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QUANTUM DEVICES and NANOSTRUCTURES QDN-2

July 19-27, 2001
International School of Solid State Physics
Ettore Majorana Foundation and Center for Scientific Culture, Erice, Italy

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2nd International School on
QUANTUM DEVICES and NANOSTRUCTURES
QDN-2

QDN-2
Erice, Italy
July 19-27, 2001

Friday, July 20, 2001

9:00/9:30	Opening Remarks (G. Benedek, G. McGuire, F. Beltram)
9:30/11:30	O. Shenderova (North Carolina State University, USA) **Introductory Remarks on Nanostructures**
11:30/12:00	Coffee Break
12:00/13:00	O. Shenderova **Introductory Remarks on Nanostructures**

Lunch

17:30/19:30	R. Ferrando (Universita' di Genova, Italy) **Simulations of Free and Supported Clusters**

Saturday, July 21, 2001

9:30/11:30	P. E. Lindelof (Øersted Laboratory, Denmark) **Quantum Transport in Nanostructures**
11:30/12:00	Coffee Break
12:00/13:00	U. Valbusa (Universita' di Genova, Italy) **Nanostructuring Surfaces via Ion Erosion**

Lunch

17:30/18:30 P. E. Lindelof (Ørsted Laboratory, Denmark)
Quantum Transport in Nanostructures

18:30/19:30 U. Valbusa (Universita' di Genova, Italy)
Nanostructuring Surfaces via Ion Erosion

Sunday,July 22, 2001

Excursion to Selinunte and Segesta

Monday, July 23, 2001

9:30/11:30 M. Reed (Yale University, USA)
Molecular Electronics

11:30/12:00Coffee Break

12:00/13:00 P. Milani (Universita' di Milano, Italy)
Nanostructured Thin Films via Cluster-Assembling

Lunch

17:30/18:30 P. Milani (Universita' di Milano, Italy)
Nanostructured Thin Films via Cluster-Assembling

Tuesday, July 24, 2001

9:30/10:30 M. Reed (Yale University, USA)
Molecular Electronics

10:30/11:30 N. Tolk (Vanderbilt University, USA)
Interface Analysis with Tunable Ultrafast Laser Sources

11:30/12:00 Coffee Break

12:00/13:00 N. Tolk (Vanderbilt University, USA)
Interface Analysis with Tunable Ultrafast Laser Sources

Lunch

17:30/19:30 Poster Session

Wednesday, 25 July, 2001

9:30/10:30 N. Tolk (Vanderbilt University, USA)
Interface Analysis with Tunable Ultrafast Laser Sources

10:30/11:30 J. Ballato (Clemson University, USA)
Micro-Photonics

11:30/12:00 Coffee Break

12:00/13:00 J. Ballato (Clemson University, USA)
Micro-Photonics

Lunch

17:30/18:30 J. Ballato (Clemson University, USA)
Micro-Photonics

18:30/19:30 R. Fazio (Universita' di Catania)
Mesoscopic Superconductivity

Thursday, 26 July, 2001

9:30/11:30 R. Fazio (Universita' di Catania)
Mesoscopic Superconductivity

11:30/12:00 Coffee Break

12:00/13:00 S. Tarucha (University of Tokyo, Japan)
Physics and Applications of Quantum Dot Structures

Lunch

17:30/19:30 S. Tarucha (University of Tokyo, Japan)
Physics and Applications of Quantum Dot Structures

Friday, 27 July, 2001

9:30/11:30	E. Cappelluti (Universta' di Roma "La Sapienza", Italy) **Electron-Phonon Interaction in Low Carrier Density Systems**
11:30/12:00	Coffee Break
12:00/13:00	E. Cappelluti (Universta' di Roma "La Sapienza", Italy) **Electron-Phonon Interaction in Low Carrier Density Systems**
13:00/13:15	Closing Remarks

Electrical Transport and Charge Injection in SiGe/Si Nanowires with Gates

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R. Leoni, G. Castellano, G. Torrioli and V. Foglietti
Istituto di Elettronica dello Stato Solido, IESS-CNR, Via Cineto Romano 42, 00156 Roma, Italy

