# SYMPOSIUM F

## Group IV Semiconductor Nanostructures

November 29 - December 2, 2004

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**8:45 AM *F1.1**
**Silicon-Based Integrated Optics: Waveguide Technology to Microphotonics.** Siegfried Janz[1], Pavel Cheben[1], Andre Delage[1], Boris Lamontagne[1], Marie-Josee Picard[1], Dan-Xia Xu[1], Kuan-Pei Yap[2] and Winnie Ye[2]; [1]Inst. for Microstructural Sciences, National Research Council Canada, Ottawa, Ontario, Canada; [2]Dept. of Electronics, Carleton University, Ottawa, Ontario, Canada.

Silicon is the most widely used platform for planar waveguide circuits, being the natural substrate for conventional and high index contrast waveguide systems. High index contrast systems such as silicon-on-insulator (SOI) and Si3N4 allow a reduction in structure size to the wavelength of light or smaller. These microphotonic components can facilitate the penetration of integrated optics from the telecommunications domain to all areas where optical analysis and diagnostics are used. Microphotonic waveguide spectrometers based on designs originally intended for WDM systems can have both bandwidth and resolution comparable to laboratory monochromators. These integrated devices can replace present day bulk optic spectrometers for sensing and chemical analysis wherever small size, stability and portability are essential. Many other possibilities for photonic devices may emerge when the ability to make microphotonic devices is combined with new concepts using photonic crystals and microresonators. Intense interest has also arisen in microphotonics to address the increasing bottleneck in data transmission over the buses connecting chips, boards, and computers. As microphotonic waveguide devices become a viable technology, several challenges must be overcome. The three most fundamental issues are waveguide loss, input and output coupling of light, and the control of polarization sensitivity. Each of these becomes increasingly difficult to manage as the waveguide dimension approaches the wavelength of light (e.g.   1 um). Furthermore, the fabrication processes used should be the same as, or modest extensions of, those used today in silicon foundries. In addition to applications of Si-based microphotonics, we will review our work and those of others in these three areas. Mechanisms leading to high waveguide loss, and means to mitigate this loss will be explored. A new input coupling scheme based on depositing graded index (GRIN) films on top of the microphotonic waveguide layer will be described. This coupler design can be applied to SOI or Si3N4 waveguides by using a-Si or silicon oxynitride films. The coupler is formed by film deposition, photolithography and etching, with no need for high-resolution e-beam lithography or three-dimensional machining. Numerical simulations show that the GRIN coupler remains effective for films composed of discrete index steps. Finally, we describe a unique solution to the problem of polarization birefringence in SOI waveguides using stress induced by an SiO2 cladding. Experimental measurements are in good agreement with theoretical results using integrated mechanical and electromagnetic finite element method calculations. The stress induced index change can fully correct polarization sensitivity of Si waveguides over wide range of dimensions and shapes. This simple approach eliminates need to design waveguides with carefully tailored dimensions and aspect ratios for the purpose of birefringence control.

**9:15 AM F1.2**
**Light Confinement in Sub-Wavelength Regions via Anderson Localization in High Index Contrast All-Dielectric Structures.** Jacob Thomas Robinson[1], Christina Manolatou[1], Michal Lipson[1] and Hod Lipson[2]; [1]Electrical and Computer Engineering, Cornell University, Ithaca, New York; [2]Mechanical and Aerospace Engineering, Cornell University, Ithaca, New York.

Si photonics provides a platform for monolithic integration of optics and microelectronics. The challenge in building active Si-based photonic devices compatible with conventional Si electronics is the weak dependence of the index and absorption on the photo-induced free-carrier effect. This weak dependence creates the need for very high power control signals in order to create all-optical switches and modulators. In order to alleviate this problem and develop all-optical devices which can operate at reasonable power levels, light must be confined and enhanced to create stronger photo-induced effects. This light enhancement is usually achieved with resonators defined by simple geometric shapes in high index material or photonic crystals. Micron-size integrated photonic devices including sensors, filters, and switches that rely on such resonators have been demonstrated. Alternate methods of confining and enhancing light provide the opportunity to develop novel devices with reduced dimensions, power consumptions, and increased speeds. In this paper we present a highly light-confineing structure with sub-wavelength dimensions. The mechanism of light confinement is based on interference effects from multiple scatterings (Anderson Localization). Anderson Localization

can be achieved in a Si/SiO2 composite when the distance between scattering interfaces is on the order of a wavelength. This can be achieved with standard Si nanofabrication techniques and incorporated into integrated devices. To achieve a structure with both strong confinement and enhancement the scattering composite must be arranged such that the interference effects limit localization to a small spatial cavity as well as couple efficiently to the input source. To accomplish this, the structure was designed using an Evolutionary Algorithm which optimized the intensity enhancement. The optimized structure consists of a single mode input waveguide and a region of Si and SiO2 rods which form the scattering interfaces. 2D Finite-Difference Time-Domain (FDTD) method with an excitation wavelength of 1550 nm reveals confinement to about a 100 by 100 nm region in Si. We also demonstrate a corresponding intensity enhancement of over 300 times the input intensity. The resonance in this structure has a Q of over 400. This strong light-confining structure can be used to achieve ultra-fast all-optical modulation in Si with low power. We show that using free-carrier injection from two-photon absorption (TPA) a modulator based on this structure could have a few ps lifetime and a 30-50% modulation depth with an in-plane pump power of about 1 pJ.

**9:30 AM F1.3**
**Si-rich Si3N4/SiO2 CMOS Compatible Light Emitting Complex Photonic Structures.** Luca Dal Negro, Jae Hyung Yi, Yasha Yi, Xiaoman Duan, Jurgen Michel and Lionel C. Kimerling; MIT, Cambridge, Massachusetts.

The possibility to fabricate one dimensional (1D) light emitting complex photonic structures like quasicrystals, aperiodic dielectrics and random systems, represents an alternative and barely explored approach with respect to the widely investigated field of periodic photonic crystals. However, the exploratory study of aperiodic photonic structures can represent indeed an exciting opportunity in order to fully understand the potential of such materials in relation to light localization, photon transport and light emission properties. In particular, when light emitting materials are combined with complex photonic structures, this approach can directly lead to the demonstration of novel multifrequency optical devices based on localized light modes and strong field enhancement effects. Here we report on a new material approach based CMOS compatible PE-CVD deposition of SiO2 and Si-rich Si3N4 layers followed by thermal annealing treatments. This approach is nicely suitable for the realization of light emitting complex dielectrics. Efficient broad band light emission and good quality photonic structures have been both demonstrated paving the way to the realization of multifrequency complex structures with enhanced light emission. In particular, we will report on the first fabrication of good quality light emitting Thue-Morse aperiodic structures where strong field enhancement effects and multifrequency response are demonstrated for the first time. In addition, within a fully VLSI-CMOS compatible annealing window, it was possible to activate broad band (800nm-1700nm) light emission homogeneously from the inside of the complex photonic structures, allowing direct access to the study of light propagation and light states in complex photonic structures like quasicrystals and aperiodic dielectric materials.

**9:45 AM *F1.4**
**Silicon Self-Assembled Photonic Band Gap Crystals.** David J. Norris, Chem. Eng. & Mat. Sci., Univ. of Minnesota, Minneapolis, Minnesota.

Photonic crystals are structures composed of artificial atoms that are approximately one thousand times larger than in traditional molecular crystals. When photonic crystals are properly tailored, they can exhibit a remarkable optical property, a range of colors for which light is not allowed to exist inside the material. This behavior, known as the photonic band gap, could be utilized to confine, manipulate, and guide light. Thus, these materials offer a route to novel photonic technologies. For this goal, conventional microfabrication techniques have been successfully adapted to obtain photonic band gap crystals. However, here we will address a completely different approach. Namely, what type of photonic band gap structures can be achieved by self-assembly? Can we spontaneously assemble the appropriate complex, ordered structures by manipulating simple building blocks? We will review efforts to use the self-assembly of colloidal particles to obtain high-quality silicon photonic band gap crystals. Despite the simplicity of this approach, experiments have recently shown that these structures can exhibit optical properties consistent with a photonic band gap. Further, since the photonic crystal is grown as a thin coating, it is extremely useful for both fundamental and technologically relevant studies. Finally, we will discuss our current knowledge of how self-assembly works and how it can be further modified to obtain even more complex structures.

**10:30 AM F1.5**
**Optically Controlled Photonic Crystal Nanocavity in Silicon.**

Stefan Francis Preble, Vilson Almeida and Michal Lipson; Electrical and Computer Engineering, Cornell University, Ithaca, New York.

Silicon, the dominant material in the microelectronic industry, is highly desirable as the platform for photonic chips. Photonic crystal structures that bend, split, couple and filter light have recently been demonstrated in silicon, but the flow of light in these structures is predetermined by the structure design and cannot be modified. All-optical control of light on silicon is challenging due to its lack of non-linear optical properties. Here we propose and demonstrate the all-optical control of a one-dimensional photonic crystal nano-cavity embedded in a Silicon waveguide. The resonance of the cavity is tuned by injecting free carriers into the nanocavity region using an optical pump beam. By strongly confining light in the photonic crystal nanocavity the sensitivity of light to small refractive index changes is enhanced. The small cavity volume ( 0.1 $\mu m^3$) and unpassivated sidewalls enable ultra-fast switching speeds with low pulse energies. The devices are fabricated using electron beam lithography and reactive ion etching. Using a pulse energy of only 40pJ, a refractive index change of approximately $10^{-2}$ is obtained. This small index change, due to the high confinement nature of the cavity structure, leads to a strong change in transmission spectrum. Consequently, the resonance is shifted by more than its full width at half maximum ( 8nm), and the transmission of the device is modulated by more than 96%. The free carrier relaxation time in such a compact structure is less than 500ps, leading to switching speeds on the order of 1Ghz. Such a device could open the door to the large-scale integration of ultra-fast modulators and switches.

### 10:45 AM F1.6
**Photoluminescent Coupled Multiple Microcavity Structures from Porous Silicon.** Vivechana Agarwal and Jose Alfredo Soto Urueta; CIICAP-Universidad Autonoma del Estado de Morelos, Cuernavaca, Mexico.

Fabrication of porous silicon one dimensional photonic crystals having 20 to 30 coupled microcavities (up to 200 layers) have been made. The photonic bandgap upto 1000nm and photoluminescence in the range 700-850nm has been observed. Here we present the fabrication, structural and optical characterisation of such structures which may be promising for variety of applications[1]. [1]V.agarwal et.al. Phys. Rev. Lett. 92(2004)097401

### 11:00 AM F1.7
**Compact Electro-Optic Modulator on Silicon-on-Insulator Platform.** Sameer Pradhan, Vilson Almeida and Michal Lipson; School of Electrical & Computer Engineering, Cornell University, Ithaca, New York.

Silicon based optoelectronic and photonic devices and circuits are attractive due to their fabrication compatibility with the CMOS process. The main methods to alter the refractive index in Si are the thermo-optic effect and the electro-optic effect. The thermal change of the real optical refractive index in Si is large. However, the thermo-optic effect is slow and can be used only up to 1 MHz modulation frequencies. For higher modulation frequencies electro-optic devices are required. Refractive index change using free carrier injection is a relatively fast process and is, therefore, used to change both the real refractive index and optical absorption coefficient. However the index change mechanism due to free carriers is weak in Silicon and usually requires long structures for modulation. The shortcoming of the weak electro-optic effect can be overcome using a resonant cavity and high-index contrast waveguides. The resonant cavity increases the optical path length of the modulator and maximizes the interaction between the optical mode and transmission medium. without increasing the physical device length. As a result, the transmittance near resonance of a ring resonator cavity is very sensitive to small refractive index changes, making it very appropriate for modulation. The resonance condition of the ring resonator is given by f0=K(c/neff)(1/2.pi.R) where c = speed of light in free space, neff = effective refractive index of the ring, R = radius of the ring, K = integer corresponding to the multiple resonant wavelengths. By changing the refractive index under carrier injection, the resonant frequency of a ring resonator can be changed. We fabricated and characterized a tunable electro-optic modulator using high-index contrast Si-SiO2 ring resonators on silicon-on-insulator (SOI) substrate. The devices were fabricated using standard CMOS compatible process technology. A high-index contrast 450nmx250nm Si-SiO2 waveguide structure is defined on a SOI substrate using e-beam lithography followed by reactive ion plasma etching (RIE). Low-resistance doping regions were defined around the rings using ion-implantation. The waveguides were passivated and planarized by a combination of growth and deposition of oxide. Finally, ohmic metal contacts (Ti) and probe pads (Ti/Au) were deposited. The refractive index of the ring was changed by applying voltage across anode and cathode probe pads. Optical modulation is achieved using plasma dispersion effect due to current injection under forward bias of the

p-i-n junction. The resonance of the ring resonators shows a clear blue-shift under carrier injection. A modulation depth up to 50% is measured for a probe wavelength of 1549nm. The drive current for a bias voltage of 0.87V is 1.76uA/um, which corresponds to a dc power consumption of 1.53uW/um. Transient analysis of the modulator indicates that the device is rise and fall times are 1.25ns which corresponds to a modulation bandwidth of 775MHz.

### 11:15 AM F1.8
**DNA Biosensor Based on Highly Confining Silicon Photonic Micro-Cavity.** Bradley Schmidt, Vilson Almeida and Michal Lipson; Electrical and Computer Engineering, Cornell University, Ithaca, New York.

There is a growing need for the development of integrated biosensors. Many current systems for bio-detection are either large, or lack the desired level of sensitivity. We demonstrate a micron-size silicon photonic structure for use in a highly sensitive integrated biosensor array that has a very low limit of detection, approaching single molecule detection. The sensor uses the high field confinement inside a Fabry-Perot micro-cavity to enhance the effective absorption cross-section of metal nano-particles that are used as tags for analyte biomolecules of interest. The micro-cavity was designed and fabricated on a high refractive index contrast silicon waveguide on Silicon-On-Insulator platform. The device is 450 nm wide and less than 5 microns in length, allowing for a high density of devices on a single chip. Experimental results show that such a device is sensitive enough to detect the presence of a discrete number of 10 nm diameter gold nano-particles. The detection is achieved by measuring the decrease in optical transmission due to the absorption losses of the metal particles at a wavelength of 1.5 microns. These results are in agreement with 3-D Finite-Difference Time-Domain simulations of the micro-cavity structure. The simulations predict a 7-9% loss in transmission through the structure for each nano-particle in the sensing area. The transmission changes less than 2% due to the variation in the location of the particles within the sensing area. Detection of various concentrations of DNA was performed using the device. Concentrations ranged in value from $10^4$ to $10^9$ copies/mL with sample volumes between $10^{-10}$ and $10^{-5}$ L. A polymer lift-off technique was used to place small areas (40-100 nm in diameter) of DNA as biorecognition elements on top of the micro-cavity. This DNA layer was used to specifically bind and detect the presence of a discrete number of c-DNA molecules tagged with 10 nm gold particles. Such a structure allows for on-chip integration of biosensor components with high sensitivity and low limits of detection, approaching single molecule detection for various analytes such as DNA, RNA, proteins, and antigens.

### 11:30 AM F1.9
**Raman Gain in Silicon Using Highly Confined Waveguide Structure.** Qianfan Xu, Vilson R. Almeida and Michal Lipson; Cornell University, Ithaca, New York.

Silicon-on-insulator (SOI) waveguide is a promising platform to monolithically integrate various optical devices with electronics. However, light emission and amplification is difficult to achieve on Silicon due to its indirect bandgap. Stimulated Raman scattering could be used for overcoming the limitation of Silicon as an active device, taking advantage of the high Raman scattering efficiency in crystalline silicon and the high field confinement in the sub-micron-size stripe waveguides. However, Raman gain in Silicon was shown to be limited by absorption from the two-photon-absorption (TPA)-generated free carriers at high pump powers. Here we demonstrate high gain of 4.2 dB in Silicon in a 7-mm-long strip waveguide with a mode-area of 0.15 $\mu m^2$ at the pump peak power of 1.5 W. In order to isolate the Raman effect from the free-carrier absorption we use pulsed pumping scheme that prevents free carriers to build up over time. The Raman gain we demonstrate is one-order-of-magnitude higher than the previous reported gain in ridged SOI waveguide. This high gain is due to the high-confinement waveguide used. The gain with pulsed pump can be used to amplify return-to-zero signal in telecommunication system, to compensate nonlinear losses in all-optical switch based on silicon, and to pump and actively mode-lock a Silicon-based laser.

### 11:45 AM F1.10
**One-dimensional photonic band gap superstructures based on porous silicon.** Denis G. Gusev, Andrey A. Fedyanin and Oleg A. Aktsipetrov; Physics Department, Moscow State University, Moscow, Russian Federation.

Photonic band gap (PBG) structures demonstrated spectacular properties associated with specific light propagation. The possibility to control the light localization and to fulfill the phase-matching conditions makes photonic-crystal microcavities perspective for optoelectronic and nonlinear-optical applications. Mesoporous silicon is a promising material for fabrication one-dimensional PBG

structures. Photonic crystals formed from mesoporous silicon are made by the electrochemical etching of silicon by means of periodic variation of chemical reaction parameters during the etching process. This paper presents fabrication and characterization of superstructures: coupled microcavities (CMC's) and "photonic molecules" (PM's) based on porous silicon. Coupled microcavities consist of several photonic crystals separated with two or more microcavity layers. Photonic molecules are PBG structures consisted of two identical microcavities separated by thick layer (spacer). The CMC's and PM's are made by the electrochemical etching of heavily doped Si(001) wafers. The pore size is controlled by the variation of the current flowing through the wafer perpendicular to its surface. The layer thickness is controlled by etching time. Studied CMC's samples have two identical half-wavelength-thick cavity spacers surrounded by Bragg reflectors. External photonic crystal consists of 4 periods of porous silicon bilayers, which are two quarter-wavelength-thick porous silicon layer with difference porosities. The thickness of intermediate Bragg reflector is varied from 0.5 to 4.5 bilayers. The center of photonic band gap of CMC's is 900 nm ($\lambda$). The spectrum has a plateau with high reflectivity. The modes of coupled microcavities are split with spectral (angular) gap between them determining by intermediate Bragg reflector transmittance. The photonic molecules consists of two identical microcavities with 5 periods of porous silicon bilayers in each Bragg reflector separated by thick layer. The thickness of this layer is changed in series from $\lambda$ to $2\lambda$ with step $\lambda/4$. The linear spectrum of photonic molecule has one or three modes, which are determined by the thickness of the spacer between microcavities. Microcavities separated by spacer with thickness divisible by even number of $\lambda/4$ possess three resonance state. On the contrary PM's with spacers thickness divisible by odd number of $\lambda/4$ have only one resonance state, which are similar to triplet and singlet states of diatomic molecules. The second- and third-harmonic generation spectroscopy in wave-vector domain is performed to characterize the fine spectroscopic features of complicate PBG superstructures. Nonlinear power dependence of nonlinear-optical response on electric field of fundamental radiation provides unique information about local field distribution across this complicate layered structures.

SESSION F2: Si/SiGe Heterostructures and Devices
Chairs: E. A. Fitzgerald and Leonid Tybeskov
Monday Afternoon, November 29, 2004
Constitution B (Sheraton)

**1:30 PM *F2.1**
**Formation of High Quality SiGe Hetero-Structures and their New Device Applications.** Yasuhiro Shiraki, Advanced Research Laboratories, Musashi Institute of Technology, Tokyo, Japan.

