difference method. In addition to the ground state properties and relaxation processes, we use time-dependent density functional theory to calculate the excited states of the nanoparticles.

In our research, we focus on semiconducting nanoparticles, e.g. ZnO and GaN clusters, doped with magnetic and non-magnetic impurities. Effects of self-purification, structural relaxation, formation energies, e.g., are investigated.

Light absorption of silicon nanoparticles

A. Gondorf¹, C. Meier¹, S. Lüttjohann¹, M. Offer¹, A. Lorke¹, H. Wiggers²

¹ Experimental Physics, University of Duisburg-Essen, Lotharstrasse 1, D-47048 Duisburg, Germany

² Combustion and Gas Dynamics, University of Duisburg-Essen, Lotharstrasse 1, D-47048 Duisburg, Germany

We have studied silicon nanoparticles fabricated by gas-phase condensation and in-flight sintering using absorption and photoluminescence (PL) spectroscopy. We observe a quantum size effect in PL as well as in absorption. By analysis of absorption spectra we are able to identify the character of the band gap of the nanoparticles as indirect. This result is supported by measurements of the decay time of the photoluminescence of excitons. The decay time is four magnitudes larger than in direct semiconductors. Moreover we are able to see in the absorption spectra the influence of the size distribution of the particles. The size distribution follows the lognormal distribution. We have developed a model for ensembles of particles with a lognormal size distribution which can explain the influence of the size distribution on the absorption.

Synthesis and Electrical Characterisation of Phosphor Doped Silicon Nanoparticles

S. Hartner

University of Duisburg-Essen, Lotharstr.1, 47057 Duisburg, Germany

Semiconducting nanoparticles are of great interest for future applications in printable electronics. These applications require knowledge and control of the electrical properties of the particles used. Therefore, the influence of a dopant such as phosphorus on the electrical properties of silicon nanoparticles is of great technological importance.

Phosphorus doped silicon nanoparticles were synthesized in a low pressure microwave plasma reactor by thermal decomposition of silane and phosphine in an Ar/H₂ plasma. The gases were supplied to the reactor with a molar ratio of phosphorus to silicon in the range of 1:4100 to 1:600. Using particles mass spectrometry and gas absorption (BET), the size of the particles was found to be in the range of 7 to 9 nm. This suggests an average concentration between 2 to 5 (P/Si = 1:4100) and 15 to 32 (P/Si = 1:600) P-atomes/ particle.

The nanosized silicon powders were compacted into pellets with a diameter of 5mm and an average thickness of 0.09 mm by applying a force of 20 kN for a period of 30 min. The electrical properties of the pellets were investigated by impedance spectroscopy (IS). The measurements were performed in hydrogen atmosphere at a temperatures ranging from 320 K to 650 K. As expected for semiconducting materials the spectra show an increase in conductivity with rising temperature. By varying the molar ratio of dopant and silicon from 1:4100 to 1:600, the conductivity increases by about two orders of magnitude. Evaluation of the Arrhenius diagrams led to activation energies between 250 meV and 160 meV compared to 380 meV for undoped silicon. A possible explanation for this behavior might be a change in the electronic environment of the electrons/holes with increasing average number of dopant atoms per nanoparticle. Coulomb interaction may lower the binding energy of these electrons/holes leading to a decrease in effective activation energy.

In the experiments phosphorus doped silicon nanoparticles were generated. Their conductivity could be varied by the amount of phosphine added to the synthesis reaction. Thereby particles matching defined specifications can be created for devices based on semiconducting nanoparticles.

Synthesis and Electrical Characterisation of Phosphorus-doped Silicon Nanoparticles

S. Hartner, K. Hitzbleck, H. Wiggers, A. Lorke

Universität Duisburg-Essen, Lotharstraße 1-21, 47057 Duisburg

Semiconducting nanoparticles are of great interest for future applications in printable electronics. These applications require knowledge and control of the electrical properties of the particles used. Therefore, the influence of a dopant such as phosphorus on the electrical properties of silicon nanoparticles is of great technological importance.