Electron beam lithography and dry etching fabrication techniques were used to define nanowires on (100)Si/SiGe heterostructures with a high mobility 2D electron gas. In addition a gate electrode, covering the whole wire region, has been implemented to modulate the electron gas density. The leakage current through the gate oxide was found to be negligible up to several applied volts.
Electrical characterizations were performed in the temperature range 0.3 - 30 K.
A set of short wires (500nm) was fabricated to investigate the transport properties in ballistic regime. The I-V curves of the wires show a non-conductive region at low source-drain voltages, whose amplitude can be varied by acting on the gate bias, and an exponential increase of the current for higher voltage is observed. The non-conductive gap disappears at high positive gate bias. The source-drain I-V characteristics can be fitted by the functional dependence of the Fowler- Nordheim voltage-induced tunneling. The barrier height for the non-conductive state is found to increase linearly, up to few meV, upon increasing the negative gate voltage.
The source-drain current exhibits an hysteretic behaviour as a function of the gate voltage that can be explained assuming charge trapping in defect states of the oxide layer and/or at the interface between the Si cap layer and the SiGe heterostructure.
The relevance of these findings for the present research concerning the conductance in mesoscopic structures will be discussed.

Growth of Self-aligned InAs Quantum Dots on InGaAs/GaAs Strained Layer Superlattices by Molecular Beam Epitaxy

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Formation of semiconductor InAs quantum dots (QDs) has been extensively investigated in order to discuss the fundamental physics of low-dimensional systems and to develop high performance quantum effect devices such as QD lasers and single-electron transistors. Usually, InAs QDs are obtained by Stranski-Krastanow (SK) growth mode using lattice mismatch between substrate and epilayer. On the other hand, we have reported that the deformation of the surface lattices in the InGaAs/GaAs strained layer superlattices (SLSs) is locally and linearly distributed even if the layer thickness is thinner than the critical value [1]. This result shows the possibility that the self-aligned QDs are grown on the InGaAs/GaAs SLSs. For such surface sensitive growth, it was thought that the formation of QDs was influenced by thermal cracking of arsenic flux.

In this study, we examine the growth of InAs QDs by solid-source molecular beam epitaxy (MBE) using arsenic cracking cell. And the effects of InGaAs/GaAs SLSs to alignment of InAs QDs were discussed.

At first, (100)-oriented GaAs substrate was chemically etched by solution of H_2SO_4: H_2O_2: H_2O = 4: 1: 1 for 10min at 330K and mounted onto molybdenum sample holder by indium solder. Surface oxide layer was thermally removed by high temperature surface cleaning method [2] in the preparation chamber of MBE without arsenic flux at 920K for 30min. The growth temperature for SLS and QD was 720K. The SLSs with 3 to 7 periods were consisted of alternation of 7nm-thick $In_{0.1}Ga_{0.9}As$ and 10nm-thick GaAs. The growth rate of InAs QDs was 0.01 monolayers (MLs)/s and the coverage was varied from 4.1MLs to 9.1MLs. Either As_4 or As_2 flux cracked at 1220K was irradiated during the QD growth. Then, the samples were introduced into *in-situ* atomic force microscope (AFM) system to observe detailed surface structure.

For the sample grown by As_2 flux, higher density of InAs QD was obtained as compared to the sample grown by As_4 flux. The standard deviation of diameters of QD for the sample grown by As_2 was smaller than that for As_4 irradiation. These results agreed with the knowledge that the surface atoms for the case of As_2 irradiation were more active than those for As_4 irradiation. But, the self-alignment of QD toward [0-11] and [011] directions was occurred in the both cases of As_2 and As_4. Moreover, number of the self-aligned QDs increased with the increase of the SLS period. It was considered that the InAs QDs obtained here aligned on the deformed lattice of the SLS from the our previous result that the linear deformation of the surface lattice of SLS was increased with the increase of the SLS period [1].

In conclusion, cracking of arsenic flux is effective to uniform the QD size and InGaAs/GaAs SLS is advantageous to align the QD formation.

[1] K.Iizuka, T.Yoshida, T.Suzuki and H.Hirose, J.Cryst.Growth **111** (1991) 429.
[2] K.Iizuka, K.Matsumaru, T.Suzuki, H.Hirose, K.Suzuki and H.Okamoto, J.Cryst.Growth **150** (1995) 13.

A Theoretical Approach to the Modelling of the Interaction of Carbon Nanotubes with Transition Metals