Since advanced crystal growth techniques such as molecular beam epitaxy (MBE) and UHV-CVD were well established, it has become possible to introduce hetero- and quantum-structures into silicon (Si). These structures enable us to develop advanced Si devices based on new concepts which were mainly established in the field of compound semiconductors. The front runner of these devices is hetero-structure bipolar transistors (HBTs). The cut-off frequency of HBTs exceeds 300 GHz and they are now in the mass production phase. Another hopeful electronic device application is field-effect transistors (FETs), particularly based on strained silicon and germanium and modulation-doping (MOD) structures. They can provide extremely high mobility and therefore high performances, much better than conventional Si MOSFETs. The mobility of n-channel MOD structures, for instance, reaches almost one million cm2/Vs, while the hole mobility of strained Ge layers exceeds the mobility of bulk Ge. Another interesting application of SiGe hetero-structures is light emission. Although the materials are indirect band-gap semiconductors, luminescence efficiency was found to be significantly improved by introducing new quantum structures. Light emitting diodes (LEDs) and micro-cavities were fabricated to demonstrate their high potential as opto-electronic devices, particularly optical interconnection and parallel processing in VLSI circuits. It is obvious that these device applications are strongly dependent on the material qualities of SiGe hetero-structures. In this talk, the development in the material growth which makes new device applications of SiGe hetero-structures, particularly quantum structures, possible is reviewed and the future prospect is discussed.

**2:15 PM F2.2**
**Direct Spectroscopy of the Valley Splitting in a Silicon/Silicon-Germanium Two Dimensional Electron Gas.**
Srijit Goswami[1], J. L. Truitt[1], Charles Tahan[1], Levente J. Klein[1], K. A. Slinker[1], D. W. van der Weide[2], Susan N. Coppersmith[1], Robert Joynt[1], R. H. Blick[2], J. O. Chu[3], J. A. Ott[3], P. M. Mooney[3] and M. A. Eriksson[1]; [1]Physics, University of Wisconsin-Madison, Madison, Wisconsin; [2]Electrical and Computer Engineering, University of Wisconsin-Madison, Madison, Wisconsin; [3]IBM Research Division,

T.J. Watson Research Center, Yorktown, New York.

The strain in silicon/silicon-germanium quantum wells reduces the usual six-fold degeneracy of the silicon conduction band, leaving a pair of degenerate bands in the growth direction. Quantum confinement in the silicon well further splits this degeneracy, leading to a small, but extremely important energy gap (the valley splitting) between these lowest two levels. We show that microwave spectroscopy can be performed between these two states. Transport measurements at 0.25K in a silicon/silicon-germanium two dimensional electron gas (2DEG) are used to detect microwave absorption at the valley splitting energy. The observed lineshapes are similar to those observed in electrically detected electron spin resonance signals. The valley splitting is found to increase linearly with an applied perpendicular magnetic field. The valley splitting peak shows a dramatic (7-fold) increase in width as the temperature is increased from 0.25 K to 0.4K. These results indicate that in moderate magnetic fields the silicon valley degeneracy can be completely removed in low temperature quantum devices.

**2:30 PM F2.3**
**Formation of Ge Nanostructures by Phase Separation During MOVPE of (III-V)$_{1-x}$(Ge$_2$)$_x$ Alloys.** Andrew Gordon Norman, Jerry M. Olson, Manuel J. Romero, Pat Dippo and Mowafak Al-Jassim; National Renewable Energy Laboratory, Golden, Colorado.

We report a new method of forming single crystal Ge nanowires and nanocrystals. The Ge nanostructures are produced by the phase separation of (III-V)$_{1-x}$(Ge$_2$)$_x$ alloys during metal organic vapor phase epitaxy (MOVPE). For the (GaInP)$_{1-x}$(Ge$_2$)$_x$ alloy system, by adjusting the growth conditions, we have formed Ge nanowires of up to 2 $\mu$m length, with controlled diameters ranging from 5 nm to greater than 50 nm, embedded in a high band gap GaInP matrix. By changing the (GaInP)$_{1-x}$(Ge$_2$)$_x$ alloy composition we are able to control the density of the nanostructures. Restricting the epitaxial layer thickness results in the formation of Ge nanocrystals. These Ge nanostructures have been studied structurally and chemically using transmission electron microscopy. Optical properties have been measured by a combination of photoluminescence, optical absorption, and cathodoluminescence. Room temperature photoluminescence has been observed from these samples, with broad peaks centered at about 1 eV. The onset of optical absorption at room temperature in these phase-separated (GaInP)$_{1-x}$(Ge$_2$)$_x$ alloy layers containing Ge nanostructures is observed at energies between 0.7 and 0.8 eV.

**2:45 PM *F2.4**
**High Mobility SiGe Heterostructures.** Eugene Arthur Fitzgerald, Materials Science and Engineering, MIT, Cambridge, Massachusetts.

We have shown that thin layers of tensile Si and compressed SiGe can be layered at the nanometer-scale in the vertical direction (growth direction) of a MOSFET structure and drastically increase the lateral mobility of electrons and holes. Such vertical engineering using thin layers and strain can also be used to design peak mobility at the desired vertical field. Unlike Si which has fewer degrees of freedom, the SiGe system allows for the interchange of band offset, layer thickness, and vertical field in material design. At high fields, we have shown that a tensile Si/compressive Ge heterostructure on relaxed Si0.5Ge0.5 can achieve an electron mobility enhancement of 2x and a hole enhancement of 10x. Materials engineering offers a continual evolution in lattice-constant engineering, potentially leading to other promising heterostructures in the future.

**3:30 PM *F2.5**
**Towards Heterogeneous Integration of Semiconductor Nanostructures – SiGe on Si.** Kang L. Wang, Hyung-jun Kim, Song Tong and Fei Liu; Electrical Engineering Department, University of California-Los Angeles, Los Angeles, California.

There has been tremendous progress in SiGe microelectronics. High performance HBT and other devices as well as their integration on Si CMOS platform have been demonstrated. In addition to the use of SiGe HBT for high frequency mixed signal mode applications, integration with optoelectronics devices will enable a major cost reduction in optical communications, in which Si-based efficient light sources and fast detectors are critical. This talk will addresses the use of self-assembled Ge quantum dots grown on Si for this potential application. We will discuss the challenges in the growth of the self assembled dots: control of size and registration or placement of dot arrays. The size control based on the growth parameters, including T, deposition rate, etc. will be addressed. Likewise, mechanisms of registration of dots on Si will be discussed. One example on the use of the strain field to provide the registration of dots is used to illustrate the possible means of guided assembly. Optical properties both in interband and intersubband transitions will be reported. The above successful demonstration of the growth of Ge on Si in nano-structural forms suggests a general technique to extend the growth of other

lattice mismatched materials in nano forms on Si CMOS. Indeed, all kinds of III-V dots, nanowires, and nanotubes have been produced, such as carbon nanotubes, Si/Ge nanowires, ZnO nanowires, and GaN nanowires. Based on the latter nanowires, PN junctions and CMOS like devices have been demonstrated. These results suggest a general approach to achieve emerging heterogeneous integration of nanostructures and devices from different nanomaterials for nanosystems.

**4:00 PM F2.6**
**Structural and Optical Properties of $Sn_xGe_{1-x}$ Quantum Dots and Quantum Wires.** <u>Jordana Bandaru</u>, Douglas Bell and Shouleh Nikzad; Jet Propulsion Laboratory, Pasadena, California.

$Sn_xGe_{1-x}$ layers and quantum dots (QDs) are of great interest as materials that could provide tunable direct band gaps, allowing completely group IV-based optoelectronic devices. These materials could be used in a wide range of applications such as emitters, infrared detectors, and thermophotovoltaics. However, substantial challenges remain in the growth and processing of these materials. We have grown $Sn_xGe_{1-x}$ films by low temperature Molecular Beam Epitaxy (MBE), using low growth temperatures ($<200°C$) in order to grow fully strained layers. X-ray diffraction, transmission electron microscopy, and Rutherford backscattering spectroscopy data indicate high-quality epitaxial films. Post-growth annealing was used to form QDs. Either QDs or quantum wires may be formed depending on annealing parameters. The effects of varying substrate temperature between 400C (wires) and 750C (QDs) on size and distribution of quantum structures were explored and will be discussed. Sn concentration (0-10%) and film thickness (40nm - 200nm) were also varied. In addition, annealing of samples with Ge cap layers was compared to that of uncapped samples. A Ge cap was used in order to limit Sn surface segregation and to control dislocation formation in the $Sn_xGe_{1-x}$ layer during the annealing process. Optical properties probed by Fourier transform infrared spectroscopy (FTIR) will be presented. FTIR spectra clearly show the decrease in band gap of $Sn_xGe_{1-x}$ layers with increasing Sn fraction up to 10%. Photomodulated reflectance (PR) is another sensitive method for probing critical points in electronic band structure, and can detect both direct and indirect transitions. PR results for $Sn_xGe_{1-x}$ layers will also be presented.

**4:15 PM F2.7**
**Time-Resolved Photoluminescence in Si/SiGe Nanostructures.** <u>Boris Kamenev</u>[1], Jean-Marc Baribeau[2], David Lockwood[2] and Leonid Tsybeskov[1]; [1]Electrical and Computer Engineering, New Jersey Institute of Technology, Newark, New Jersey; [2]Institute for Microstructural Sciences, National Research Council, Ottawa, Ontario, Canada.

We present comprehensive studies of spectrally and time-resolved photoluminescence (PL) in Si/SiGe nanostructures with Ge content controllably varied from 10 to 60%. Using a pulsed laser excitation source with adjustable parameters, we show that PL rise/decay time has several components and their ratio strongly depends on the excitation conditions such as pulse intensity, duration, etc. We present a model where different PL bands originate within nearly pure Ge clusters and/or Si-SiGe interfaces.

**4:30 PM F2.8**
**Top-gated Quantum Dots in Silicon/Silicon-Germanium Two-Dimensional Electron Gases.** <u>Keith A. Slinker</u>[1], K.L.M. Lewis[1], C.C. Haselby[1], Levente J. Klein[1], J.L. Truitt[1], Srijit Goswami[1], D.E. Savage[1], M.G. Lagally[1], D.W. van der Weide[1], J.O. Chu[2], P.M. Mooney[2], Susan N. Coppersmith[1] and Mark A. Eriksson[1]; [1]University of Wisconsin - Madison, Madison, Wisconsin; [2]IBM Watson Research Center, Yorktown Heights, New York.

Electrons in silicon/silicon-germanium two-dimensional electron gas quantum dots are a promising architecture for spin based quantum computation. Top gated quantum dots allow precise tuning of electron shape and interdot coupling. We report the observation of Coulomb blockade in dots defined by a combination of etching and metal top gating. A narrow channel or mesa is fabricated by electron beam lithography and subsequent reactive ion etching. Metal gates are deposited across the channel to define the leads of the dot. The sides of dot are defined either by surface depletion from the etched sidewalls or by metal plunger gates. Low temperature measurements (1.8K) show a single electron charging energy of about 2meV. We observe steps in the differential conductance known as the Coulomb staircase with varying source-drain bias. We also report on the use of gate dielectrics to further reduce the leakage current from the top gates.

**4:45 PM F2.9**
**Nanometer-scale control of Ge island nucleation sites on Si(001) using a Ga focused ion beam.** <u>Alain Portavoce</u>[2], Mark C. Reuter[1], Robert Hull[2] and Frances M. Ross[1]; [1]IBM TJ Watson

Research Center, Yorktown Heights, New York; [2]Department of Materials Science and Engineering, University of Virginia, Charlottesville, Virginia.

Novel microelectronic devices such as quantum dot cellular automata and photonic waveguides require nanoscale control of quantum dot positions. This can present a challenge in fabrication since the quantum dots are typically formed by strain-driven self-assembly, leading to random nucleation positions. In this presentation we will show that low-dose implantation of Ga using a focused ion beam (FIB) can be used to control the nucleation sites of Ge islands grown on the Si(001) surface, allowing us to fabricate arbitrary patterns of quantum dots without creating significant surface topography. The experiments were carried out in a UHV system incorporating a FIB, a transmission electron microscope with gas handling capabilities enabling CVD growth to take place in the polepiece, and an electron beam evaporator in a side chamber. By using this system we can pattern a thin specimen using the FIB, anneal it in the TEM and then observe in real time the self assembly of islands as Ge is deposited onto the specimen, all without breaking vacuum. We find that with suitable implantation and annealing conditions this patterning technique slightly modifies the surface roughness and possibly the subsurface strain field. This increases the island nucleation probability on irradiated areas and therefore allows the control of island positions on the nanometer scale. Furthermore, we find that the islands nucleated on implanted areas have a different shape from Ge islands grown on unmodified Si(001) surfaces, and exhibit a lower wetting layer thickness and a smaller critical size for dislocation nucleation. We will describe the kinetics of island growth, which we can extract from videos recorded during deposition onto FIB-patterned surfaces, and we will also describe the structure and properties of the islands produced. Furthermore, by comparing UHV-CVD with MBE deposition of Ge, we will show that gas reactivity is not the principal factor allowing organisation; instead the island nucleation barrier is modified on irradiated areas. Finally, we will discuss the optimum conditions for forming arbitrary patterns of islands and the possibilities of using this technique during fabrication of quantum dot-engineered devices.

SESSION F3: Poster Session
Chairs: Christophe Delerue and Masakazu Ichikawa
Monday Evening, November 29, 2004
8:00 PM
Exhibition Hall D (Hynes)

**F3.1**
**Charge Transport in Silicon Nanocrystal Arrays.**
<u>Rishikesh Krishnan</u>[1], Philippe Fauchet[1], Todd Krauss[3], Qianghau Xie[2], Xiang-Dong Wang[2] and Joseph Kulik[2]; [1]Electrical and Computer Engineering, University of Rochester, Rochester, New York; [2]Department of Chemistry, University of Rochester, Rochester, New York; [3]Physical Analysis Lab Arizona, Freescale Semiconductor, Tempe, Arizona.

Single layers of isolated, size-controlled silicon nanocrystals were prepared by thermal crystallization of a thin amorphous silicon layer sandwiched between silicon dioxide layers. A subsequent oxidation treatment ensured controlled increase in their lateral separation. The size of the nanocrystals, separation of the nanocrystals (from < 1 nm to 4 nm), stoichiometry of the resulting oxide and surface morphology were monitored with transmission electron microscopy, scanning transmission electron microscopy, atomic force microscopy, x-ray photoelectron spectroscopy, and Raman spectroscopy. Mesoscopic charge transport studies performed with an electrostatic force microscope (EFM) revealed rapid lateral transport of charges when the nanocrystals were tightly packed (<1 nm average separation) and interconnected. As the inter-nanocrystal separation was increased, lateral charge transport was rapidly suppressed. Nanocrystals separated by up to 3.6 nm retained the injected charges in a well-defined localized region ( 275 electrons inside a 62 nm diameter region) for a time of the order of several days. The ability to switch from a very short to a very long retention time using the same structure by simply changing the post-growth processing conditions is attractive for various applications. The ability to obtain a long charge retention time and place the nanocrystals at well-defined depths indicates that our structures may be useful for charge storage applications such as in non-volatile memory devices. We believe that our structures with long retention times could also be used as charge templates for self-assembly applications.

**F3.2**
**Addition Energies of Semiconductor Quantum Dots from First Principles.** <u>Alberto Franceschetti</u>, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Transport properties of semiconductor nanostructures are characterized by a complex interplay between quantum confinement effects and Coulomb blockade effects. Previous calculations of electron and hole addition energies in quantum dots have been based on the evaluation of electron-electron and hole-hole Coulomb and exchange integrals, which are clouded by uncertainties in the dielectric screening function appropriate for low-dimensional quantum structures. Here we use density-functional theory in the local-density approximation to calculate the electron and hole addition energies of Si and InAs quantum dots in the 1-3 nanometer size regime from first principles. The addition energies are given directly by total-energy differences, thus circumventing the need to introduce an approximate dielectric function. Our results clarify the role of the surface and the relative importance of single-particle splittings vs. Coulomb interactions in the addition spectra of quantum dots. We also show how the results of our calculations can be used to extract the parameters of a model dielectric function that can be used to predict the addition spectra of quantum dots in different dielectric environments.

### F3.3
**Computer Simulation of Charging/Erasing Transients of a Ge/Si Hetero-Nanocrystal-Based Flash Memory.**
Dengtao Zhao, Yan Zhu, Ruigang Li and Jianlin Liu; Electrical Engineering, Quantun Structures Laboratory, Riverside, California.

The transient process of the programming/erasing is very important for a nanocrystal-floating-gate flash memory. In this work, a computer simulation was carried out to investigate the charging, retention and erasing processes of our proposed Ge/Si hetero-nanocrystal floating gate flash memory. The simulation was based on Poisson equation and tunneling current. The transient gate current, transient drain current and the average charge in one dot were simulated respectively. Evident hysteresis features can be observed in the transient processes in a voltage-sweeping measurement mode. The hysteresis strongly depends on the voltage sweeping speed. The presence of Ge on Si dot can enhance the hysteresis process which suggests the enhanced data storage. While measuring the transient process in a constant voltage mode, the time decay of transient current and charge are weakened if Ge is used on the Si dot, indicating a longer retention time for Ge/Si-floating-gate flash memory.

### F3.4
**Threshold Voltage Shift in Hetero-nanocystal Floating Gate Flash Memory.** Yan Zhu, Dengtao Zhao, Ruigang Li and Jianlin Liu; EE department, University of California, Riverside, Riverside, California.

Owing to the band offset at the interface of hetro-nanocrystal, flash memory using hetero-nanocrystals as floating gate can have a longer retention time while keeping almost the same programming speed. As an index of memory window, the threshold voltage shift that results from the charge stored in the floating gate is one of the most important parameters for the flash memory. In this presentation, we show our simulation results of threshold voltage shift of our proposed Ge/Si hetero-nanocrystal floating gate memory devices. First, numerical investigations were carried out by solving 2-D Poisson-Boltzmann equation. The simulation shows that the presence of the Ge on Si dot can remarkably prolong the retention time, indicated by the time decay behavior of the threshold voltage shift. It also shows that increase of thickness of either Si or Ge dot will introduce a reduction of the threshold voltage shift. The shift also strongly depends on the dot density. However, only a weak dependence of threshold voltage shift on the tunneling oxide thickness was found. A capacitor model was also proposed to explain the dependence of threshold voltage shift on variable parameters, which agrees well with the results of 2-D Poisson-Boltzmann numerical method.

### F3.5
**Source-Drain Engineering Challenges in Finfet Device Fabrication.** Daniel Pham, International Sematech, Austin, Texas.

Daniel Pham+, Hong-Jyh Li++, Billy Nguyen, Gabriel Gebara, Dana Larison, Barry Sassman, Larry Larson. International SEMATECH, +Freescale Semiconductor Assignee, ++Infineon Assignee. Austin, TX, USA Double-gate devices are considered most promising for scaling into the sub-20nm regime due to a steeper sub-threshold slope, reduced short channel effects, improved mobility, and drive current. The FINFET is one of the most attractive double-gate structure and most compatible with today s standard processing technologies. One of the challenging issues of fabricating FinFETs device is the doping of the source-drain junction in the Fin area. In planar device junction formation, the dopant is implanted onto a planar surface and can be monitored and analyzed by several standard techniques. These methods cannot be applied for FinFET junction formation due to the ultra-thin vertical dimension of the Fin. Implanting perpendicular to the wafer surface might not be the effective way to distribute the dopant uniformly across the Fin height due to the small surface area

of the Fin. Also, due to silicon channeling, angle implantation might create dopant channeling through the ultra-thin Fin. Our simulation data illustrate the results of dopant distribution into a single Fin structure (35nm W x 55nm H) after several boron implantation conditions. The results demonstrate that a high angle of implantation at certain energy is needed to maximize the dopant distribution in the Fin. However, the maximum usable implant angle is limited by the packing density of the Fins. Further more, the amorphization in the fin area due to implantation might occur. As previously observed in FDSOI, amorphization of the thin silicon layer might suppress the regrowth due to lack of silicon crystal which might lead to higher resistivity and higher leakage. Several simulation data are verified with electrical resistivity measured on the Fin test structure.