Phosphorus doped silicon nanoparticles were synthesized in a low pressure microwave plasma reactor by thermal decomposition of silane and phosphine in an Ar/H₂ plasma. The gases were supplied to the reactor with a molar ratio of phosphorus to silicon in the range of 1:4100 to 1:600. Using particles mass spectrometry and gas absorption (BET), the size of the particles was found to be in the range of 7 to 9 nm. This suggests an average concentration between 2 to 5 (P/Si = 1:4100) and 15 to 32 (P/Si = 1:600) P-atomes/ particle.

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In the experiments phosphorus doped silicon nanoparticles were generated. Their conductivity could be varied by the amount of phosphine added to the synthesis reaction. Thereby particles matching defined specifications can be created for devices based on semiconducting nanoparticles.

Synthesis, Deposition and Electrical Characterization of Tungsten oxide thin film for gas sensing

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Thin films of tungsten oxide have been prepared by molecular beam deposition of nanoparticles. The particles are synthesized in a low-pressure, premixed flame reactor using WF₆ as precursor material. A particle mass spectrometer is used for size selection. The flame conditions are adjusted to synthesize WO_x particles with $2.6 < x < 3$. Thin films of particles in the size regime between 5 and 9 nm are deposited on interdigital capacitors for electrical characterization. Also, small discs of compacted material are investigated by AC-methods. To identify possible mechanisms leading to gas-sensitivity, temperature-dependent impedance spectroscopy on the as-prepared WO_x thin films has been carried out between 313K and 503K. Two contributions to the overall impedance are detected and analyzed by fitting the data using equivalent circuits. One contribution can be attributed to grain-boundary conductivity (GB), the other to electrode-particle (EC) conductivity. Both increase with increasing temperature as expected for semi-conducting material. Activation energies of -1.93eV and -101meV for GB and the EC contacts are respectively extracted from Arrhenius diagrams. Furthermore, we find that the specific conductivity of the samples increases with decreasing oxygen content. The sensitivity of WO₃ thin films to NO and CO was analyzed. Even WO_x -films, consisting of only a few mono layers of particles, are remarkably sensitive, with a higher sensitivity for NO than for CO at 583 K.

Conductivity of transparent ITO nanoparticle/polymer composite layers

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We studied the conductivity and optical absorption behavior of transparent composite layers consisting of conductive polymer poly(3,4-ethylenedioxythiophene)/poly(4-styrene sulfonate) (PEDT:PSS) mixed with high conductive ITO nanoparticles. Below the percolation threshold of the ITO nanoparticles, at volume fraction of ~ 0.16 , the conductivity reduces with increase of the ITO content. The reason for the decrease is a compensation of carriers between the p-doped PEDT:PSS and the n-doped ITO. By applying a simple harmonic oscillator approximation, based on superposition of two phase system and compensation of carriers we have accomplished to model the optical characteristic. Furthermore, the reduce in the total numbers of carriers by compensation leads to conductivity decrease.

First-principles studies on dilute magnetic semiconductors

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Dilute magnetic semiconductors (DMS) based on wide bandgap semiconductors such as ZnO and GaN are promising materials for spintronic applications because of their relatively high Curie temperatures (T_C above the room temperature). There is substantial debate whether the origin of magnetism is Zener type, which would explain magnetism for more-or-less random distribution of impurities, or whether magnetic atoms form small clusters within the host material that produce the observed ferromagnetism. In the present work we performed density functional calculations on $Zn_{100-x}Co_xO$ and $Ga_{100-x}Mn_xN$ to study their properties with substitutional impurities. The calculations are done using the projector augmented wave method (PAW) and the generalized gradient approximation (GGA) for the exchange-correlation. A large supercell is used in our studies to incorporate the dilute doping of transition metal atoms to as low as 5 at.% into the host semiconductor. The effects of co-doping with Cu and Al in $Zn_{100-x}Co_xO$ are also investigated.