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Single-wall carbon nanotubes (SWNTs) have attracted great interest among scientist, because of their potential applications in molecular nanotechnology and electronics. Nowadays reasonable quantities of higly purified SWNTs are produced, making experimental investigations on their chemistry more reliable. Recently successful controlled fluorination of the SWNTs sidewalls provided a precursor for the attachment of functional groups to the exterior of SWNTs.[1] The syntesis of chemical derivates based on carbon nanotubes makes these systems ideal candidates as building blocks for the construction of nanostructured molecular devices. Theoretical modelling could be helpful in the understanding of the structures and the mechanical and electronic properties of these systems. In this paper a theoretical investigation has been performed on the functionalization of carbon nanotubes with transition metals. Traditional *ab initio* computational approach to the SWNTs constitutes a challenging task, because of their size. Fragments of reduced molecular size have been adopted to model the whole system and to find out information on the reactivity attitude of carbon nanotubes. Accurate calculations at DFT-NL level have been perfomed on the interaction of molecular models with transition metals. Relatively small hydrocarbons topologically resembling the honeycomb lattice of nanotubes are taking into account. Because such fragments are planar molecules, a suitable geometric constraints has been imposed in order to reproduce the curved surface of the carbon atoms in (n,0) zig-zag and (n,n) armchair nanotubes. The electronic characteristics of these systems are compared with nanotube fragments (n,0) and (n,n) of finite size. Particularly we analyze the possibility of an η^2 interaction on the C-C bond and an η^6 interaction on the benzene ring. A metal fragment well-suited for an η^2 bond is $M(PH_3)_2$ M=Ni,Pd,Pt , whereas a $Cr(CO)_3$ fragment has been chosen for an η^6 bond. The nature of the metal-ligand interaction has been examined through the characterization of the optimized geometries and the analysis of the electronic structures of the involved fragments. The molecular model approach allows us to outline the effect of the curvature on the nanotubes reactivity. The results have been compared with those on fullerene models,[2] in order to extrapolate information on the different attitude of nanotubes and fullerenes systems towards transition metal fragments.

[1] E. T. Mickelson, C. B. Huffman, A. G. Rinzler, R. E. Smalley, R. H. Hauge, J. L. Margrave, *Chem. Phys. Lett.*, 296, 188, (1998); P. J. Boul, J. Liu, E. T. Mickelson, C. B. Huffman, L. M. Ericson, I. W. Chiang, K. A. Smith, D. T. Colbert, R. H. Hauge, J. L. Margrave, R. E. Smalley, *Chem. Phys. Lett.*, 310, 367, (1999); K. F. Kelly, I. W. Chiang, E. T. Mickelson, R. H. Hauge, J. L. Margrave, X. Wang, G. E. Scuseria, C. Radloff, N. J. Halas, *Chem. Phys. Lett.*, 313, 445, (1999).
[2] F. Nunzi, A. Sgamellotti, N. Re, A pyracylene model for the interaction of transition metals with fullerene: a density functional study, *submitted to J. Chem. Soc., Dalton Trans.*.

Self-Consistent Tight Binding Adapted for Large Metallic Hydro-Carbon Systems: Case Study of Field Emission Related Properties for Nano-Diamond Clusters Coatings

Denis Areshkin, Olga Shenderova, and Donald Brenner

North Carolina State University, USA

We use self-consistent environment dependent tight binding scheme to simulate eigenvalue spectra electron density, Coulomb potential distribution, and wave function geometry for metallic hydro-carbon systems. Self-consistent field iterations start at high temperature. A variant of Newton-Raphson method for nonlinear systems of equations is used to accelerate simultaneous self-consistency convergence and temperature reduction to any desired value. Special consideration is given to achieve cubic scaling of the algorithm with the system size. The usual number of iterations for metallic system is 6 to 8, while Mulliken Population convergence better than 0.005 is achieved in a single iteration for semiconducting systems. To demonstrate the method capabilities we perform the analysis of the field emission related properties for nano-diamond coatings.

Alkali Adsorption on III-V Semiconductors: Chain Formation and Adsorption Sites

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We present a high-resolution photoelectron spectroscopy study of the room temperature Cs and K adsorption on InAs(110) surfaces. The adsorption sites have been monitored by means of In-4d, As-3d, Cs-4d and K-2p core levels. The In-4d and As-3d show Cs- and K- induced extra components due to electronic rehybridization to the substrate atom, indicating two inequivalent adsorption sites for both alkali adsorbates. The Cs-4d data shows two distinct components, while K-2p seems to have a single component. Since alkali chain formation on III-V has been so far reported only for Cs, data comparison with recent STM images [1] and theoretical calculation [2] suggests that chains formation in the Cs/III-V(110) systems should be mainly driven by the electronic interaction between the two Cs adatoms forming a dimer.