### F3.6
**Structural characterization and Coulomb blockade of a-SiNx/ nanocrystalline Si /a-SiNx asymmetric double-barrier structures.** Xinfan Huang, Liangcai Wu, Min Dai and Kunji Chen; Nanjing University, Nanjing, China.

The nanocrystalline silicon (nc-Si) based asymmetric double-barrier structure with the principle of direct tunneling and charge storage have attracted great interest due to its potential application in nano-electronic devices, such as single electron memory. In such structure, the operation with a small number of stored electrons can be realized which is based on quantum confinement and Coulomb blockade principle in the nc-Si. In this paper, we fabricated the a-SiNx/nc-Si/a-SiNx double-barrier structures (with the nc-Si size of 2 nm, 4 nm, and 7 nm, respectively) on the p-type Si substrates by plasma-enhanced chemical vapor deposition (PECVD) technique and by subsequent furnace annealing. In planar and cross-section transmission electron microscopy (TEM) photographs, we observed separate nc-Si grains almost of the same size as the thickness of as-deposited a-Si layers due to the constrained crystallization principle. The density of the nc-Si is of the order of 1011cm-2. By Raman scattering spectroscopy, we further verified the existence of nc-Si in the structures. By using capacitance-voltage (C-V) measurements, we studied the electrical properties of the structures. At room temperature, two capacitance peaks were observed due to resonant tunneling and Coulomb blockade in low frequency C-V curves of both samples with 2 nm- and 4 nm-thick nc-Si layers, respectively. From the interval between the two peaks, the Coulomb charging energy of nc-Si dot with the diameter of 2 nm and 4 nm were estimated to be 175 meV and 102 meV respectively, which are in good agreement with the results obtained by theoretical calculation (180 meV and 90 meV respectively). While in the C-V curves of the sample with 7 nm-thick nc-Si layer, three peaks were observed. The frequency dependence of the resonant tunneling of electron was also investigated, which demonstrated that each capacitance peak in C-V curves was caused by injecting a single electron into every nc-Si. We estimated the density of nc-Si grains to be about 1011 cm-2 based on that, which is in agreement with the result of TEM photographs. This a-SiNx/nc-Si/a-SiNx asymmetric double-barrier structure is one of the basic units of nc-Si floating gate FET, which could be applied for future room temperature nanoelectronic devices such as nanomemory.

### F3.7
**Possible Operation of Periodically Layered Nanocrystalline Porous Silicon as An Acoustic Band Crystal Device.**
Akira Kiuchi, Bernard Gelloz and Nobuyoshi Koshida; Tokyo Univ. A&T, Tokyo, Japan.

Previously [1], we reported that porosity-modulated periodic structure of nanocrystalline porous silicon (nc-PS) operates as a nonlinear optical device under photoexcitation or injection of carriers as well as a microcavity. This is based on the controllability of refractive indices of nc-PS in a wide range. Because of a hard mechanical property of crystalline silicon, there should be a possibility that periodic nc-PS structure is useful for application to a key component of the acoustic band crystal (ABC) device. As the first step, it is shown here by a theoretical calculation that acoustic stop bands are generated in the periodic nc-PS structures. The acoustic wave propagation in the periodically stacked nc-PS layers was calculated in a simplified one-dimensional model with a modulated elastic constant in a similar way to the case of compound semiconductor superlattices [2]. The major device parameters are the pitch of the two nc-PS layers with different porosities and the respective portion of the thickness. For the elastic constants of nc-PS layers, the values reported by Bellet [3] were used in corresponding to the porosity. Emphasis is paid upon the frequency region for the occurrence of the acoustic stop band in terms of the device parameters. The major results are as follows: (1) Acoustic stop bands are produced in various frequency regions dependent on the parameters of periodic nc-PS structures. (2) The frequencies corresponding to acoustic stop bands strongly depends on the pitch of two nc-PS layers with different porosities. (3) Another important parameter for the stop bands frequency is the porosity of the respective nc-PS layers by which the elastic constant is

determined. (4) As the contrast in the elastic constant between the two nc-PS layers is increased, the stop band frequency tends to decrease. (5) When the device are composed of many stacked nc-PS layer pairs with low (20%) and high (90%) porosities (the pitch of the two layers and their proportion are 10 $\mu$m and 0.5, respectively, in this case) the minimum frequency of the acoustic band gap is about 40 MHz. The above results show a new possibility of nc-PS layer for the ABC device applications. In appropriate combination between the ABC operation with the thermally induced ultrasonic emission [3] and with the optoelectronic characteristics, some applications will be opened toward function-integrated devices. 1. M. Takahashi and N. Koshida, J. Appl. Phys. 86, 5274 (1999). 2. B. Jusserand et al., Phys. Rev. 33, 2897 (1986). 3. D. Bellet, in Properties of Porous Silicon, Chapt 4, ed. L. Canham (IEE, 1997) pp.127-131. 4. H. Shinoda, T. Nakajima, M. Yoshiyama and N. Koshida, Nature 400, 853 (1999).

### F3.8
**Thermal conductivity of porous silicon evaluated from phase characteristics of photoacoustic spectroscopy.** Masato Ohmukai, Hirokazu Shimizu and Yasuo Tsutsumi; Electrical and Computer Eng., Akashi College of Technology, Akashi, Hyogo, Japan.

Porous silicon, well known as a visible luminescent material, has been revealed to be an attractive candidate for the application to ultrasonic emitter recently. Since the ultrasonic emission is induced thermally it is important to evaluate thermal properties of porous silicon. We are investigating the evaluation of thermal conductivity of porous silicon using phase delation in photoacoustic signals. We report the dependence of thermal conductivity on anodization time during forming porous silicon.

### F3.9
**Extreme Aspect Ratio Semiconductor Structures.**
A. Amezcua[1], P. Sazio[1], H. Fang[2], D.-J. Won[2], T. Scheidematel[2], B. Jackson[2], Neil F. Baril[2], J. Badding[2] and V. Gopalan[2]; [1]Optoelectronics Research Center, University of Southampton, Southampton, United Kingdom; [2]Materials Research Institute, Pennsylvania State University, University Park, Pennsylvania.

We have succeeded in synthesizing semiconductors (Si and Ge) inside a highly ordered array of nanometric holes in over centimeters length scales. These high-index contrast, extreme aspect ratio structures have fascinating optical properties, including light guiding, optical modulation, and a convenient way of forming two and three dimensional photonic crystal structures without lithography. The synthesis and optical guiding properties of these structures will be presented. This development also opens up new avenues for highly ordered semiconductor nanowires research from quantum confined effects to optical lasing.

### F3.10
**On-chip Silicon based Waveguide with 1D Photonic Crystal Cladding.** Yasha Yi, Peter Bermel, Shoji Akiyama, Xiaoman Duan and Lionel C. Kimerling; DMSE, M.I.T, Cambridge, Massachusetts.

We developed a new type of on-chip silicon waveguide - the Photonic Crystal(PC) Cladding waveguide, in which the cladding layers are comprised of high index contrast dielectric layers (e.g., Si/SiO2 or Si/Si3N4). A unique feature of this waveguide is that the refractive index in the new PC cladding waveguide core has a large flexibility, low index core (e.g. SiO2) or hollow core waveguide can be realized on silicon chip. In parallel to the conventional index guiding waveguide, the PC cladding waveguide can be designed as slab waveguide, ridge waveguide, and channel waveguide, which have low index core (SiO2 or air) and high index contrast dielectric cladding pairs (Si/SiO2 or Si/Si3N4). Besides, our fabrication process is entirely Si-CMOS-compatible. The mode dispersion and field profiles of these waveguides are studied and found to be very similar to that of metallic waveguides. To demonstrate the PBG guiding mechanism, we prism couple to the asymmetric PC cladding waveguide, and the effective index of the propagation mode is measured directly. The measured effective mode index is less than either of both Si and Si3N4 cladding layers, which is a clear demonstration of the photonic band gap guiding principle. The slab waveguide loss measurement shows low loss of 0.5 dB/cm for both TE and TM modes at 1550 nm. We have also fabricated and measured PC cladding channel waveguide, light is demonstrated to guide in the low index core materials, the waveguide loss and bending loss are also measured and analyzed, which form the foundation for future integration on Si chips. The future challenge on the film stress control due to multilayer stacking is also discussed. Potential applications include high power transmission, low dispersion, thin cladding thickness, nonlinear properties' engineering, and biomaterials sensor on silicon chip.

### F3.11
**High-Speed All-Optical Modulation in Silicon using Two-Photon Absorption and High-Finesse Cavities.**

Christina Manolatou and Michal Lipson; ECE, Cornell University, Ithaca, New York.

The ability to control light with light in Silicon in an integrated fashion would enable the integration of a variety of optical and electronic devices in a single CMOS compatible platform. Most integrated devices in Silicon are passive where the flow of light cannot be altered once the structure is fabricated. Achieving active devices in Silicon is a challenge due to its weak nonlinearity and transparency at telecom wavelengths which require large devices and high-power excitation. Our theoretical analysis shows the feasibility of high-speed, low-power, all-optical modulation in Silicon using free-carrier injection by two-photon absorption (TPA) in highly confining resonant structures. The modulation scheme relies on the sensitivity of the resonator response to small changes its refractive index resulting from the free-carrier plasma effect. TPA allows use of a control beam (pump) at the same wavelength range and coupled through the same waveguide as the signal being controlled (probe). The strong field enhancement inside the resonant cavity, proportional to its finesse, reduces the pulse energy required for given modulation by a few orders of magnitude compared to a non-resonant structure. We investigate theoretically the dependence of the modulation on cavity characteristics and free-carrier lifetime and show that by shrinking the cavity size we can increase the modulation speed while reducing the pump energy. Our analysis shows that modulation depths of at least 50% are achievable with pump pulse width of a few ps and energies on the order of 1 pJ.

### F3.12
**Field Enhancement Mechanisms and Electron Field Emission Properties of WC-SiC Nanocomposite Thin Layers.** W.M. Tsang[1], S.P. Wong[1,2] and J.K.N. Lindner[3]; [1]Dept of Electronic Engineering, Chinese University of Hong Kong, Shatin, Hong Kong; [2]Materials Science & Technology Research Center, Chinese University of Hong Kong, Shatin, Hong Kong; [3]Institut fur Physik, University of Augsburg, Augsburg, Germany.

A WC-SiC nanocomposite thin layer structure consisting of nano-grains of WC embedded in SiC has been fabricated on an n-type Si substrate by ion beam synthesis (IBS) using a metal vapor vacuum arc ion source. A SiC layer was first formed by high dose carbon implantation into the silicon substrate. Subsequent W implantation was performed to form the WC-SiC nanocomposite structure which can only be successfully achieved under appropriate implantation and annealing conditions. Characterization of the implanted samples was performed using atomic force microscopy (AFM), conducting AFM, x-ray diffraction, x-ray photoelectron spectroscopy, and transmission electron microscopy. Excellent field emission properties with an ultra-low turn-on field of 0.35 V/$\mu$m from such a nanocomposite structure have been achieved. By a systematic study of the correlation between the field emission properties from these ion beam synthesized structures and their surface morphology and local surface electrical conductivity, it was demonstrated that for electron field emission from these IBS samples there were two distinct electric field enhancement mechanisms, one corresponding to the surface morphology effect and the other corresponding to the local electrical inhomogeneity effect. In addition, we further propose an internal field enhancement mechanism for the WC-SiC nanocomposite structure. Combining the three field enhancement effects, we can provide a consistent explanation of the excellent field emission properties from the WC-SiC nanocomposite structure. Details of the internal field enhancement mechanism will be described and its consequences will be discussed. This work is supported in part by the Research Grants Council of Hong Kong SAR (Ref. CUHK4200/01E) and by the Germany-Hong Kong Joint Research Scheme of RGC, Hong Kong SAR and DAAD, Germany.

### F3.13
**Structure and Field Emission Properties of SiC Nanotip Arrays by Using ECR-CVD as Self-Masked Dry Etching technique.** Hung-Chun Lo[1,4], Chia-Fu Chen[1], Chih-Hsun Hsu[2], Jih-Shang Hwang[3], Li-Chyong Chen[2] and Kuei-Hsien Chen[4]; [1]Department of Materials Science and Engineering, National Chiao Tung University, Hsinchu, Taiwan; [2]Center for Condensed Matter Sciences, National Taiwan University, Taipei, Taiwan; [3]Institute of Optoelectronic Sciences, National Taiwan Ocean University, Keelung, Taiwan; [4]Institute of Atomic and Molecular Science, Academia Sinica, Taipei, Taiwan.

We report here arrays of SiC/Si nanotips with high aspect ratios ( 100) and sharp apexes ( 1 nm) by direct etching from Si substrates. Well-aligned nanotip arrays were fabricated by single-step electron cyclotron resonance (ECR) plasma process using gas mixtures of silane, methane, argon and hydrogen. Detailed structure analyses using high resolution transmission electron microscopy (HR-TEM) revealed that the process is a self-mask etching process in that, accompanying the etching of Si, deposition of SiC nanoclusters occurred simultaneously, therefore, forming protecting caps on the

tips. The nanotip arrays so produced showed magnificent field emission property with typical field emission current of 0.5 mA/cm$\hat{2}$ at an applied field as low as 0.8V/$\mu$m. Furthermore, the nanotip arrays also exhibited excellent stability, as evident by temporal evolution of the emission current at a constant applied voltage measurement which showed less than 3% fluctuation in one hour. Formation of the gate-controlled SiC nanotip arrays with defined pattern have also been demonstrated. The SiC nanotip arrays produced by ECR-plasma process of monolithic Si wafer offers a Si process compatible, reliable and economic field emission electron source alternative to carbon nanotubes.

## F3.14
**A Low Temperature Inverse Micelle Solvothermal Approach for Shape- Controlled Synthesis of Germanium Nanocrystals.** <u>Wenzhong Wang</u>, Jianyu Huang, Dezhi Wang, Shankar Kunwar and Zhifeng Ren; Physics, Boston College, Chestnut Hill, Massachusetts.

We report a simple low temperature inverse micelle solvothermal route to synthesize large quantity single crystal germanium (Ge) nanocrystals. By adjusting the growth parameters, such as the concentration and type of the surfactant, nanocrystals with different morphology, including nanospheres, nanocubes, etc, have been successfully prepared. The as-prepared nanocrystals were characterized by X-ray diffraction, transmission electron microscopy, high resolution transmission electron microscopy and energy dispersive X-ray spectroscopy. The X-ray powder diffraction patterns show that the as-prepared nanocrystals are diamond-type cubic pure Ge. The Ge nanocrystals prepared using surfactant pentaethylene glycol monododecyl ether (C12E5) as capping agent at high concentration contain a few different shapes including sphere, triangle, hexagon, etc. Pure Ge nanospheres were prepared using low concentration surfactant C12E5 as capping agent. The nanospheres have an average diameter of 20 nm. Using surfactant heptaethylene glycol monododecyk ether (C12E7) as capping agent, we prepared Ge nanocubes with edge length of about 100 nm. The preparation of Ge nanocrystals was performed in a 125 mL Parr reactor (Model 4750, Parr Company, Moline, IL). A typical preparation procedure of Ge nanocrystals is as follows: 80 mL hexane, 0.6 mL GeCl4, 0.6 mL phenyl-GeCl3, 1.8 mL C12E5, and 5.6 mL Na (25 wt% dispersion in toluene) were added to a 200 mL flask. Then the mixtures were stirred in a magnetic stirrer for 30 min before being transferred to a Parr reactor. The Parr reactor was kept at 280 oC for 72 h without any stirring and shaking, and then cooled to room temperature. A black powder was collected and washed with excess amount of hexane, alcohol, and distilled water to remove any NaCl byproduct and hydrocarbon residue, and then dried at 60 oC for 12 h in an oven.

## F3.15
**Ge and Si Nanostructures Deposited by PLD.** <u>Daria Riabinina</u>, Federico Rosei and Mohammed Chaker; INRS-EMT, University of Quebec, Varennes, Quebec, Canada.

Semiconductor nanostructures are of great interest because of their numerous potential applications. Indeed, quantum dots (QD) as the active gain medium in semiconductor lasers may be one of the early applications of nanotechnology within active devices of commercial use. Ge on Si nanostructures is the key system for the integration and development of optoelectronic devices in the existing silicon-based industry [1,2]. Pulsed laser deposition (PLD) has established itself as a very versatile method for thin film growth of almost any kind of materials. During PLD, the interaction between an intense laser and a target material results in the creation of a plasma that contains several species including atoms, ions, electrons and small clusters. This plasma is highly directional and allows the transfer of matter from the target to the substrate. It is known that highly nanocrystalline and cluster-assembled films can be prepared by single beam PLD when deposition is performed into a moderate pressure gas [3]. Recent studied were performed on the size of Si nanoclusters deposited by PLD [4,5]. The size of the deposited nanostructures can be controlled by tuning the deposition conditions. In this work, we study the size correlation of Ge and Si nanoclusters with the deposition conditions such as gas pressure, target-substrate distance and laser fluence. Characterization of the surface morphology was performed by ex situ atomic force microscopy (AFM). The pressure of inert gas (He) was varied from 1 to 10 Torr. For an increase of He pressure it was observed that size of Ge nanoclusters decreases. Decreasing the laser fluence from 5 J/cm2 to 0.5 J/cm2 resulted in increase in the size of Ge nanoparticles. Furthermore, we demonstrated in this work that Si nanoparticles dimensions as a function of deposition conditions do not have similar trends as in the case of Ge. The size-controlled growth of semiconductors nanostructures at room temperature is a major advantage of PLD technique. Usually semiconductors nanostructures are grown by molecular beam epitaxy or chemical vapour deposition. The major problem of these techniques is the limited control of the size and shape of zero-dimensional nanostructures. PLD is an alternative

technique of the growth of semiconductors nanostructures with a good control of their size distribution. 1. N. Motta, J. Phys. : Cond. Matt. 14 (2002) 8353. 2. F. Rosei, J. Phys.: Cond. Matt. 14 (2004) S1373. 3. D.H. Loendes, D.B. Geohegan, A.A. Puretsky, D.P. Norton, C.M. Rouleau, Science 273 (1996) 898. 4. L. Patrone, D. Nelson, V.I. Safarov, M. Sentis, W. Marine, J. Appl. Phys. 87 (2000) 3829. 5. A.V. Kabashin, J.-P. Sylvestre, S. Patskovsky, M. Meunier, J. Appl. Phys. 91 (2002) 3248.

## F3.16
**Si1-xGex Nanocrystals Observed by EFTEM: Influence of the Dry and Wet Oxidation Process.** Angel Cuadras[1], Jordi Arbiol[2], <u>Joan Ramon Morante</u>[3], Tomas Rodriguez[4] and Andres Rodriguez[4]; [1]Electronic Engineering, Universitat Politecnica de Catalunya, Castelldefels, Barcelona, Spain; [2]Scientific and Technical Facilities, Universitat de Barcelona, Barcelona, Barcelona, Spain; [3]Electronics, Universitat de Barcelona, Barcelona, Barcelona, Spain; [4]Electronic Technology, Universidad Politecnica de Madrid, Madrid, Spain.