Preparation of nanoparticle films for single particle spectroscopy

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Silicon nanoparticles exhibit efficient photoluminescence (PL) in the visible spectral range. However, due to size-distribution effects the spectroscopic properties of single nanoparticles cannot be assessed. Therefore, to develop a microscopic understanding of excitonic effects in silicon, one has to perform single nanoparticle spectroscopy.

A major obstacle for single particle spectroscopy is the difficulty to deposit diluted layers of isolated nanoparticles on a substrate surface. In the case of the silicon nanoparticles studied here, which are synthesized from the gas-phase without, i.e., organic surface functionalization or modification, there is also a strong tendency to agglomeration.

By dispersing the nanoparticles in different solutions, we try to deposit films of isolated particles. We use different organic and aqueous solvents. In the latter case, we find that by varying the pH value we can modify the zeta-potential and reach a stabilized solution. After deposition, we find ring-like structures with a particle-size gradient that leads to a position-dependent energy shift in the PL signal. This can be explained in the framework of the DLVO theory.

We compare the deposition results for silicon nanoparticles to results obtained using commercially available PbS nanoparticles with functionalized surfaces.

Direct assembly of nanoparticles

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Advances in nanoparticle technology enable the production of new types of electronic devices, catalytic systems and complex functional surface coatings. For most of these applications, random deposition or self-assembled arrangement of the particles on surfaces are sufficient. However, an increasing number of potential applications such as single electron transistors and quantum computers require exact placement of single nanoparticles with sub-10 nm resolution and specific size. Till date, techniques that provide an exact online placement of countable and size-selected nanoparticles for functional devices have not been reported. For this purpose a cluster-jet system, based on a gas-phase nanoparticle synthesis source, connected to a focussing collimator system has been developed. The objective of this technique is to assemble countable single nanoparticles with spatial resolution of 10 nm or below onto a pre-structured substrate. In the first stage of this system, nanoparticles in the size regime between 3 and 10 nm are synthesized in a low pressure microwave plasma reactor. This reactor has the unique advantage of generating particles with defined size distribution, structure, morphology and low degree of agglomeration due to coulomb repulsion during particle formation and growth. Separated single particles are extracted by means of a particle laden molecular beam. A mass filter consisting of a particle mass spectrometer (PMS) coupled to the reactor is used to select nanoparticles of a specific size, according to their mass, charge and kinetic energy. In order to achieve the designated lateral resolution, the particle laden beam will be collimated by electromagnetic lenses and focused onto a pierced AFM-tip. Operation of the focusing mechanism and tip preparation have been successfully performed separately and are currently being adapted to the use in the cluster-jet system. After completion, this technique is intended to enable the assembly of nanoparticles in almost any desired two-dimensional structure onto a substrate.

Experimental and modelled transconductance of InAs Nanowire-FET

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Silicon-doped InAs Nanowhiskers were grown by a low-pressure metal-organic vapour phase epitaxy using the vapour-liquid-solid growth mode using Au nanoparticles [1,2]. Omega-shaped-gate n-doped InAs Nanowhisiker metal-isolator semiconductor field-effect transistors (MISFET) have been fabricated by e-beam lithography. A set of nanowire transistors with variable SiNx gate dielectric thickness from 30 nm to 90 nm has been fabricated. All nanowire transistors exhibited high performance n-type semiconductor output characteristics with well-defined linear and saturation regimes.

The experimental transconductance of the nanowire transistors substantially increased while reducing the SiNX gate dielectric layer thickness. We achieved a maximum normalized transconductance (g_m/d) of 3.5 S/mm at room temperature for 30 nm gate dielectric layer. The scalability of the transconductance could be clearly demonstrated by variation of gate dielectric thicknesses. Using a MISFET model is sufficient to achieve a good correlation to experimental transconductance data. The transconductance g_m is proportional to the gate capacitance C [3]. It is shown that the transconductance g_m follows closely to the expected inverse $\ln(h/r)$. This comparison shows that InAs nanowire transistors exhibit extremely high performance which can be modelled precisely as a prerequisite for future circuit implementation.