[1] S. Modesti *et al.*, Surf. Sci. 447 (2000), 133-142
[2] A. Calzolari *et al.*, Surf. Sci. 454-456 (2000), 207

A Quantum-Dot Cellular Automata Shift Register

Ravi Kummamuru, Alexei O. Orlov, John P. Timler, R. Ramasubramaniam, Craig S. Lent,
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Quantum-dot Cellular Automata (QCA) is a computational paradigm [1] where the position of single electrons within cells composed of coupled quantum dots, is used to encode and process binary information. In the past few years the basic QCA devices were experimentally tested and good agreement with theoretical predictions was demonstrated [2]. Clocked QCAs [3,4,5] are an advanced version of QCA devices where the switching of electrons is controlled by a clock signal, and energy is supplied to the cells by the clock lines, rather than by inputs alone. As a result, in contrast to the edge driven cellular architectures, power gain and pipelining can be achieved in clocked QCA systems. Recently, a functional clocked cell [5] and a QCA latch [6] were fabricated and tested.

Here we present the latest device in the family of clocked QCA systems - a two cell shift register [4,7]. The device consists of two capacitively coupled QCA latches. Each QCA latch consists of three micron-sized aluminum islands, or dots, separated by aluminum oxide tunnel junctions. Both the latches are leadless, i.e. they are not connected to any external charge reservoirs. The current device was tested at 70mK. In this poster, demonstration of the shift register operation and analysis of types and rates of errors in the device will be discussed.

[1] C.S. Lent, P.D. Tougaw, W. Porod, and G.H. Bernstein, Nanotechnology 4, p. 49, 1993.
[2] A .O. Orlov, I.Amlani, G.H.Bernstein, C.S.Lent, and G.L.Snider, Science, **277**, 928 (1997); I. Amlani, A.O. Orlov, G.Toth, C. S. Lent, G. H. Bernstein, and G. L. Snider, Science (284), 289 (1999)
[3] C. S. Lent and P. D. Tougaw, Proceedings of the IEEE. 85, 541 (1997).
[4] G. Toth, C. S. Lent, J.Appl.Phys. 85, 2977 (1999).
[5] A.O. Orlov, I.Amlani, R. K. Kummamuru, R. Ramasubramaniam, G. Toth, C. S. Lent, G. H. Bernstein, and
G. L. Snider, Appl. Phys. Lett, 77(2), pp. 295-297 (2000).
[6] A.O. Orlov, R. K. Kummamuru, R. Ramasubramaniam, G. Toth, C. S. Lent, G. H. Bernstein, and G. L. Snider, Appl. Phys. Lett, 78(11),pp. 1625-1627 (2001).
[7] A. N. Korotkov, K. K. Likharev, J.Appl.Phys. 84, 6114 (1998).

Nanoscale patterning of thin aluminum film using AFM lithography

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In the last decade there has been an increasing interest in fabricating nanodevices for investigating quantum effects and for application in the nanoelectronics. As an alternative to standard microelectronic fabrication, several fabrication techniques assisted by scanning probe microscopy have been developed and some attempts to realize nanodevices have been successful. Due to the intrinsic low throughput, this kind of fabrication approach is not suitable for mass production. Nevertheless the scanning probe assisted lithography has some advantages that make it suitable for prototype fabrication: low cost, high positioning accuracy, in-situ and real time characterization of the processes.
Presently most of the efforts are directed towards field assisted techniques, such as the local oxidation induced by the probe of an atomic force microscope: both semiconductors and metals can be oxidized at a nanometer scale by scanning a negatively biased tip over the grounded sample.
In this work we focused on the patterning of the aluminum by anodization because this process exhibits a high efficiency and is compatible with MOS technology. An oxide pattern is defined by AFM anodization on aluminum films and subsequently aluminum or aluminum oxide structures are obtained by using a highly selective wet etching. This procedure that recalls the resist-mask fabrication with conventional lithography (exposure and development) requires a minimal sample preparation. The structures obtained can be used as masks for reactive ion etching processes. We report examples of sub-100 nm pattern transfer on the substrate using the AFM-fabricated masks and dry etching. Results on aluminum electrode pairs separated by a nanometer size gap are also reported.

Direct Surface Force Measurement of Particles from Micron- to Nano-Size

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Dispersion and agglomeration of nanosize particles have been the critical issues in many processes including ceramic processing and chemical mechanical planarization (CMP). Generally, decreasing particle size lowers the packing density due to a finite thickness of a repulsive layer. Therefore, high solids loadings could not be achieved yet for particles around 10 nm in size in aqueous media. Additionally, on decreasing particle size from micron to true nano size continuum or mean field theories such as DLVO-theory can no longer be applied. To date no direct method for the measurement of surface forces of single nanosize particles exists. Direct surface force measurement of nanosize particles in an atomic force microscope has been limited so far by the shape and material properties of the tip. It is proposed that a single multiwalled carbon nanotube (MWNT) can be used as a probe of nanosize particle. In this poster we will present a modified colloid probe technique using MWNT and force measurements in various conditions.

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