Si and Ge nanocrystals (NC) embedded in oxide matrix have attracted much attention due to their potential optoelectronic and photonic applications. They could combine efficient and tunable light emission at room temperature together with full compatibility with standard complementary metal-oxide-semiconductor technology. Moreover, a major interest in small-size group-IV NCs relies in the fact that they can have direct optical transitions. Yet, a generalized standard way to grow and produce high quality Si1-xGex NC embedded in oxide matrix, with a good control over size and distribution is not available. In the present contribution we report about the formation of NC in an oxide matrix after polycrystalline Si0.7Ge0.3 oxidation. For it, we have thermally oxidized polycrystalline Si0.7Gex on SiO2 for obtaining NC embedded in the thermal oxide. We have performed wet oxidations at 650 °C and dry oxidations at 850 °C. High Resolution Transmission Electron Microscopy (HRTEM), Electron Energy Loss Spectroscopy (EELS) and Energy Filtered Transmission Electron Microscopy (EFTEM) have been used to characterize the NC after wet and dry oxidations. EFTEM images and EELS analysis show the evolution of the oxidation of polycrystalline Si0.7Ge0.3 layer, leading to the formation of a layer with Ge-rich nanoclusters zones. We have found that the polycrystalline layer is gradually consumed during oxidation, first homogenously both in wet and dry oxidation and later more irregularly. Significant differences arise from wet and dry oxidation. In dry oxidation, the initial polycrystalline Si0.7Ge0.3 layer leads to silicon oxide while Ge is segregation. Once the silicon is completely oxidized, we observe the presence of unoxidized Ge clusters as EFTEM images clearly show. However, it is difficult to assess the presence of Ge in the oxide by means of EFTEM, although infrared spectroscopy (FTIR) shows fingerprints of it. On the contrary, wet oxidation lead to a progressive oxidation of the layer, both of Ge and Si, that maintain island of material which form like NC in the oxide. These NC can be detected even when the layer is completely oxidized, showing a more homogeneous size distribution than dry oxidations. These NC are also Ge-richer in comparison with as-grown Si0.7Ge0.3 layer. In conclusion, wet oxidation seems to be preferable to oxidize polycrystalline Si1-xGex to obtain Ge-rich NC embedded in an oxide matrix, as both Ge and Si are oxidized, in contrast to dry oxidation, where Ge is mainly segregated.

## F3.17
**Rapid Growth of Ge Quantum Dots Prepared by High-Vacuum Ion-Beam Sputtering.** <u>Hsin-Hsien Wu</u>, Material, Cheng Kung University, Tainan, Taiwan.

Numerous efforts have been made for the research and development of quantum dots due to its technological importance. The fabrication of quantum dots is almost exclusively accomplished by molecular-beam expitaxy (MBE) technique. Recently an e-beam evaporation process was also attempted. In this study, a new approach using high-vacuum ion-beam sputter deposition technique was investigated for the fabrication of high-density Ge quantum dots (GeQD). The new approach eliminates the need of expensive MBE equipment. As received (100) silicon wafers and surface modified (100) silicon wafers were used as the substrates. Various substrate temperatures, ranging from 500 C to 800 C, were used. The ion beam intensity and energy was varied through adjusting the inlet gas flow rate and the electron cyclotron resonance (ECR) voltage, respectively. In selected experiments, an assisted ion source was used to enhance the incident beam energy. Ge quantum dots obtained have densities ranging from 5 x 108 cm-2 to 5 x 109 cm-2. The dot size varied from 80 to 700 nm, all with an aspect ratio of 1/10, approximately. The as-grown samples were characterized using atomic force microscopy (AFM) for surface morphology, high resolution transmission electron microscopy (HRTEM), micro-Raman spectroscopy for microstructure, and photo luminescence (PL) for quantum confinement effect. Among the result, a unique PL peak at 971 nm was observed.

**F3.18**
**Abstract Withdrawn**

**F3.19**
**Formation of Sn Nanodots on a (001) Si Surface and their Incorporation in an Overgrown Si Layer.**

John Lundsgaard Hansen[1], Arne Nylandsted Larsen[1], Shusaku Hayama[2] and Gordon Davies[2]; [1]Institute of Physics and Astronomy, Aarhus University, Aarhus C, Denmark; [2]Institute of Physics, King's College London, London, United Kingdom.

The interest in tin quantum dots (QDs) in crystalline silicon is motivated by possible applications for optical components. A predicted direct band gap for $Si_{1-x}Sn_x$ ($0.9 < x \le 1$) [1] and an increase in the band gap energy (from 0.08 eV for $\alpha$-Sn) when forming QDs is the basis for this interest. In this paper we present a method to form a two-dimensional layer of Sn nanocrystals in an epitaxial Si layer grown on a n+ (001) Si crystal. Using this method gives a high degree of freedom to adjust the density and size of the dots since the dots initially are created on the Si surface, that is, lower deposition temperature gives a higher density of dots, and a smaller amount of Sn deposited on the surface gives a decrease in dot size. The formation of Sn dots on the surface can best be described as formation in the Volmer-Weber mode [2]. Incorporation of the Sn dots into the overgrown Si layer will change the form and composition of the Sn dots to a SiSn alloy with a shape elongated in the growth direction. A high temperature treatment of the structure recreates the dot shape as phase separation or void-mediated formation [3] occurs. The optical properties will be discussed where a comparison between different ways of creating the Sn QDs will be made. [1] A. Richard, Soref and Clive H. Perry, J. Appl. Phys. 69 (1991) 539 [2] E. Søndergård, R. Kofman, P. Cheyssac, A. Stella, Surf. Sci. 364 (1996) 467 [3] Y. Lei, P. Möck, T. Topuria, N. D. Browning, R. Ragan, K. S. Min, and H. A. Atwater, Appl. Phys. Let., 82 (2003) 4262

**F3.20**
**Abstract Withdrawn**

**F3.21**
**Epitaxial Sn-Si Islands Formed at the $SiO_2$/Si Interface by Sn Implantation and Annealing.**

Joao M.J. Lopes[1], Paulo F.P. Fichtner[2,1], Fernando Claudio Zawislak[1], Ricardo M. Papaleo[3,1], Francisco Lovey[4], A. Condo[4] and A. Tolley[4]; [1]Departamento de Fisica, Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, Brazil; [2]Escola de Engenharia, Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, Brazil; [3]Faculdade de Fisica, PUC-RS, Porto Alegre, RS, Brazil; [4]Departamento de Materiales, Centro Atomico Bariloche, Bariloche, Argentina.

Thin films of $SiO_2$ on Si (100) were implanted with 120 keV Sn ions at a fluence of $1.5E16$ cm$^{-2}$. After high temperature (900-1100 °C) thermal annealings, an array of Sn-Si islands were observed at the $SiO_2$/Si(100) interfaces due to migration of the implanted Sn ions (initially located at around the middle of the oxide layer). The island system was characterized by transmission electron microscopy (TEM), scanning force microscopy (SFM) and Rutherford Backscattering Spectrometry under channeling conditions (RBS/C). TEM observations on cross-section samples showed either trapezoidal or pyramidal islands (about 1-2 nm high and with a 4-7 nm wide base) epitaxially attached to the Si matrix. SFM images of the Si surface, obtained after oxide removal, revealed also $\approx$1-2 nm high protrusions, packed in a relatively ordered arrangement at an area density of roughly $2E11$ cm$^{-2}$. TEM images of the lattice suggest that the islands have a diamond-like structure, with a lattice parameter slightly larger than that for pure Si crystals. This causes additional strain contrast and plane misalignment with respect to the Si matrix. In fact, the presence of Sn atoms in substitutional positions was demonstrated by RBS/C. The breakdown of the planar $SiO_2$/Si interface and the appearance of the island system is discussed in terms of elastic strain energy accumulation due to the lattice misfit. The influence of the damage produced by Si and O recoils on the stability of the $SiO_2$/Si interface and on the island formation is also discussed.

**F3.22**
**Gated SiGe Single and Double Quantum Dots for Quantum Computation.**

Levente J. Klein[1], S. Goswami[1], K. A. Slinker[1], K.L.M. Lewis[1], Robert Blick[1], J.O. Chu[2], P.M. Mooney[2], Susan N. Coppersmith[1] and M.A. Eriksson[1]; [1]Department of Physics, University of Wisconsin Madison, Madison, Wisconsin; [2]IBM T.J. Watson Research Center, Yorktown Heights, New York.

Spins of localized electrons in quantum dots are promising candidates for quantum information processing. Here we present Coulomb blockade measurements of quantum dots formed in the two-dimensional electron gas of a silicon/silicon-germanium heterostructure. The quantum dots are formed by electron beam lithography and subsequent reactive ion etching. Lateral side gates fabricated from the two-dimensional electron gas itself nearby the dot [1], allows the tuning of the quantum dot potential. Stability plots of the conductance through the quantum dots acquired at low temperature (0.2 K) show stable single electron charging. Recent advances show low charge noise, with no switching events observed over hours of continuous measurement. A large spin relaxation time is expected in Si due to small spin orbit coupling. A fundamental goal of these experiments is the observation of electron spin resonance in an individual quantum dot. As a step towards this goal, we observed electrically detected electron spin resonance in Hall bars formed in silicon/silicon-germanium two-dimensional electron gas. Finally, for tunnel coupled quantum dots, we present well defined stability plot of the conductance as a function of the gate voltage on each dot. Single electron charging of each quantum dot is achieved. [1] "Coulomb Blockade in a Si:SiGe Two-Dimensional Electron Gas Quantum Dot" L.J. Klein et al. Appl. Phys. Lett. 84, 4047 (2004).

**SESSION F4: Si/SiGe THz Devices**
Chair: Jean-Marc Baribeau
Tuesday Morning, November 30, 2004
Constitution B (Sheraton)

**8:30 AM *F4.1**
**Towards a Si/SiGe Quantum Cascade Laser for Terahertz Applications.** Douglas J. Paul, Department of Physics, University of Cambridge, Cambridge, Cambridgeshire, United Kingdom.

There are many potential applications of terahertz radiation including medical and dental imaging, security imaging, bioweapons detection, molecular spectroscopy and pollution monitoring. Terahertz applications have been slow to develop due to the lack of any practical and cheap source of radiation. Recently a GaAs quantum cascade laser has been demonstrated to operate at low temperatures in the terahertz with power outputs up to 80 mW. While the indirect bandgap of silicon has precluded the development of a silicon-based laser due to the inefficient recombination of electrons and holes, the unipolar quantum cascade laser concept should allow a Si-based laser to be produced. Below the optical phonon energy (62 meV or 14.9 THz in silicon), group IV materials have the significant advantage over III-V materials of no polar optical phonon scattering potentially allowing higher operational temperatures. Progress in developing a Si/SiGe quantum cascade laser will be presented including evidence of population inversion along with waveguide designs and measurements. Strain symmetrised Si/SiGe quantum cascade interwell structures with up to 600 active periods will be presented demonstrating tuneable terahertz electroluminescence around 2 THz. The experimental results have excellent agreement with theoretical spectra calculated using a self-consistent 6 band k.p band structure solver. The use of buried silicide layers produced using a technique similar to bond and etch back silicon-on-insulator will be shown to aid the vertical confinement of the optical mode allowing modal overlap and waveguide losses comparable to demonstrated GaAs terahertz quantum cascade lasers. Electroluminescence around 3 THz will be demonstrated from quantum cascade devices fabricated from Si/SiGe heterostructures grown on buried silicide wafers. Potential problems relating to impurity electroluminescence, high current densities, dislocations and waveguide fabrication will be discussed. Pump-probe measurements using a free electron laser have extracted a non-radiative lifetime of 25 ps from a 95 micron wavelength (3.2 THz) quantum cascade emitter. Monte Carlo modelling of the subband scattering mechanisms and dynamics produce a comparable value of 14 ps. The near temperature independence up to 300 K of the non-radiative lifetimes will also be presented.

**9:00 AM *F4.2**
**Recent Results on the Road to a Si/SiGe Quantum Cascade Laser.** Ulf Gennser[1], Alex Borak[2], Maxi Scheinert[2], Laurent Diehl[2], Soichiro Tsujino[2], Claudiu Falub[2], Hans Sigg[2], Elisabeth Mueller[2], Detlev Gruetzmacher[2], Yves Campidelli[3], Olivier Kermarrec[3], Isabelle Sagnes[1], Daniel Bensahel[3] and Jerome Faist[4]; [1]LPN-CNRS, Marcoussis, France; [2]Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland; [3]ST Microelectronics, F-38926 Crolles-Cedex, France; [4]Universite de Neuchatel, CH-2000 Neuchatel, Switzerland.

Quantum cascade (QC) lasers emitting in the mid or far infrared, with continuous wave room temperature operation, are very interesting devices for niche applications such as chemical sensors or medical imaging. Of particular interest, the QC laser design, exploiting intersubband transitions instead of band-to-band recombination, does not a priori limit itself to direct bandgap materials, and the possibility of realising a silicon based intersubband laser has recently attracted serious interest. Pseudomorphic Si/SiGe QC structures have been realised, exhibiting electroluminescence in the 9 $\mu$m range, with non-radiative lifetimes around 0.5 ps. Using

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SiGe pseudo-substrates, strain compensated Si/SiGe QC structures grown at low T ($\approx$300 $^\circ$C) and containing up to 30 cascades have been realised, with interface roughness as low as 0.3 nm. Using a 'bound-to-continuum' (B-C) design to enable the rapid extraction of carriers via a superlattice miniband, electroluminescence in the 7 $\mu$m range has been demonstrated at current densities of up to 8 kA/cm$^2$, though with a reduced quantum efficiency compared to the pseudomorphic case. A major complication is the use of the valence band, where the Si/SiGe heterostructures have their maximum band offset. Hence, a B-C design based on heavy hole states will have interspersed light hole states that may reduce the non-radiative lifetime. However, studies of simple tunnelling structures show that the scattering in these structures is sufficiently low, so that the total angular momentum is conserved during tunnelling. As a consequence, the minigaps between heavy hole levels can effectively block transport, even in the presence of light hole states. Achieving lasing with these highly strained valence band heterostructures requires the solution of a host of problems in terms of the material, the laser design and the intersubband physics of the valence band. Current research is focused on developing high conductivity, low optical loss contact structures and new waveguide designs; increasing the quantum efficiency of the strain compensated cascade structures; and understanding the effect of the interspersed light hole states.

**9:30 AM *F4.3**
**The emission of Terahertz radiation from doped silicon devices.** James Kolodzey, Pengcheng Lv, R. Thomas Troeger, Sangcheol Kim and S. K. Ray; Elec. & Comp. Eng., University of Delaware, Newark, Delaware.

Recent interest in biological imaging, remote sensing, and biochemical spectroscopy has made nanoscale Terahertz (THz) emitters based on semiconductors become extremely attractive. THz lasers with good performance (emitting over 1 milliWatt CW at 10 K) have been fabricated from the group III-V compounds by molecular beam epitaxy, but such devices are complex with over 500 quantum wells and barriers and are incompatible with low cost Si processing. Similar devices from the SiGe system have had difficulties because the strain limits the total number of active layers, and have produced relatively poor performance (peak powers near 5 nW), even using strain symmetric active regions on virtual substrates of relaxed SiGe buffers. We report here on the characteristics of a new type of THz emitting device with higher powers (above 0.1 milliWatt) based on radiative impurity transitions in doped silicon, which can be simply fabricated without Ge alloying. The THz emitters were fabricated from both p-type and n-type doped silicon wafers with typical resistivities of 5 Ohm-cm, using conventional photolithography and metal contact lift off. Samples were electrically pulsed and the electroluminescence was measured by Fourier Transform Infrared spectrometry. At 4.2 K, the emission spectra showed several peaks centered around 8.1 THz for the boron doped device, 7 to 13 THz for the gallium doped device, and 6.6 THz for the phosphorus doped device. The electroluminescence was attributed to radiative transitions from excited p-like to s-like hydrogenic states, with emission energies in remarkable agreement with the known dopant absorption levels. Current versus voltage measurements suggested an excitation mechanism based on impact ionization of neutral dopants by hot carriers. The net quantum efficiency (emitted photons per injected electron) was estimated to be up to 0.2%. The temperature dependence will be reported with operation above 30 K.

SESSION F5: Si/SiG3 Three-Dimensional
Nanostructures
Chair: J. Kolodzey
Tuesday Morning, November 30, 2004
Constitution B (Sheraton)

**10:15 AM *F5.1**
**Progress in the Growth and Characterization of Ge Quantum Dots and Islands.** Jean-Marc Baribeau, Institute for Microstructural Sciences, National Research Council Canada, Ottawa, Ontario, Canada.

Self-assembled quantum dots have the potential to become the building blocks of the next generation of microelectronic, optoelectronic and photonic devices. $Si_{1-x}Ge_x$ alloys grown on Si (001) are among the best-studied semiconductor systems in which, under appropriate growth conditions, self-organization takes place at the nanometer scale [1]. In this talk, we review progress in the understanding of $Si_{1-x}Ge_x$ island growth and dot formation on Si (001). We discuss the evolution of the island morphology with $Si_{1-x}Ge_x$ coverage, and look at the effect of various growth parameters or post-growth treatments on the shape of the islands and dots. We describe the structural, vibrational and optical properties of $Si_{1-x}Ge_x$ islands and review recent progress in the determination of

their composition and strain distribution. The spatial distribution of the three-dimensional islands and their vertical correlation in mutilayer stacks is also described. We discuss various approaches that have been examined to engineer $Si_{1-x}Ge_x$ quantum dots and in particular control their size, density and spatial distribution. For example, we show how C pre-deposition on Si (001) can influence nucleation and growth of Ge islands. We also describe growth condiditons that lead to the formation of surface cusps on Si (001) and show how these surface features can promote nucleation of dots. Finally, we briefly review recent progress in the use of $Si_{1-x}Ge_x$ island superlattices in device applications. [1] J.-M. Baribeau, N.L. Rowell and D.J. Lockwood, Self-Assembled $Si_{1-x}Ge_x$ Dots and Islands, in Self-Organized Nanoscale Materials, edited by M. Hidachi and D.J. Lockwood (Kluwer/Plenum, New York, 2005).

**10:45 AM F5.2**
**1D Alignment of Nanoscale Ge Islands on Grooved Si(001) Surfaces.** Takeshi Kitajima[1], Bing Liu[2] and Stephen R. Leone[2]; [1]Electrical and Electronic Engineering, National Defense Academy of Japan, Yokosuka, Kanagawa, Japan; [2]Departments of Chemistry and Physics, and Lawrence Berkeley National Laboratory, University of California Berkeley, Berkeley, California.

Positioning of size controlled quantum dot arrays is one of the main issues of nanoscale surface design and materialization. The combination of lithographic patterning and self-assembly of nanoscale 3D islands via the Stranski-Krastanov growth mode of lattice-mismatched Ge/Si heteroepitaxy can provide ordered dot arrays. Here we present 1D alignment of size-controlled Ge 3D islands on electron beam patterned Si surfaces with V-grooves. The Si(001) surface is patterned into lines by V-grooves using electron beam lithography and subsequent chlorine plasma etching. The typical width and depth of the groove is 100 nm and 20 nm, respectively. The sample is grown in a MBE chamber, which also has an ion gun and AES. After the surface cleaning and annealing, 6 ML of Ge is supplied at the rate of 1 ML/min and the sample temperature is kept at 850 K. Surface morphology of the grown sample is measured by ex situ atomic force microscopy (AFM). Two types of patterns are prepared for the growth. One is a line pattern with <100> directed grooves and the other has <110> directed grooves. On the <100> line pattern, both of top Si(001) surface atoms between the grooves and Si(103) vicinal side facet atoms of the V-groove accommodate Ge islands. On the <110> line pattern, only top Si(001) atoms have islands and the Si(113) vicinal side facet atoms are free of islands. The absence is most likely due to the lower surface free energy of the (113) facet. Islands on the top (001) surface atoms of both the <110> and <100> line patterns are dome-type islands of 50 nm width and 4 nm height on average when the line width is more than 100 nm. When the line width is less than 100 nm, islands on the top surface of the <110> line pattern is extended in the <110> direction. This shows that the islands grow faster in the <110> direction due to a bias for Ge dimer diffusion on the modified surface morphology. On the <100> line pattern, the island shape shows no change. Islands on the (103) vicinal facet in grooves of the <100> line pattern are pyramid-type islands of 35 nm width and 2 nm height on average. The island base is directed toward the <100> direction and shows similarity to the pyramid-type islands on the (001) surface. The density of these islands are about twice the island density on the top surface and islands form one dimensional arrays because of the limited width of the side facet. The nucleation of pyramid islands on the side facets of the grooves might be due to the high surface free energy of the (103) surface, which have one dangling bond for each step. During growth, the Ge wetting layer on the Si surface should minimize its energy via diffusion of Ge toward the grooves by covering the dangling bonds with excess Ge. Preferential nucleation of islands in the groove on a 4 ML sample support this hypothesis. We believe this is the first example of an artificial 1D regimented array of pyramid-type islands of less than 50 nm size.