[1] R. S. Wagner and W. C. Ellis, Appl. Phys. Lett., 4, 89 (1964)

[2] K. Hiruma, T. Katsuyama, K. Ogawa, M. Koguchi, H. Kakibayashi, and G. P. Morgan, Appl. Phys. Lett., 59, 431 (1991)

[3] Hou T. Ng, J.Han, Toshishige Yamada, P. Nguyen, Yi P. Chen, and M. Meyyappan, Nano Lett., Vol.4, 1247, (2004)

Time-Resolved Photoluminescence Spectroscopy on undoped and Cr-doped ZnO Nanoparticles

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Due to their large band gap of 3.37eV ZnO nanostructures are promising candidates for room temperature UV light emitting applications. Furthermore, doping of ZnO with transition metals such as Cr, Mn etc. is predicted to induce ferromagnetism at room temperature. Thus, it is important to understand the recombination processes as well as the recombination dynamics particularly at room temperature.

In this work we present time resolved and time integrated photoluminescence (PL) measurements of undoped and Cr-doped ZnO. The low temperature PL spectra for undoped and Cr-doped samples are dominated by several narrow emission lines attributed to free and bound exciton transitions followed by their longitudinal optical phonon replica. The narrow linewidth (FWHM) of 2.9meV indicates that the samples are of high optical quality, which allows us to observe pronounced PL emission up to room temperature. Hereby, donor and acceptor bound excitons exhibit clearly different decay times, which can be explained by a different degree of localization.

Similar optical quality was obtained in Cr-doped ZnO nanoparticles. The incorporation of Cr is unambiguously proved by EELS and EXAFS. However, magnetic field dependent photoluminescence measurements do not show any significant influence of the magnetic ions on the magneto-optical properties. This can be explained by X-ray absorption near edge structure (XANES) analysis of the samples which reveals that chromium is mainly not incorporated on a Zn-site.



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Thursday, 7.12.

- | | | |
|-------|-------------------------------|---|
| 09:00 | Welcome | Prorektor Eckart Hasselbrink |
| 09:15 | invited lecture | Kevin Hennesy (ETH Zürich) |
| 10:00 | coffee break / poster session | |
| 10:30 | invited lecture | Cedrik Meier (U Duisburg) |
| 11:15 | invited lecture | Marius Grundmann (U Leipzig) |
| 12:00 | lunch break | |
| 13:00 | invited lecture | Jose Ulloa (TU Eindhoven) |
| 13:45 | coffee break / poster session | |
| 14:45 | invited lecture | Daniel Haegele (U Bochum) |
| 15:30 | invited lecture | Andreas Wieck (U Bochum) |
| 16:15 | coffee break / poster session | |
| 16:45 | invited lecture | Victor Klimov (LANL) |
| 17:30 | invited lecture | Carola Kryschi (U Erlangen-Nürnberg) |
| 18:15 | informal labtours | |

Friday, 8.12.

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|-------|---|--|
| 09:00 | invited lecture | Thomas Ihn (ETH Zürich) |
| 09:45 | coffee break / poster session | |
| 10:15 | invited lecture | Margit Zacharias (U. Paderborn) |
| 11:00 | invited lecture | Peter Klar (U Giessen) |
| 11:45 | lunch break | |
| 12:45 | invited lecture | Hisazumi Akai (U Osaka) |
| 13:30 | coffee break / poster session | |
| 14:30 | invited lecture | Myrtil Kahn (CNRS Toulouse) |
| 15:15 | invited lecture | Andreas Waag (TU Braunschweig) |
| 16:00 | coffee break / poster session | |
| 16:30 | invited lecture | Masako Ogura (U Osaka) |
| 17:15 | invited lecture | Karsten Albe (TU Darmstadt) |
| 18:00 | invited lecture | Daniel Gamelin (U Washington) |
| 18:45 | transfer to restaurant | |
| 19:00 | dinner at Schifferbörse Duisburg (open end) | |