**11:00 AM F5.3**
**Formation of Ultrahigh Density $\beta$-FeSi$_2$ Nanodots by Codeposition of Fe and Si on Oxidized Si(111) Surfaces.** Yoshiaki Nakamura[1,2], Yasushi Nagadomi[1] and Masakazu Ichikawa[1,2]; [1]Dept. of Applied Physics, The Univ. of Tokyo, Tokyo, Japan; [2]CREST, Japan Science and Technology Agency, Tokyo, Japan.

Semiconducting $\beta$-FeSi$_2$ is attractive as a promising material for a Si-based light emitter with a wavelength ($\approx$1.5$\mu$m) of optical fiber communication. It has been reported that strained $\beta$-FeSi$_2$ on Si (111) can be a direct-gap semiconductor [1]. Therefore we expect that $\beta$-FeSi$_2$ nanodots on Si (111) have high light-emitting efficiency because coherent nanodots preserve strain caused by the lattice mismatch and a nanodot has almost no impurities due to its small size. In this work, we report formation of $\beta$-FeSi$_2$ nanodots with ultrahigh density by codeposition of Fe and Si on oxidized Si (111) surfaces. Samples cut from an n-type Si (111) wafer were introduced into the ultrahigh vacuum (UHV) chamber at the base pressure of

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$\approx 1 \times 10^{-8}$ Pa, equipped by scanning tunneling microscopy (STM) and reflection high-energy electron diffraction (RHEED) apparatuses. Clean Si (111)-(7x7) surfaces were prepared by flushing at 1250 °C in the UHV chamber. The samples were oxidized at 600 °C for 10 min at the oxygen pressure of $2 \times 10^{-4}$ Pa in the chamber to form ultrathin Si oxide films with a thickness of 0.3 nm. Si with an amount of 0.5 bilayer (BL) was predeposited onto the ultrathin Si oxide films at 500 °C to create nucleation sites before codeposition of Fe and Si. Then Fe and Si were simultaneously deposited onto the samples with a stoichiometric ratio of deposition rates (1:2) up to amounts of 4 monolayer (ML) and 4 BL, respectively at growth temperatures within 400-600 °C. For the sample grown at 500 °C, STM images showed that semispherical nanodots were formed with the average size of $\approx 5$nm and the density of $\approx 2 \times 10^{12}$ cm$^{-2}$. RHEED patterns of this sample indicated that $\beta$-FeSi$_2$ nanodots were epitaxially grown on Si (111). On the other hand, RHEED patterns showed that the main phase of the nanodots was c-FeSi for the sample grown at 400 °C and $\alpha$-FeSi$_2$ for the sample grown at 600 °C. We annealed $\beta$-FeSi$_2$ nanodot samples at 550 °C to improve the nanodot crystallinity, which was confirmed by RHEED patterns. STM images of annealed samples showed a larger dot size of $\approx 7$ nm and a smaller dot density of $\approx 1 \times 10^{12}$ cm$^{-2}$ by coalescence. To investigate the effect of the nucleation sites created by Si predeposition, we made samples without predeposition. For the samples made by codeposition of Fe and Si at 500 °C without predeposition, STM images showed similar nanodots in size, density, and shape to the case of samples made with nucleation sites. However, RHEED patterns indicated mixed phases of c-FeSi and $\alpha$-FeSi$_2$ were formed in nanodots. We could form $\beta$-FeSi$_2$ nanodots with ultrahigh density ($> 10^{12}$cm$^{-2}$) by codeposition of Fe and Si at 500 °C after predeposition of Si, and improve the crystallinity of $\beta$-FeSi$_2$ nanodots by annealing at 550 °C. This work was partly supported by JSPS.KAKENHI (15201023). References [1] L. Miglio, V. Mergalli, and O. Jepsen, Appl. Phys. Lett. **75**, 385 (1999).

**11:15 AM F5.4**
**Growth and Overgrowth of Ge/Si Quantum Dots: An Observation by Atomic Resolved HAADF-STEM Imaging.** D. Zhi[1], P. A. Midgley[1], R. E. Dunin-Borkowski[1], B. A. Joyce[2], D. W. Pashley[3], Andrew L. Bleloch[4] and P. J. Goodhew[5]; [1]Materials Science and Metallurgy, University of Cambridge, Cambridge, United Kingdom; [2]Physics, Imperial College, London, United Kingdom; [3]Materials, Imperial College, London, United Kingdom; [4]UK SuperSTEM Laboratory, Daresbury, United Kingdom; [5]Engineering, University of Liverpool, Liverpool, United Kingdom.

Self-assembled formation of quantum dots is of increasing interest for application in optical, nanoelectronic, biological, and quantum computing systems. From fabrication technology point of view, there can be great advantage if it all could be made on Si substrate. Furthermore, Si-Ge is also a model semiconductor system for fundamental studies of the growth and their properties. In practice, as the MBE growth of heterostructure is an inherently non-equilibrium process, the resultant of the formation of self-assembled nanostructures are extremely complex and very sensitive to their growth and overgrowth conditions. The morphology, structure, and composition of the QDs can all be changed during the growth; therefore it will be very crucial to understand their structures of different stages at atomic scale. In this presentation, our efforts are focused on characterizing and understanding the QD growth phenomenon by high-resolution HAADF-STEM imaging. Both the formation of uncapped QD and the effect of encapsulation process were investigated based on the analysis of the direct imaging. The morphological and compositional evolution of the QDs and wetting layers was directly observed at atomic scale for the first time. The results show that during the encapsulation, Ge content in the centre of QD keeps unchanged (100%), despite of significant intermixing, lateral spreading, and lateral inhomogeneous Ge distribution inside a Ge QD. Initially non-uniform wetting layer for the uncapped Ge QD becomes uniform after encapsulation, and a 3-monolayer-thick core with 60% Ge content is formed in the 2nm-thick wetting layer with an average Ge content of 30%. Moreover, the above results were obtained by direct Z-contrast STEM imaging without involving complex image simulation procedures.

**11:30 AM *F5.5**
**Heteroepitaxial Growth on Vicinal and Nanostructured Si(001): From Kinetic Growth Instabilities to Perfectly Ordered Dot Arrays.** F. Schaffler, Institut fur Halbleiterphysik, Johannes Kepler Universitat Linz, Linz, Austria.

The Si(001) surface is intrinsically unstable against kinetic step bunching during Si homo- and SiGe heteroepitaxy [1]. While this phenomena has for some time been associated with a strain-driven equilibrium mechanism [2], it is now clear that it is of purely kinetic origin. Recent kinetic Monte Carlo (KMC) simulations in connection with a basic stability analysis provide strong evidence for step bunching being caused by the interplay between the

adsorption/desorption kinetics at atomic height steps and the pronounced diffusion anisotropy on the reconstructed Si(001) surface [3]. The simulations, which were performed on large unit cells and coverages of up to 1000 atomic layers, show excellent agreement with STM experiments, and qualitatively reproduce the pronounced temperature dependence of the step bunching phenomena [4]. The detailed understanding of step bunching on Si(001) allowed us to tailor the period and height of the bunches by controlling substrate miscut, growth temperature, deposition rate and layer thickness. Using vicinal Si(001) substrates with 4° miscut along [110], homoepitaxial layers with ripple periods of $\approx 100$nm were prepared. These were then employed as templates for the ordering of SiGe or Ge dots grown in the Stranski-Krastanov mode. When the period lengths of the template coincide with the mean spacing of the dots, only one dot row fits into one period. We could show that the dots then nucleate at the step bunches, where the energetically favorable {105} facets of the dots are most easily created. This way 1D ordering of SiGe dots on a nanometer scale can be achieved in an entirely self-organized manner. To realize perfectly ordered SiGe and Ge dots in 2D and 3D, we used arrays of pits that were defined by lithography and reactive ion etching. For small enough periods, only one dot per unit cell is created, which nucleates at the lowest point of the pit. XTEM images reveal that the nucleation site is defined by the intersection of neighboring facets, which form either upon annealing of [5], or by Si buffer layer deposition on, the nanostructured template [6]. By exploiting the strain-driven vertical ordering of Ge dots in a Si/Ge dot superlattice, perfect 3D ordering of Ge dots could be demonstrated. Lithographically defined ordering of SiGe and Ge dots fulfills an essential precondition for all but the most trivial applications of self organized dots, namely their addressability. Combined with vertical ordering that allows the topmost dot layer to be exploited as a sacrificial, self-aligned mask for selective ion implantation, electric contacts to individual dots become now feasible. [1] C.Schelling et al., Phys. Rev. Lett. 83, 995 (1999) [2] J.Tersoff et al., Phys. Rev. Lett. 75, 2730 (1995) [3] J.Myslivecek et al., cond-mat/021231 [4] J.Myslivecek et al., Surface Sci. 520 193 (2002) [5] H.Lichtenberger et al., Appl. Phys. Lett. 82, 3650 (2003) [6] Z.Zhong et al., J. Appl. Phys. 93, 6258 (2003)

SESSION F6: Si Nanocrystals and Porous Si:
Light-Emitting and Other Properties I
Chairs: L. Pavesi and A. Williamson
Tuesday Afternoon, November 30, 2004
Constitution B (Sheraton)

**1:30 PM *F6.1**
**Visible Multi-Color Luminescence from Nanocrystalline Silicon.** Tomio Izumi[1] and Keisuke Sato[2]; [1]Reserch Institute of Science & Technology, Tokai University, Hiratsuk, Kanagawa, Japan; [2]Dept. of Electronic and Computer Engineering, Tokyo Denki University, Hatoyama, Hikigun, Saitama, Japan.

Efficient visible luminescence from nanocrystalline silicon (nc-Si) at room temperature has attracted worldwide attention because of its potential application to Si light emitting devices. The nc-Si was formed in silicon dioxide (SiO2) thin films by co-sputtering of Si and SiO2, and subsequently annealing at high temperature above 900°C. The size of the nc-Si was controlled by changing conditions such as oxidation temperature and HF treatment. ITO and Al electrodes were connected with lead wire in Ag paste to apply the voltage between two electrodes of the EL device. The EL device showed a rectifying behavior. The HF treated EL device (EL-1) and the oxidized EL devices (EL-2 and EL-3) at 600°C and 900°C was at threshold voltage of 4.0 V, 9.0 V and 9.5 V, respectively. The light emissions from these these EL devices were observed by applying the forward vias above these threshold voltages. The EL-1, EL-2 and EL-3 emitted red, green and blue lights at 670, 560 and 410 nm, respectively. The particle size of the nc-Si in these EL devices was 2.5, 2.3 and 1.9 nm for red, green and blue luminescence, respectively. The light emission from these EL devices could be strongly and stable seen with naked eye in air. In this paper, we fabricates the EL devices using HF treated and surface-oxidized nc-Si to realize the silicon-based EL display, which has high brightness, and good stabilit, low voltage and multi color. Moreover, we discuss the formation process of the nc-Si and the emission mechanism. HR-TEM, ESR, FTIR and PL measurements were used for evaluation of the luminescent mechanism of the nc-Si.

**2:00 PM *F6.2**
**Origin of the multiexponential decay dynamics in light-emitting silicon nanocrystals.** Cecile Reynaud[1], Olivier Guillois[1], Nathalie Herlin-Boime[1], Gilles Ledoux[2,3] and Friedrich Huisken[2]; [1]LFP, CEA-CNRS URA 2453, Gif sur Yvette Cedex, France; [2]Institute for Solid State Physics, University of Jena, Jena, Germany; [3]LPCML, CNRS, Villeurbanne, France.

Light-emitting silicon nanocrystals (nc-Si) have attracted much interest due to their importance for optoelectronic devices. Electron hole recombination in a quantum confined system is generally considered as the theoretical frame explaining the photoluminescence (PL) origin. However, there is still a living debate about the PL properties. This is particularly true for the temporal PL behavior. The decay is not single exponential and decay curves well described by a stretched exponential law were systematically reported for all types of nanocrystalline silicon. Such decay kinetics is expected when there are several pathways of deexcitation with different characteristic times, and generally indicates a significant disorder in the material. In the case of silicon nanostructures, the origin of the stretched exponential decay is often attributed to interactions between the nanocrystals, with excitation transfer from the smaller particles to the bigger ones. In contrast to these approaches, the absence of carrier hopping has been demonstrated experimentally in porous silicon [Mihalcescu 1998]. In order to elucidate this question, time-resolved photoluminescence measurements on films made from gas phase grown silicon nanocrystals [Ehbrecht 1999; Ledoux 2000] have been carried out. The gas-phase synthesized nanoparticles are extracted as a supersonic beam, size-selected, and deposited downstream as films of variable densities. The nanoparticle number densities were determined by atomic force microscopy. The PL spectroscopy was carefully studied, as a function of the film density. Incident UV excitation intensity was recorded, the sample absorption measured and the PL yield determined. PL decay dynamics were recorded at different PL wavelengths. The photoluminescence properties appear independent of the film density. Even in the very low density film ( 4?109 particles/cm2) where nanoparticles are completely isolated from each other, the decay kinetics corresponds to a stretched exponential law [Guillois 2004]. This means that carrier hopping alone cannot explain the stretched exponential decay. The origin of the stretched exponential decay must be linked to an intrinsic characteristic of the nc-Si. In this paper, the experimental results will be described in details and compared to the theoretical predictions available in the frame of the quantum confinement model. Then, the possible origins of the multiexponential character of the decay dynamics will be discussed, and the particular properties of the PL in indirect band-gap semiconductors emphasized. [Ehbrecht 1999] M. Ehbrecht, F. Huisken, Phys. Rev. B 59, 2975 (1999) [Guillois 2004] O. Guillois, N. Herlin-Boime, C. Reynaud, G. Ledoux, F. Huisken, J. Appl. Phys. 95, 3677 (2004) [Ledoux 2000] G. Ledoux, O. Guillois, F. Huisken, B. Kohn, V. Paillard, D. Porterat, C. Reynaud, Phys. Rev. B 62, 15942 (2000). [Mihalcescu 1998] I. Mihalcescu, J. C. Vial, R. Romestain, Phys. Rev. Lett. 80, 3392 (1998)

**2:30 PM *F6.3**
**Optical Properties of Si Nanocrystals.** <u>Alexander L. Efros</u>, Center for Computational Material Science, NRL, Washington DC, District of Columbia.

The strong photoluminescence of Si nanocrystals and porous Si, which can be considered as an ensemble of Si nanocrystals, has stimulated great interest in their optical properties. In my talk I will review the major experimental results on the linear and nonlinear optical properties of Si nanocrystals and will analyze these results in the framework of existing theoretical models. At the end I will discuss the several potential optical applications of ensembles of Si nanocrystals.

**3:15 PM *F6.4**
**First Principles Simulations of Group IV Semiconductor Nanomaterials.** <u>Andrew J. Williamson</u>, Physics, Lawrence Livermore National Laboratory, Livermore, California.

The results of recent first-principles calculations of the structural, electronic and optical properties of group IV semiconductor nanomaterials will be presented. At the nanoscale, the surface to volume ratio increases dramatically and new phenomena, such as quantum confinement, arise. Accurate description of these phenomena requires simulations with atomistic detail and accurate treatment of electron correlation. I will describe some of our recent algorithmic improvements to density functional and quantum Monte Carlo electronic structure calculations which enable these techniques to be applied to experimentally realistic size semiconductor nanomaterials. Using these techniques we are able to accurately predict the size dependence of the structural and optical properties of silicon, germanium and carbon nanoparticles. Calculations used to interpret optical and X-ray absorption and photoemission measurements and subsequently predict atomic surface reconstructions, chemical surface doping and structural phase transformations will be discussed.

**3:45 PM F6.5**
**Foerster Effect between Semiconductor Nanoparticles.** <u>Christophe Delerue</u> and Guy Allan; ISEN, IEMN, Lille, France.

The Foerster resonance energy transfer between molecules has been studied for more than fifty years. It has been recently observed in

quantum dot arrays [1] and could be a loss mechanism for quantum dot lasers. This effect can also be used to transfer excitons in a controlled way. Using the tight-binding approximation, we calculate the transition rate between two semiconductor nanocrystals as a function of their distance and their size. We consider intra- and inter-band transitions and show the differences between direct (InAs) and indirect (Si) gap semiconductors. We compare the results with the simple Foerster theory of dipole-dipole interaction and with the radiative lifetime. [1] S.A. Crooker et al., Phys. Rev. Lett. 89, 186802 (2002)

**4:00 PM *F6.6**
**Optical Gain in Silicon Nanocrystals.** <u>Lorenzo Pavesi</u>, Physics, University of Trento, Povo (Trento), Italy.

Optical gain in Si nanocrystals grown by a wealth of different techniques has been observed. The material gain value has been extracted from the modal gain measured with the time-resolved-variable-stripe-length (TRVSL) technique by taking into account the propagation losses and the modal confinement factors of the embedding waveguide structure. Further pump-probe measurements have confirmed the presence of net optical gain. A four level model of this phenomenon has been proposed where the interface between the Si nanocrystals and the embedding matrix is playing a critical role. An interesting dependence on the silicon nanocrystal mean radius as well as on the optical confinement factor and active material refractive index has been observed. A critical balance between stimulated emission and losses mechanisms such as Auger non-radiative recombination or excited state absorption or propagation losses emerges from our data. We acknowledge University of Catania, CNR-IMM of Catania, University of Modena, Technical University of Munich, Rochester University, Max Planck Institute of Halle, Research Institute in Prague, University of Barcellona, University of Helsinki, where the samples reviewed here have been produced.

**4:30 PM *F6.7**
**Silicon Nanocrystals: Photosynthesizers for Molecular Oxygen.** <u>Dmitri Kovalev</u>, Physics Department, Technical University of Munich, Garching, Germany.

The energy transfer of electronic excitation plays an essential role in numerous scientific branches such as photophysics and biochemistry. To elucidate the fundamental physical effects occurring during energy transfer processes semiconductor nanostructures are viewed as a promising systems. Oxygen molecules in the electronic ground state are chemically inert due to their spin-triplet characteristic. The transition from the ground triplet state to one of the excited singlet states and vice versa requires the change of electron spin state (spin-flip process) and direct states conversion via absorption/emission of photons is spin-forbidden in the first approximation. However, excitation of an intermediate substance (photosensitizer, usually dye molecule) and subsequent transfer of energy to oxygen activates the molecule to an excited spin-singlet state. We demonstrate that the efficiency of photosensitization of oxygen molecules mediated by excitons confined in silicon nanocrystals is extremely high: 100% at cryogenic and 75% at room temperature. The remarkable photosensitizing properties of silicon nanocrystal assemblies result from a broad energy spectrum of photoexcited excitons, a long triplet exciton lifetime and a highly developed surface area. We present experimental proof for the efficient generation of singlet oxygen molecules. We show that energy transfer proceeds via direct electron exchange and is accompanied by phonon emission cascade. From time-resolved measurements the characteristic time of energy transfer is found to be in the range of microsec-onds. Magnetooptical experiments reveal the importance of the spin orientation of the exchanged electrons for the energy transfer rate. Room temperature photooxidation of silicon nanocrystals evidences the direct chemical action of photosensitized oxygen molecules.

**F7.1**
**Improved Optoelectronic Characteristics of Nanocrystalline Porous Silicon by High-Pressure Water Vapor Annealing.** <u>Bernard Gelloz</u>[1], Akira Kojima[2], Hajime Sano[1], Masao Niibe[1], Tetsuya Uchida[1] and Nobuyoshi Koshida[1,2]; [1]Elec.&Elec. Eng., Tokyo Univ. A&T, Tokyo, Japan; [2]Quantum14 Co., Tokyo, Japan.

Nanocrystalline porous silicon (PS) is a promising material for achieving various optoelectronic device applications, such as

light-emitting diodes, waveguides, lab-on-chip, potential lasing capabilities, etc [1]. However, its luminescence quantum efficiency remains rather low. Best values to date are about 3% [2] for the photoluminescence (PL) and 1.1 % [3] for the electroluminescence (EL). The luminescence stability of nanocrystalline PS for a long-term operation is also a critical issue which needs to be solved before any applications could be considered. Complete surface passivation is especially important to suppress the generation of non-radiative recombination centers. A possible solution to this problem is to cover the nanocrystalline Si surface with a high quality SiO2 layer with minimized interfacial defects. In order to achieve this high quality surface passivation, a high-pressure H2O vapor annealing technique that is useful for improving the electrical properties of poly-crystalline silicon TFT devices [4] has been applied to nanocrystalline PS. The annealing effects on various optoelectronic properties of PS prepared under various conditions have been studied as a function of the annealing pressure (1 to 3 MPa), temperature (150 to 300 C), and treatment time (1 to 3 h). The microscopic characterizations of the high-pressure-annealed samples have been carried out, including studies on complimentary effects of electrochemical oxidation. It has been observed that the PL of PS is drastically enhanced by the high-pressure anneal under relatively low temperatures, while the emission wavelength remains unchanged. This treatment is very effective to quench non-radiative defects at the nanocrystalline Si surfaces by decreasing the interfacial mechanical stresses, to enhance the carrier localization in Si nanocrystals, and consequently to improve both the luminescence efficiency and stability. The improvement in the optical properties produces desirable effects on the electrical properties as well. Due to a significant decrease in the carrier trap densities at the interfacial oxides, for instance, ballistic electron emission from the PS diodes we reported previously is significantly stabilized. In addition, EL characteristics should be improved, since carrier injection efficiency into luminescent silicon nanocrystals is enhanced. [1] B. Gelloz and N. Koshida, Handbook of Electroluminescent Materials, Chap. 10, 393, edited by D.R. Vij, Institute of Physics Publishing, Bristol and Philadelphia. (2004). [2] J.C. Vial et al. Phys.Rev. B 45,14171 (1992). [3] B. Gelloz and N. Koshida, J. Appl. Phys. 88 (7), 4319 (2000). [4] T. Sameshima, M. Satoh, K. Sakamoto, K. Ozaki and K. Saitoh, Jpn. J. Appl. Phys. 37 L1452 (1998).

## F7.2
**Composition of Ge/Si Islands in the Growth of Ge on Si(111).** <u>Fulvio Ratto</u> and Federico Rosei; EMT, INRS, Varennes, Quebec, Canada.

The heteroepitaxial growth of group IV semiconductors represents a field of enormous interest, due to the possibility it offers to engineer the optoelectronic properties of the resulting structures with vast flexibility1,2. In particular, the Stranski-Krastanov (SK) growth mode of Ge on Si surfaces may yield a real breakthrough in the semiconductor industry. Indeed, the self-assembled Si/Ge 3D islands may act as quantum dots, whose luminescence properties could be used to develop novel optoelectronic devices, compatible with the existing Si-based technology. For these reasons, the growth of Ge on Si substrates has been the subject of numerous theoretical and experimental reports during the past two decades3,4. Nevertheless, several critical issues are still preventing the adoption of Si/Ge nanostructures for device fabrication. One of the points of major concern regards the actual stoichioemtry inside individual 3D islands. Intermixing is known to occur since the early stages of growth of Ge on Si surfaces. A detailed description of the chemical composition gradient inside single dots is necessary to model the potential barriers which cause carrier confinement inside the system. Further, mapping the Si/Ge concentration inside self-assembled islands could cast some light on the nature of the main diffusion mechanisms that produce the alloying itself, thus eventually leading to their control. Our results on the growth of Ge on Si(111) are obtained by Low Energy Electron Microscopy (LEEM) and X-Ray Photoemission Electron Microscopy (XPEEM). The latter yields photoelectron spectra with a high lateral resolution, thus allowing mapping the Si/Ge concentration in the topmost layers of the system5. Ge was deposited by MBE on Si(111) substrates kept at temperatures ranging from 400 to 600 C. The surface morphology was analyzed by LEEM and Si2p and Ge3d XPEEM core level spectra and related images were acquired on individual islands. An analytical framework developed ad hoc allowed us to obtain an unprecedented mapping of the surface stoichiometry with a 30 nm lateral resolution6. A Si enrichment of the islands borders seems to be consistent with diffusion mechanisms which are mainly mediated through surface mobility. Our analysis represents a fundamental improvement in relation to previous results obtained using other experimental techniques, which could not provide the necessary spatial resolution. 1) F. Rosei, J. Phys.: Condens. Matter 16 1373 (2004). 2) C. Teichert, Phys. Rep. 365, 335 (2002). 3) I. Berbezier, A. Ronda, A. Portavoce, J. Phys.: Condens. Matter 14 8283 (2002). 4) P.C. Kelires, J. Phys.: Condens. Matter 16, 1485 (2004) 5) F. Ratto, F. Rosei, A. Locatelli, S. Cherifi, S. Fontana, S.

Heun, P.D. Szkutnik, A. Sgarlata, M. De Crescenzi, N. Motta, Appl. Phys. Lett. 84, 4526 (2004). 6) F. Ratto, F. Rosei, A. Locatelli, S. Cherifi, S. Fontana, S. Heun, P.D. Szkutnik, A. Sgarlata, M. De Crescenzi, N. Motta, in preparation.

## F7.3
**Uniform dome-shaped self-assembled Ge islands by UHV/CVD after boron pre-deposition.** <u>Ning Deng</u>, Wentao Huang and Peiyi Chen; Institute of Microelectronics, Beijing, China.

The effects of pre-deposition of boron with different B2H6 flux on the self-assembled growth of Ge islands on Si(100) substrate by UHV/CVD are studied by atomic force microscopy (AFM). Proportion of dome-shaped Ge islands increases with the increasing of flux of B2H6 [Fig 1]. Quite uniform dome-shaped Ge quantum dots with size and height distribution of less than ±3%, which is much more narrow than the size distribution of typical self-assembled Ge dots, are obtained after appropriate boron pre-deposition[Fig 2]. The lateral size and height of these dots are 60 and 10nm respectively and the density is about 8E9cm-2. Based on the shape transition model we proposed elsewhere, the uniform size and shape distribution after boron pre-deposition was explained. During the growth, boron atoms will diffuse into Ge islands. The reduced lattice mismatch results in a larger critical size for shape transition from pyramids to domes, then uniform dome-shaped Ge islands can be obtained. The results show that method of boron pre-deposition can be used to fabricate quite uniform Ge quantum dots to meet the requirements of opto-electronic devices.

## F7.4
**Classical Versus First-Principles Structural Relaxation: Calculated Electronic Excitations and Optical Properties of Ge Nanocrystals Embedded in a SiC Matrix.**
<u>Giancarlo Cappellini</u>[1,3], Hans-Christian Weissker[2], Davide De Salvador[4], Jurgen Futhmueller[2], Friedhelm Bechstedt[2], Guido Satta[1,3] and Luciano Colombo[1,3]; [1]Physics Department, University of Cagliari, Cagliari, Italy; [2]IFTO, FSU, Jena, Germany; [3]SLACS, INFM, Cagliari, Italy; [4]Physics Department, University of Padova, Padova, Italy.

We discuss and test a combined method to efficiently perform ground- and excited-state calculations for relaxed structures using both a quantum first-principles approach and a classical molecular-dynamics scheme. We apply this method to calculate the ground state, the optical properties, and the electron excitations of Ge nanoparticles embedded in a cubic SiC matrix. The combined method is shown to be applicable to embedded nanocrystals in large simulation cells for which the first-principle treatment of the ionic relaxation is presently out of reach, whereas the electronic, optical and excitation properties can already be obtained via first-principles techniques [1]. [1] J.Furthmueller,G. Cappellini, H.Ch.Weissker, F.Bechstedt, Phys. Rev. B 66, 045110 (2002)

## F7.5
**Self-Assembled Ge/Si Quantum Dot Superlattices: Analysis using Raman Spectroscopy and Capacitance Measurements.**
Ariano R. Rodrigues[1], Giovani Zanelatto[1], Adenilson Jose Chiquito[1], Alexander I. Milekhin[2] and <u>Jose Claudio Galzerani</u>[1]; [1]Physics, Universidade Federal de Sao Carlos, Sao Carlos (SP), SP, Brazil; [2]Institute of Semiconductor Physics, Novosibirsk, Russian Federation.

The three-dimensional confinement of charge carriers in quantum dots is responsible for their electronic and optical properties, which differ substantially from those of bulk materials. The interesting properties of the quantum dots qualify them as promising materials for the design of microelectronic and optoelectronic devices with improved characteristics. Among them, the multilayer nanostructures, such as Ge/Si are of special interest due to their possible application in various devices and integration with modern silicon technology. In this work, the vibration spectra of self-assembled structures with germanium quantum dots were studied using Raman scattering; capacitance measurements were also accomplished. The structures were prepared by molecular-beam epitaxy of germanium and silicon layers on Si (001) substrates, based on the Stranski-Krastanov growth mechanism. After a 500 Å buffer Si layer, ten monolayers of germanium was grown, followed by a 500 Å silicon layer. The process was repeated five times. The growth temperature of germanium was set at 300, 400, 500 and 600 °C. Resonant Raman scattering was accomplished with excitation energies provided by Ar+Kr+, titanium-saphire and dye (rhodamine 590) lasers. The spectra were acquired at the temperature 8 K. The longitudinal optical phonon confined in the dots was monitored, revealing that the dots are strained in these structures; the intensity and the frequency position of this Raman line are analyzed as a function of the excitation energy for each sample. The resonance maximum at 2.4 eV observed in the case of the sample grown at 300 °C is attributed to the $E_1$ exciton (1) in the strained Ge dots. For 400 °C, however, the $E_0$ resonance was

also detected, around 2.55 eV. The amplitude of the resonance curve falls to a half as compared to the former, as an indication that the sizes of the dots have diminished. For these two samples, it could be clearly observed that the confined phonon frequency shifts downward, suggesting a size distribution of the quantum dots. For the sample grown at 500 °C, the resonance amplitude drastically decreases, and the phonon frequency behavior with the excitation energy cannot be unambiguously followed anymore. The analysis of the sample grown at the highest temperature revealed no contribution of the quantum dots. The capacitance versus voltage measurements using standard lock-in techniques confirmed the presence of the Ge quantum dots in the 300 and 400 °C samples only. (1) S. H. Kwok, P. Y. Yu, C. H. Tung, Y. H. Zhang, M. F. Li, C. S. Peng and J. M. Zhou, Phys. Rev. B59(7), 4980 (1999).

## F7.6
**Measurement of the Concentration-Dependent Si-Ge Interdiffusivity During Oxidation Enhanced Interdiffusion in Si-Ge Heterostructures.** Nevran Ozguven, Daniel B. Aubertine and Paul C. McIntyre; Materials Science and Engineering, Stanford University, Stanford, California.

We present a study of the effects of Si surface oxidation, a well-established method for injection of interstitial defects into silicon, on Si-Ge interdiffusion in epitaxial heterostructures. Measurements were performed on single crystal $Si_{1-x}Ge_x/Si_{1-y}Ge_y$ superlattices grown by low-pressure chemical vapor deposition onto Si (001) substrates. An epitaxial Si cap, which is partially consumed during dry $O_2$ post-anneals, is grown on these superlattices for the oxidation experiments. Measuring interdiffusivity via x-ray diffraction involves monitoring the decay of x-ray (000) or (004) superlattice satellites as a function of annealing time. In a model system, where the interdiffusivity is concentration independent, the logarithm of the superlattice satellite decay rate is linearly proportional to the interdiffusivity. Typically, a straightforward analysis of this type is not possible with SiGe because the interdiffusivity is a strong function of Ge concentration. In previous work we have shown that by using $Si_{1-x}Ge_x/Si_{1-y}Ge_y$ superlattices with an as-grown composition amplitude of less than 2% Ge we are able to extract the interdiffusivity at a multilayer's mean composition. In this presentation, we describe an observed enhancement of the Si-Ge interdiffusion kinetics for the case of oxidation anneals when compared to inert atmosphere anneals. The x-ray scattering method is used to quantify the effects of nonequilibrium point defect concentrations created during Si oxidation on the interdiffusivity of Si and Ge over the temperature range 770°C to 870°C.

## F7.7
**Evolution of the Luminescence Spectrum During the Dry and Steam Oxidation of SiGe Films.** Andres Rodriguez[1], Jesus Sangrador[1], Tomas Rodriguez[1], Angel Carmelo Prieto[2], Manuel Avella[2] and Juan Jimenez[2]; [1]Tecnologia Electronica, E.T.S.I. de Telecomunicacion, Universidad Politecnica de Madrid, Madrid, Madrid, Spain; [2]Fisica de la Materia Condensada, E.T.S.I. Industriales, Universidad de Valladolid, Valladolid, Valladolid, Spain.

Nanoparticles embedded in a dielectric medium can be used for either electronic memories or photonic devices. Up to date, there are only a few reports about the synthesis of nanoparticles of SiGe by oxidation and/or annealing of SiGe films, though the oxidation of SiGe has been studied in the past. In this work, a comparative analysis of the two oxidation processes in SiGe layers using Raman and FTIR spectroscopies is presented. When SiGe films are oxidized in a pure oxygen ambient, Ge is segregated from the growing silicon oxide and a progressive Ge enrichment of the remaining layer occurs, ending with the formation of elemental Ge, which is subsequently oxidized. For advanced oxidation, Ge oxides appear and nanoparticles of Ge were found to form. When the SiGe films are oxidized in steam, the oxide layer contains a mixture of Si-O and Ge-O bonds from the very beginning of the oxidation process. Ge segregation also occurs, but it is much less important in this process than in the dry one. The cathodoluminescence of these samples was also studied, showing the existence of blue luminescence at 3.1 eV, which is related to the presence of defects at the interface between Ge nanocrystals and the oxide matrix, and a UV band at 4 eV. To clarify the origin of the luminescence bands, dry and steam oxidation processes were carried out using SiGe films of different thickness. In dry oxidized SiGe, the luminescence emission appears only when the film is close to full oxidation, no matter its original thickness, reaches a maximum and then vanishes when the oxidation is completed. In steam oxidized SiGe layers, however, the luminescence progressively increases in intensity as the oxidation proceeds and reaches a maximum when the layer is fully oxidized. The origin of the luminescence is discussed in terms of the nature of the oxides and the presence of nanoparticles in each stage of the oxidation.

## F7.8
**Dislocation and Strain Distribution Analysis for SiGe Buffer Layers Formed on Silicon on Insulator Substrates.** Noriyuki Taoka[1], Akira Sakai[1], Shogo Mochizuki[1], Osamu Nakatsuka[2], Shigeaki Zaima[1], Yukio Yasuda[1], Masaki Ogawa[2], Tsutomu Tezuka[3], Naoharu Sugiyama[3] and Shin-ichi Takagi[3]; [1]Graduate School of Engineering, Nagoya University, Nagoya, Japan; [2]EcoTopia Science Institute, Nagoya University, Nagoya, Japan; [3]MIRAI Project, Association of Super-Advanced Electronics Technology, Kawasaki, Japan.

For Si-based electric devices with high mobility and low power-consumption, technologies which combine advantages of using silicon-on-insulator (SOI) substrates with those of strained lattice channels have been recently developed. Strain-relaxed SiGe buffer layers formed on SOI or directly on insulator (SGOI) are promising candidates for substrates to realize these devices. This paper addresses the analysis for microstructures in SGOI formed by two typical methods and clarifies the relationship between dislocation introduction and strain distribution in SGOI. One of two processes employed here to form SGOI was a Ge-condensation method in which pseudomorphic SiGe layers epitaxially-grown on SOI substrates were oxidized [1]. Strain of the SiGe layers was almost completely relaxed and low threading dislocation density was obtained. On the other hand, X-ray diffraction two-dimensional reciprocal space mapping (XRD-2DRSM) showed asymmetric diffraction profiles indicating that the SiGe layer had mosaic structures. Furthermore, in plan-view TEM images, contrasts relevant to residual strain-undulation, running approximately along two orthogonal in-plane <110> directions, were clearly observed in SGOI although no misfit dislocations lying parallel to the film surface were seen. This result strongly suggests that 60( misfit dislocations glided-out from the SiGe layers during the oxidation process while local strain-undulation caused by the dislocations still remained even after the SiGe layer was totally strain-relaxed. We have tried another process in which the strain relaxation of SiGe layers was accomplished predominantly by introducing pure-edge dislocation networks [2]. After cleaning a SOI (001) substrate surface, a low-temperature Ge layer was epitaxially grown and an amorphous Si (a-Si) cap layer was subsequently deposited; a typical sample structure was a-Si (17nm)/200(C-grown Ge (35nm)/SOI(100nm). The sample was then annealed at 1100(C in N2 ambient. The a-Si and the Ge layers were intermixed and the strain-relaxed SiGe with the pure-edge dislocation network at the SiGe/SOI interface could be formed. Furthermore, by increasing the annealing duration, enhanced solid-phase intermixing of Ge and Si resulted in the SiGe buffer layer directly formed on the insulator. Although residual threading dislocations were seen in this type of samples, XRD-2DRSM clearly revealed that the SiGe layer formed by this process exhibited much smaller mosaicity compared to those prepared by the Ge-condensation method. This work was partly supported by NEDO. [1] T. Tezuka et al., Materials Science and Engineering B89 360(2002). [2] N. Taoka et al., Material Science in Semiconductor Processing, submitted.

## F7.9
**Nanostructures in cleavage process simulation of silicon on the basis of large-scale electronic structure calculations; surface reconstruction, anisotropic strain and step formation.** Takeo Hoshi, Yusuke Iguchi and Takeo Fujiwara; Department of Applied Physics, University of Tokyo, Hongo, Bunkyou-Ku, Tokyo, Japan.

For recent years, we have developed theory and program code for large-scale electronic structure calculations [1-4]. Their mathematical foundation is to calculate the one-body density matrix of electron system, in stead of one-electron eigen states. Molecular dynamics simulations are demonstrated with up to more than ten million atoms. The large-scale calculation method can provide process simulations of silicon with the size of up to more than 10 nm. The method is applied to cleavage process [2,4], a non-equilibrium process. Cleavage dynamics is simulated with external loads. Bondbreaking and surface rebonding occur, when the bulk (sp3) wavefunctions change their character, locally, into surface (non-sp3) wavefunctions. As a remarkable feature of 10 nm scale simulations, step formations are observed. We focus the unstable cleavage with (001) plane and the stable (experimentally observed) cleavage with (111)-2x1 plane. First, the cleavage process under [001] external load is investigated. In smaller samples, with the size of about 4 nm, a (001) cleavage plane is obtained, in which the asymmetric surface dimers appear. In larger samples, with the size of 10-20 nm, however, the (001) cleavage plane becomes unstable with many step formations. The result is consistent to the experimental fact that no (001) plane appears as cleavage surface. Second, the cleavage process with [111] external load is simulated. During the cleavage propagation, the pi-bonded (Pandey) (2 x 1) structures are formed, as elementary process. An anisotropic surface strain is induced by forming the pi-bonded structure, which enhances the successive formation of the pi-bonded structure. As well

as the elementary (2 x 1) structure, different types of step formations are observed and compared to experiments [5-7]. In a case, a well-defined (2x1) domain appear after the step formation, though the cleavage surface is defective before the step formation. Moreover, in several cleavage simulations, the cleavage path is bent from the (001) plane into the (111)-2x1 plane. These results imply the (relative) stability of the (111)-2x1 cleavage mode. A common theoretical viewpoint among the above nanostructures is the competition of two anisotropic strain mechanisms; (i) strain due to the global (crack) shape and (ii) strain due to the local atomic or electronic structure. They can be different in magnitude and in symmetry. We speculate that the competition is inherent in all the structural properties on the order of 10 nm. [1] Hoshi and Fujiwara, J. Phys. Soc. Jpn (JPSJ) 69, 3773 (2000). [2] Hoshi and Fujiwara, JPSJ 72, 2429 (2003). [3] Takayama, Hoshi and Fujiwara, JPSJ 73, 1519 (2004). [4] In preparation; The current list of our works is seen in our web page: http://fujimac.t.u-tokyo.ac.jp/hoshi/ [5] Feenstra and Stroscio, Phys. Rev. Lett. 59, 2173 (1987) [6] Tokumoto et al., J. Vac. Sci. Technol. B9, 595(1991) [7] Mera et al., Ultramicroscopy 42-44, 915 (1992)

### F7.10
**Growth and Properties of Core/Shell Silicon Nanowires.**
Florian M. Kolb, Herbert Hofmeister, Eckard Pippel, Margit Zacharias and Ulrich Goesele; MPI of Microstructure Physics, Halle (Saale), Germany.

Semiconductor nanowires are potential building blocks for future nanotechnological applications. A method for silicon nanowire fabrication is the combination of silicon monoxide evaporation with gold islands on a silicon substrate [1], similar to the vapor-liquid-solid (VLS) mechanism. This method combines the simplicity of silicon monoxide evaporation with the possibility of enhanced growth control. The resulting wires have a core diameter of down to 10 nm. With this contribution we will present a detailed investigation of the growth of these nanowires and their structural properties. Post-treatment of the wires by etching and post-oxidation offers a way for further decreasing the size of the nanowires. As result we will present a model for the growth process as well as an experimentally supported explanation for nanowire diameter oscillations during the growth. The nanowires fabricated with this method consist of a crystalline silicon core and a thick amorphous oxide shell. Analyzing the oxide shell using electron energy-loss spectroscopy (EELS) including the energy-loss near-edge fine structure (ELNES) revealed that the shell consists of silicon dioxide without any silicon suboxides. The nanowires and the gold droplets on their tips were analyzed seperately using electron diffraction and high-resolution transmission electron microscopy (HRTEM). For size control we investigated the effect of gold colloid nanocrystals as starting points for the growth of the silicon/silicon dioxide nanowires. It will be demonstrated how the size of the gold is correlated to the thickness of the nanowires grown by our method. [1] F.M. Kolb, H. Hofmeister, R. Scholz, M. Zacharias, U. Goesele, D.D. Ma, S.-T. Lee, Journal of the Electrochemical Society, 151 (7) G472, (2004)

### F7.11
**Metal-Free Growth of Si Nanowires by Annealing SiOx (x<2) Films Deposited by PECVD.** Xiaoxin Wang, Jianguo Zhang and Qiming Wang; Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China.

The Si nanowire (SiNW) is an important material for nano-electronic and optoelectronic devices. Currently, Si nanowires are usually fabricated with the catalysis of metals, most of which are deep level recombination centers in Si and can deteriorate the performance of the devices based on the Si nanowires thus fabricated. In this paper, we present a new SiNW growth method free from metal catalysis by high temperature annealing of SiOx (x<2) films deposited by plasma-enhanced chemical vapor deposition (PECVD). The influence of the stoichiometry (x value) and the thickness of SiOx films, the annealing temperature and the annealing atmosphere on the SiNW growth was studied in detail. The results indicated that the SiOx film with x equal to 1 was the most favorable stoichiometry for SiNWs growth after annealing at 1000-1150°C. Thinner SiOx films below 300nm in thickness were easier for the growth of SiNWs at lower annealing temperatures. A relatively large N2 flow rate of greater than 10sccm during the furnace annealing was of importance for the SiNW growth, and SiNWs could be sharpened and elongated with the aid of H2 in our study. SiNWs of 50-100nm in diameter and tens of micrometers in length can be fabricated in this way. The formation mechanism is also discussed and is likely to be related to oxide-assisted growth (OAG) mechanism, with SiOx films serving as the Si source. As PECVD and furnace annealing processes are fully compatible with the current Si CMOS technology, this metal-free SiNW growth method has promising applications in fabricating high quality Si nanodevices based on SiNWs.

### F7.12
**Synthesis and Photoluminescence of Silicon-Germanium Alloy Nanowires.** Xiaowei Wang[1], Jiming Bao[2], Jianyu Huang[1], Dezhi Wang[1], Capasso Federico[2] and Zhifen Ren[1]; [1]Physics, Boston College, Chestnut Hill, Massachusetts; [2]Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts.

Silicon-germanium alloy nanowires were synthesized by thermal evaporation and condensation of the mixture of silicon monoxide and germanium powder without any catalyst. EDS, SAED, SEM, TEM were used to characterize the structure and chemical composition of the wire. Photoluminescence study showed that the wire had a strong infra-red emission. And the emission peak position was determined by the ratio of silicon to germanium.

### F7.13
**VLS Epitaxy of Si and Ge Nanowires: Kinetics, Morphologies, and Properties.** S. T. Picraux, T. Clement, J. L. Taraci, J. W. Dailey, David J. Smith and Jeff Drucker; Arizona State University, Tempe, Arizona.

We report on a rich variety of nanostructures which can be synthesized by varying the pressure and temperature in Vapor-Liquid-Solid epitaxy on Si, on their growth kinetics, and on the novel surface energy properties of these materials. In these studies the CVD growth of Si and Ge nanowires is seeded by metallic nanodots on (111) and (100) oriented Si. Experiments are carried out for disilane and digermane in a UHV system for pressures from 10-6 to 10-2 Torr and temperatures between 300 and 800C. The growth kinetics and morphology are observed to depend strongly on pressure for Ge, with the growth of layered heteroepitaxial islands at lower pressures and at higher pressures with a transition to rapid <111> axial nanowire growth with a growth rate that scales linearly with pressure. Growth kinetics are quantitatively compared with that for blanket growth and are contrasted to Si nanowire growth. We also report first measurements of the nucleation time for nanowire growth. Examples of the dramatic superhydrophobic and superhydrophilic behavior of functionalized Si nanowire surfaces will be presented. We combine monolayer surface chemistry with silicon nanowire substrates to create a lotus leaf like surface, and for the first time demonstrate the amplification of light-induced water contact angle switching. Measurements of the contact angle for water on both the smooth and nanowire surfaces allow direct estimation of the effects of surface morphology on hydrophobicity. These results, based on a biomimetic approach to nanotechnology, have new implications for the design of microfluidic systems.

### F7.14
**Fabrication of Uniform Arrays of Nanopillars, Nanospikes and Nanorings Using Modified Nanosphere Lithograpy.** Jefferson Earl Rose, [1]Chemistry, UCLA, Los Angeles, California; [2]Chemistry, UCLA, Los Angeles, California.

Arrays of uniform, Si nanospikes and flat top nanopillars were fabricated using nanosphere lithography and multiple step etching processes. Using a monolayer of self-assembled 470 nm polystyrene nanospheres as a mask, processing that sequences physical Ar+ pre-etching followed by SF6 chemical etching results in nanopillars or nanospikes. For the same chemical etching conditions, a low energy physical pre-etch gives nanopillars and high energy pre-etch results in nanospikes. Both nanostructures have nanowire interconnects that are intrinsic to the fabrication process and are therefore convenient means electrical wire for future devices. In addition arrays of uniform Si nanorings with flat tops were fabricated using new nanosphere chemical modification lithography. A self-assembled monolayer of 470 nm polystyrene nanospheres was chemically etched followed by mechanical agitation which resulted in a mask of nanoring patterns. Subsequent etching of Si results in nanorings that have a thickness of 100 nm, an outer diameter of 250 nm and an inner diameter of 150 nm. By varying the solvent used during processing nanorings, Si nanowire interconnects could be made optional. The silicon surfaces were studied using AFM and SEM. Single Ge quantum dots were self-assembled on Si nanopillars. The Ge quantum dots appear to be self-aligned to the center of of the Pillars. Arrays of Si nanopillars were formed by nano-sphere lithography on the surfaces of Si. The template used to form the nanopillars was a monolayer of nominally 470nm polystyrene spheres. The resulting nanopillars were 210nm high and 200nm in diameter as determined by tapping-mode AFM and SEM. The Ge was deposited by molecular beam epitaxy at surface temperature of 600 degrees C. The self-assembled and aligned Ge quantum dots were formed after deposition of 10 ML of Ge was, as determined by an in-situ quartx crystal monitor. The size of resulting Ge quantum dots was measured by AFM in the tapping mode and were found to be 85nm in diameter. Ge quantum dots were also formed on nanorings. The nanorings were formed using modified-nanosphere lithography (MNSL) a new technique. These achievements and more recent experimental results will be discussed

in detail.

## F7.15
**Fabrication of a Regular Array of Atomic Silicon Wires on Silicon.** Takeharu Sekiguchi, Shunji Yoshida and Kohei M. Itoh; Department of Applied Physics and CREST-JST, Keio University, Yokohama, Japan.

In recent years nanotechnology towards realization of quantum information processing has been extensively studied. As a candidate for quantum computer, the present group has proposed "all-silicon quantum computer" [1], which utilizes nuclear spins ($I$) of Si isotopes. We will use a vicinal surface of $^{28}$Si isotope ($I=0$) as a template for linear chains of $^{29}$Si ($I=1/2$). In the present study we report successful fabrication of atomic $^{nat}$Si chains along a regular array of a uniform step structure on a vicinal $^{nat}$Si(111) substrate. The experiments were performed in a UHV chamber, and the surface structure was observed by high resolution scanning tunneling microscopy. At first, we fabricated a regular array of atomically straight single bilayer steps on a Si(111) surface with about 1° miscut toward [−1−12]. By modifying the thermal annealing process proposed by Viernow et al.[2], the density of kinks smaller than 7×7 unit cell was reduced and the atomic structure of the step edges were unified. This step edge structure is classified as U(2,0) [3] according to the lateral shift of the 7×7 structure on the lower terrace with respect to that on the adjacent upper terrace. While the step-parallel component of this shift was absent ($\underline{0}$), the step-normal shift was ($\underline{2}+2/3$)$b$ = 0.89 nm, where $b$ = 0.33 nm is the distance between the adjacent [1−10] rows in the ideal 1×1 lattice and $(2/3)b$ is the intrinsic shift due to (111) layer stacking. Indeed, a partial 7×7 structure of $\underline{2}b$ width was observed just below each step edge and contained four adatoms in each unit cell. Furthermore, we deposited Si atoms on the surface with this uniform step structure from a Knudsen cell. By optimizing the deposition amount and the substrate temperature during the growth, a single adatom row [3] was grown along each lower edge of the steps. The single-adatom-row growth was allowed in the $2b$ wide region just below the step edge where there was no stacking fault. In contrast, such a growth was inhibited in the remaining terrace containing the stacking fault because the temperature was not high enough to relieve it. Excess Si deposition resulted in subsequent formation of ill-ordered 7×7 structures along the single adatom rows. Above the optimal temperature highly-ordered 7×7 structure was formed along each step edge without the single adatom row, while below this temperature Si clusters were formed just above the step edge. Details such as the structure model and the growth mechanism will be discussed in the symposium. [1] T.D. Ladd, et al., Phys. Rev. Lett. 89, 017901 (2002). [2] J. Viernow, et al., Appl. Phys. Lett. 72, 948 (1998); J.-L. Lin, et al., J. Appl. Phys. 84, 255 (1998). [3] W. Shimda and H. Tochihara, Surf. Sci. 311, 107 (1994).

## F7.16
**Characterization of SiC Nanowire Grown by APCVD Using Single Precursors.** Rho Dae Ho[1,2], Kim Jae-Soo[2], Byun Dong-Jin[1], Yang Jae-Woong[3], Lee Jae-Hoon[4] and Kim Na-Ri[1]; [1]Materials Science and Engineering, Korea University, Seoul, South Korea; [2]Metal Processing Center, Korea Institue of Science and Technology, Seoul, South Korea; [3]Advanced Materials Engineering, Daejin University, Pochun, South Korea; [4]Light Materials Team, Korea Institute of Industrial Technology, Chonan, Chungnam, South Korea.

SiC were the promising materials because of its typical properties like wide bandgap, high electron mobility, chemical stability and superior physical properties. Since the discovery of carbon nanotubes, one-dimensional nanoscale materials have received wide spread interested due to its potential applications of electrical and optical nanodevices. Carbon nanotube was used strengthen materials and hydrogen storage materials and optical device materials like FET (Field Emission Tip). SiC nanowire and nanorods were considered candidate materials of carbon nanotubes because of SiC's superior physical properties. Specially, SiC nanowire's physical property and thermal stability were fitted to FET materials at high vacuum and temperature conditions. So many researchers studied its capability and optical and electrical properties. Recent report of the SiC nanorod's optical property shows much low threshold voltages about 2.5　3.5 V/um These results were lower than that of carbon nanotubes, Mo, Si and C. But most of SiC nanowire growth methods produce a particle like shapes. To resolve this problem, CVD method was used in this research. And growth temperature was lower by using single precursors (HMDS, TMS and TPS) than other reports. By this research, SiC nanowire was grown on Si directly. Grown nanowires diameters was about 30　50nm and have length of several um. Measured threshold voltage was about 2　4 V/um. These data were varied with kind of catalyst and growth conditions. High blue emission peak was observed in the grown SiC nanowires by PL measurements

## F7.17
**Growth and Chracterization of SiOx Nanowires by VLS and SLS Growth Mechanism.** Rho Dae Ho[1,2], Kim Jae-Soo[2], Byun Dong-Jin[1], Yang Jae-Woong[3], Lee Jae-Hoon[4] and Kim Na-Ri[1]; [1]Materials Science and Engineering, Korea University, Seoul, South Korea; [2]Metal Processing Center, Korea Institute of Science and Technology, Seoul, South Korea; [3]Advanced Materials Engineering, Daejin University, Pochon, South Korea; [4]Light Materials Team, Korea Institute of Industrial Technology, Chonan, Chungnam, South Korea.

Since discovery of carbon nanotube's optical and electrical properties, many researchers extensively studied its application and origin of its mechanism. And other nanostructures materials's optical properties were studied too. Among the nanostructure materials, one-dimensional nanowires have attracted intensive interest due to their potential use in optoelectronic devices and fundamental importance to the study of size dependence chemical and physical phenomena. Silica is widely used in silicon based intergrated devices and can also produced as nanowires. By recent research, silica nanowires show stable and high bright emission, which is much lower than that of oxidized Silicon nanowires. The blue light emitting of silica nanowires may have potential application in intergrated optical nanodevices, high-resolution optical heads of scanning near-field optical microscopes and so on. To synthesize silica nanowire, various methods was developed. And silica nanowires that had a typical shape so called "nanoflowers" and "spring" was produced. But its typical shapes were not suitable to opto-electrical devices. In this research, we growth silica nanowires on Si, quartz, and Al2O3 substrates using vapor evaporating method. Grown silica nanowires had about 20 50nm diameter and several um length. Specially, grown nanowires microstructures were different with used substrates. And its electrical property was varied too. In this research, we discussed its phenomena and origin of growth scheme and mechanism

## F7.18
**Germanium Nanowires Growth via Vapor Transport.** Yi Ma, Xiaowei Wang, Jianyu Huang, Dezhi Wang and Zhifen Ren; Physics, Boston College, Brighton, Massachusetts.

Germanium nanowires were synthesized from the mixture of germanium oxide and graphite powder with or without Au catalyst. EDS, SAED, SEM, TEM were used to characterize the structure of the germanium nanowires. When no catalyst was used, big wires were obtained with the diameter of around 100 nm. When Au catalyst was used, the diameter of the wire was modulated by the size of gold nanoparticles. We will also discuss the growth mechanism of the nanowires.

## F7.19
**Synthesis and Characterization of ZnS/Si Wire Heterostructures.** Chunsheng Du and Ning Pan; University of California at Davis, Davis, California.

Semiconductor heterostructures with modulated composition enable the generation of devices with diverse functions. In this regard, the capability of heterostructures formation through carefully controlled interfacing in nanoscale building blocks with high surface area will be increasingly important in the assembly of electronic and photonic devices. Here we report the synthesis of silicon (Si) and zinc sulfide (ZnS) nanowire heterostructures via the solid-liquid-solid (SLS) and vapor-liquid-vapor (VLS) processes using cobalt as a metal catalyst. Si powder and ZnS powder were used as raw source materials for the growth of heterostructures. The fabrication process involved the growth of Si nanowire via SLS process followed by the growth of ZnS nanowire from the end of Si nanowire by way of a VLS process via thermal evaporation of ZnS powder in a quartz tube furnace at 1000?C, while hydrogen was introduced into the furnace at a flow rate of 50 sccm. The growth time was 15 min to 1 h. The heterostructures were thoroughly characterized by scanning electron microscopy (SEM) (Philips XL30), transmission electron microscopy (TEM) (Philips CM 120). Electron microscopic analysis showed different faceted tip geometries at the terminus of the wires. The wire diameter is around 300 nm with the height of about 60-70 microns. The compositions of the wires at both sides of the junction were analyzed on FEI XL30-SFEG high-resolution SEM equipped with energy dispersive x-ray spectroscopy (EDS) system. Our synthesis of axial heterostructures, including heterojunctions between ZnS and Si within a single wire, indicates the general potential of axial heterostructures growth for the development of nanowire-based devices. This method may be applicable to the preparation of other sulfide-silicon

heterostructures or other zinc blended semiconductors.

**F7.20**
**Optical Properties of Ge Nanowires Grown on Silicon (111) and (100) Substrates.** Boris Kamenev[1], <u>Varun Sharma</u>[1], Ted I. Kamins[2], R. Stanley Williams[2] and Leonid Tsybeskov[1]; [1]Electrical and Computer Engineering, New Jersey Institute of Technology, Newark, New Jersey; [2]Quantum Science Research, Hewlett-Packard Laboratories, Palo Alto, California.

We report Raman scattering and photoluminescence (PL) measurements in Ge nanowires (NWs) grown by chemical vapor deposition on silicon substrates with (100) and (111) crystallographic orientations. A sharp and narrow Raman peak at 300 inverse centimeters indicates single-crystal quality of Ge NWs 40 nm in diameter and approximately a micrometer in length. The absence of Si-Ge vibrations in Raman spectra shows that SiGe interdiffusion is insignificant for most of the NW volume. Low temperature PL spectra and the PL intensity temperature dependence strongly indicates that the observed emission originates mostly at Ge NW/Si substrate interfaces, where Si-Ge intermixing has been detected. We found that such interfaces are formed differently for (111) and (100) oriented Si substrates due to the strongly oriented (111) preferential growth direction of Ge NWs.

**F7.21**
**Carrier Transport in One-dimensional Ge Nanowire - Si Substrate Heterojunctions.** Boris Kamenev[1], <u>Eunkyu K. Lee</u>[1], Pavel A. Forsh[3], Ted I. Kamins[2], R. Stanley Williams[2] and Leonid Tsybeskov[1]; [1]Electrical and Computer Engineering, New Jersey Institute of Technology, Newark, New Jersey; [2]Quantum Science Research, Hewlett-Packard Laboratories, Palo Alto, California; [3]Physics Department, Moscow State University, Moscow, Russian Federation.

We present detailed ac and dc measurements on electrical and photoelectrical properties of one-dimensional hetero-junctions formed between VLS-grown Ge nanowires and crystalline Si substrates. We show that at the region of nanowire-substrate interfaces these junctions exhibit nearly ideal properties while at the nanowire end, where Au clusters are located, carrier transport is controlled by structural defects, most likely dislocations.

**F7.22**
**Generation of Silicon Nanowhiskers by Molecular Beam Epitaxy.** <u>Luise Schubert</u>[1,2], Nikolai D. Zakharov[1], Gerhard Gerth[1], Hartmut S. Leipner[2], Peter Werner[1] and Ulrich Goesele[1]; [1]Max Planck Institute of Microstructure Physics, Halle, Germany; [2]Department of Physics, Martin-Luther University, Halle, Germany.

Silicon nanowhiskers are frequently grown by chemical vapor deposition (CVD) and gas-source molecular beam epitaxy (GS-MBE). These techniques are using small droplets of metals, such as gold, as a seed for the nanowhisker growth. The silicon is preferentially incorporated via the liquid silicon-metal droplet, a mechanism referred to as the vapor-liquid-solid mechanism (VLS). At the present time, there is little information on the growth of Si nanowhiskers by molecular beam epitaxy (MBE). The poster presents our first results on a more detailed analysis of the MBE-specific VLS mechanism. All growth steps have been performed in-situ and in ultra-high vacuum (UHV). The whiskers were generated as seeds, whose size (diameter : 50nm to 150nm) depends on the amount of deposited Au and the substrate temperature. During the subsequent Si deposition (substrate temperature between 450°C and 550°C), nanowhiskers were formed with a diameter ranging from 50nm to 200nm. The length (maximum 1$\mu$m) depends on the substrate temperature and the size of the Au droplets. The relation between length and diameter of the nanowhiskers is opposite to what is reported in literature for growth via CVD. The experimenta results are discussed on the base of a model including not only the conventional VLS mechanism, but also a strong surface diffusion component.

**F7.23**
**Auger Electron Spectroscopy of Contacts to Si Nanowires.** <u>Bangzhi Liu</u>[1], Soham Dey[1], Theresa S. Mayer[2], Joan M. Redwing[1] and Suzanne E. Mohney[1]; [1]Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania; [2]Department of Electrical Engineering, The Pennsylvania State University, University Park, Pennsylvania.

Silicon nanowires (SiNWs) have drawn considerable attention recently due to their potential applications in new electronic, photonic, and mechanical devices, as well as chemical and biological sensors. The development of low-resistance, stable ohmic contacts to these nanowires is necessary for optimal performance of some of these new devices. In this study, a Physical Electronics Model 670 scanning

Auger nanoprobe is used to characterize the diffusion of metals along SiNWs before and after annealing. Special challenges are encountered in data interpretation because of the small size of the nanowires and the geometry of the samples. These challenges include shadowing, edge effects, and substrate backscattering effects, which are affected by beam energy and sample orientation. The effects are evaluated first and strategies are discussed to extract useful information from Auger electron spectroscopy of nanowires. Finally, the reactions between the contacts and nanowires are discussed in light of the changes in the contact resistance upon annealing, with special emphasis given to Ti/Au contacts for which favorable annealing conditions have been identified for reduced contact resistance.

**F7.24**
**Formation of Hydrogen-Passivated Silicon Nanochains by Pulsed Laser Ablation without Thermal Annealing.** <u>Mitsuru Inada</u>[1], Ikurou Umezu[2], Shukichi Tanaka[1], Shinro Mashiko[1] and Akira Sugimura[2]; [1]National Institute of Information and Communications Technology, Kobe, Japan; [2]Department of Physics, Konan University, Kobe 658-8501, Japan.

We have formed silicon nanochains covered with hydrogen by pulsed laser ablation of silicon target in pure hydrogen gas without annealing process. When the hydrogen gas pressure was higher than 670Pa, silicon nanochains with 4-10nm wide and length of up to several microns were formed. Transmission electron microscopy shows the nanochain consists of many links of crystalline silicon nanoparticles. Micro-Raman spectra from the nanochains show an evident downshift of silicon peak and asymmetric broadening. These results also indicate that the nanochains have crystalline silicon core with confinement effects. It is particular attention that the silicon nanochains have crystalline core without any intentionally annealing process. Fourier transform infrared absorption shows that hydrogen content in the silicon nanochains is 10-30% with Si-H$_{2,3}$ configurations. Since the nanochain has silicon core, Si-H bond is dominantly located on the surface of nanochains. This suggests the surface of nanochains ideally passivated by hydrogen. In the micro-photoluminescence measurements, we observed bright visible luminescence at around 1.6 eV. This result suggests that crystalline structure and hydrogen-passivation suppress non-radiative recombination process and increase the PL intensity of nanochains.

**F7.25**
**Growth Rate of Silicon Nanowires.** <u>Jun Kikkawa</u>, Yutaka Ohno and Seiji Takeda; Department of Physics, Osaka University, Toyonaka, Osaka, Japan.

We have measured the growth rate of silicon nanowires (SiNWs) in the temperature range between 365 and 500°C. The SiNWs were grown by a vapor-liquid-solid (VLS) growth method using Au-Si liquid droplets as catalysts and monosilane (SiH$_4$) as a vapor phase reactant, and were post-growth observed by means of transmission electron microscopy (TEM). The growth rate increases exponentially as the temperature increases. The physical meaning of this activation energy for the growth of SiNWs, which may be composed of an energy needed to remove Si atoms from a vapor-liquid interface to a liquid-solid interface and that for the decomposition of SiH$_4$, will be discussed. It is also found that SiNWs grown at the temperatures higher than about 400°C is more straight: most SiNWs grown below 400°C are rather twisted. This can be accounted for by the growth rate of SiNWs. In addition, SiNWs with smaller diameters are likely to grow more rapidly. These basic data is useful to understand the initial stage of the growth of SiNWs.

**F7.26**
**Modification of nc-Si/SiO$_2$ Nanostructures by Selective Laser Induced Heating.** <u>Boris Kamenev</u>[1], Haim Grebel[1], Viktor Timoshenko[2] and Leonid Tsybeskov[1]; [1]Electrical and Computer Engineering, New Jersey Institute of Technology, Newark, New Jersey; [2]Physics Department, Moscow State University, Moscow, Russian Federation.

We report a modification of nc-Si/SiO$_2$ nanostructures by selective laser induced heating of Si nanocrystals. Using Raman spectroscopy, we found amorphization of Si nanocrystals after irradiation by nanosecond laser pulse with energy density of 30-40 mJ/cm$^2$. This amorphization is found for structures with relatively small SiO$_2$ separating layers and, most likely, caused by the strain relaxation. The appearance of the amorphous phase results in increasing of photoluminescence efficiency. The data indicate the presence of at least two luminescence origins in the nc-Si/SiO$_2$ nanostructures.

**F7.27**
**Si nanocrystals in PECVD silicon oxides and comparison of its luminescence efficiency with implanted and annealed samples.** Mariano Peralvarez[1], M. Lopez[1], J. R. Morante[1], <u>Blas Garrido</u>[1], J. Barreto[2], V. J. Cadarso[2], M. Riera[2], K. Zinoviev[2]

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and C. Dominguez[2]; [1]Electronics Department, Universitat de Barcelona, Barcelona, Spain; [2]Institut de Microelectronica de Barcelona, CNM-CSIC, Bellaterra, Spain.

Si nanocrystals (Si-nc) embedded in SiO2 present outstanding photo and electrolu-minescent emission in the visible and are the materials of choice for the realization of efficient light sources integrated with Si technology. Several Si compatible approaches have been used to synthesize Si-nc embedded in SiO2, being ion implantation one of the most frequently reported. Some authors have reported Si-nc formation from PECVD but there is still the need to understand how the Si excess and the detailed matrix composition -presence of N and H- affect the precipitation and growth of the Si-nc and the photoluminescence (PL) efficiency. We report in this work a thorough study on the structural properties and PL efficiencies of a series of Si-nc/SiO2 composites fabricated by this method in a wide range of Si excess up to 50 atomic percent (which corresponds to x in SiOx down to 0.5). For reference, the same study has been performed in Si-nc/SiO2 materials synthesized by ion implantation and annealing. The SiOx PECVD deposited samples have a thickness between 50 and 100 nm and the phase separation, precipitation and growth of the Si-nc have been achieved by high temperature annealing at 1250 degrees C. Refractive index and thickness have been measured by ellipsometry and correlated with compositional measurements. The detailed composition profile has been determined by XPS, SIMS and FTIR analyses. H has completely disappeared in annealed samples while the N concentration is found between 5 and 10%. EFTEM demonstrates that isolated Si-nc are formed for Si excess up to 20% while for higher Si concentration a continuous Si phase is observed. The PL efficiency in PECVD samples is maximized for a Si excess of 17% which is very close to the maximum efficiency found in implanted samples for the 15% of Si excess. We have measured absorption cross-section and lifetimes of Si-nc in both deposited and implanted samples and have found that they depend only on Si excess for samples which have undergone a complete phase separation. No dependence of PL efficiency has been found on the presence of N in the matrix. We will present a detailed study and modelization of PL emission as a function of pumping power in which we have taken into account excited state absorption and Auger quenching effects. We will also report at the conference the making and characterization of LEDs fabricated from deposited samples.

SESSION F8: Si Nanocrystals and Porous Si: Light-Emitting and Other Properties II
Chairs: Albert Polman and Anthony Van Buuren
Wednesday Morning, December 1, 2004
Constitution B (Sheraton)

**8:15 AM *F8.1**
**Electric Force Microscopy of Individually Charged Silicon Nanoparticles.** <u>Thierry Melin</u>[1], Heinrich Diesinger[1], Dominique Deresmes[1], Thierry Baron[2], Sophie Barbet[1] and Didier Stievenard[1]; [1]IEMN-CNRS UMR 8520, Dpt ISEN, Villeneuve d Ascq, France; [2]LTM - CNRS UMR 5129, CEA, Leti DTS, Grenoble, France.

We report on charge injection experiments performed on single silicon nanoparticles[1,2] and their analysis by Electric Force Microscopy (EFM). An analytical model will be first presented, enabling a quantitative determination of the charge state of the semiconductor nanoparticles from EFM signals, for arbitrary tip and nanoparticle shapes[3]. Experimentally, we provide an analysis of the capacitive and charge interactions taking place in EFM of silicon nanoparticles deposited on conductive substrates. We demonstrate that the weak image interactions associated with charged nanoparticles - of dipole-dipole type- can be identified from a spectroscopic EFM analysis[4]. Finally, we address the issue of the charge injection mechanisms. From the hysteretic behaviour of the charge injection spectroscopy, we separate volume versus surface charge effects[5]. We show that charges are mostly injected in the nanoparticle volume, with however some residual injection on the nanoparticle surface. Volume charge injection mechanisms are modelled in a regime of successive charge tunnelings through the tip/nanoparticle and nanoparticle/substrate oxyde tunnel barriers, taking into account quantum confinement and electrostatic effects by solving the coupled Schrodinger and Poisson equations for the charge wavefunctions confined at the nanoparticle substrate interface. Mechanisms of charge saturation will be discussed from the comparison between experiments and theory. [1] E. Boer et al. Appl. Phys. Lett., 78 3133 (2001). [2] T. Melin, D. Deresmes and D. Stievenard, Appl. Phys. Lett., 81 5054 (2002). [3] T. Melin et al. Phys. Rev. B 69, 035321 (2004). [4] T. Melin et al., Phys. Rev. Lett. 92, 166101 (2004). [5] H. Diesinger et al. submitted to Appl. Phys. Lett (2004).

**8:45 AM *F8.2**
**Silicon Nanocrystals: From Coulomb Blockade To Memory**

**Arrays.** <u>Rajesh A. Rao</u>, Ramachandran Muralidhar, Robert F. Steimle, Sherry Straub, Bruce Hradsky, Jane Yater, Steve Anderson, Erwin Prinz, Craig Swift, Tushar Merchant, Matt Stoker, Michael Sadd and Bruce E. White; APRDL, Technology Solutions Organization, Freescale Semiconductor, Inc., Austin, Texas.

Non-volatile memory devices using discrete charge storage nodes - such as silicon nanocrystals or traps in silicon nitride (SONOS) - offer potential to lower the operating voltages compared to continuous floating gate flash due to their immunity to charge loss via isolated defects in the tunnel oxide. This results in scaling of memory module size by up to 50% at the 90nm technology node. Furthermore, discrete charge storage memory devices can be integrated with high voltage periphery and logic devices using only 4 non-critical mask adders over conventional CMOS process technology. The superior Fowler-Nordheim tunneling erase characteristics of nanocrystal memory compared to SONOS permit HCI/FN operation capability at tunnel oxide thicknesses needed to mitigate read disturb, rendering Si nanocrystals very attractive for embedded NOR memory applications. New aspects in silicon nanocrystal memory technology include Coulomb blockade or charge confinement effects, atomistic nucleation, and nanocrystal passivation to preserve them during subsequent processing and program/erase endurance characteristics. The paper will discuss the above aspects and focus on the effect of Coulomb blockade as nanocrystal size is reduced, which manifests in faster erase and larger gate disturb of unselected bits during program and READ. 4Mb NOR memory arrays have been fabricated using 90nm CMOS technology. Excellent memory characteristics including tight Vt distributions are obtained using a tunnel oxide thickness of 5nm and a 6V power supply.

**9:15 AM *F8.3**
**Enhanced Silicon Nanocrystal Photoluminescence via Au-Si Near-Field Energy Transfer Processes.** <u>Julie Suzanne Biteen</u>, Issac Garcia-Munoz, Nathan S. Lewis and Harry A. Atwater; California Institute of Technology, Pasadena, California.

We report two approaches to increase the luminescence emission intensity from Si nanocrystals (nc-Si) under optical pumping via: 1. the use of nanostructured Au as a sensitizer for nc-Si emission, and 2. near-field coupling of nc-Si emission to localized surface plasmons on rough Au surfaces to increase the radiative emission rate relative to conventional nc-Si emission. We have observed a ten-fold enhancement in photoluminescence intensity from nc-Si coupled to Au nanostructures emitting at 1.7 eV. We also observe a decrease in the radiative lifetime, and we will present data showing this effect. The emission energy is unchanged during this enhancement process. By placing nc-Si embedded in silicon dioxide in proximity to a 100-nm thick nanoporous gold (npg) film with surface roughness and voids on the order of 10 nm, we have designed a system that takes advantage of both the enhanced absorption and the enhanced radiative rate. We will discuss our results in the context of models for energy transfer from nc-Si to localized plasmons in the npg film. Energy transfer from Au to nc-Si takes advantage of the metal's relatively large absorption cross section ($10^{-10}$ $cm^2$ for Au vs. $10^{-15}$ $cm^2$ for Si) to sensitize the nanocrystals, and we will present data showing the increase in absorption cross section of nc-Si upon coupling to npg. Energy transfer from the nc-Si to the Au leads to an increased radiative rate, but does not quench PL as the rough surface of the npg film enables radiative emission from the metal. We will present data showing a decrease in lifetime, and support it with data showing that coupling to Au suppresses the saturation of PL intensity that otherwise occurs as pump power is increased. Since the efficiency of the near-field energy transfers, which are consistent with Förster (dipole-dipole) processes, depends on separation distance, we will report trends in PL intensity and lifetime upon systematic variations of the nc-Si/Au separation distance from 0.5 to 50 nm.

**9:45 AM *F8.4**
**Coupling Si Quantum Dots to Surface Plasmons.** Jeroen Kalkman and <u>Albert Polman</u>; FOM-Institute AMOLF, Amsterdam, Netherlands.

We present a new way to enhance the effective emission rate and efficiency of Si quantum dots. The quantum dots are placed near a metal-dielectric interface and decay by the generation of surface plasmons. While this in itself constitutes a loss process; the plasmons can subsequently be coupled out to the far field as light. The effective emission rate of the quantum dot-plasmon system is then determined by the sum of the quantum dot's intrinsic radiative rate and the plasmon coupling rate, and -as we will demonstrate- can thus be enhanced by several orders of magnitude. Surface plasmons are electromagnetic modes that propagate at the interface between a metal and a dielectric. When an excited Si quantum dot is placed close to such an interface, a near-field interaction between the oscillating dipole and the metal occurs, leading to the generation of a surface plasmon at the dipole's frequency. We describe this interaction

in terms of a semi-classical model, also taking into account distance-dependent variations in the local density of states and coupling to lossy surface modes. The surface plasmon, propagating along the metal-dielectric interface, can subsequently be coupled out into the far field using a properly engineered grating that relaxes the momentum mismatch between the plasmon and a far-field photon. We show that in well-engineered structures the plasmon propagation losses are small and the efficiency of converting the plasmon to light can be close to unity. We provide direct experimental evidence of enhanced decay rates of Si quantum dots by energy transfer to surface plasmons at a $Ag/SiO_2$ interface. Quantum dots are made in $SiO_2$ at different depths using ion implantation, whereupon the sample was covered with an optically thick silver film. For quantum dots placed d=40 nm away from the $SiO_2$-Ag interface, a two-fold increase in decay rate is observed at $\lambda$=750 nm, while no effect is observed at d=100 nm, both in agreement with our calculations. Strong stretched exponential decay characteristics are observed for quantum dots very close to the metal, also in agreement with our model that takes into account the quantum dot depth distribution and convoluted homogeneous broadening effects. With our model supported by experiments, we performed calculations on systems that will show much larger enhancements e.g. using Au rather than Ag. Very large effects are expected for coupling to metal films with finite thickness, where complex plasmon coupling behavior between the two metallo-dielectric interfaces causes a 1000-fold enhanced coupling rate from Si quantum dots to the surface plasmons. By using this plasmon coupling concept, the saturation output power of LEDs based on Si quantum dots can be enhanced by orders of magnitude. Efficient coupling to surface plasmons also circumvents non-radiative quench processes in Si quantum dots, thus leading to an enhanced effective emission quantum efficiency.

**10:30 AM *F8.5**
**Influence of the Strain, Surface Structure and Particle-Particle Interaction on the Occupied and Empty Density of States in Group-IV Nanostructures.** Anthony van Buuren, Christoph Bostedt, Trevor Willey, R. W. Meulenberg and Lou Terminello; Chemistry and Materials Science Department, Lawrence Livermore National Laboratory, Livermore, California.

The observed size depended change in the optical properties in semiconductor quantum dots has been generally explained in terms of a quantum confinement argument. Until recently the effect of the strain, surface reconstruction and particle-particle interaction on the electronic and structural properties of quantum dots has been neglected due to the inherent difficulty in measuring these properties. Traditional analysis techniques of nanostructures, such as optical spectroscopy of the band gap transitions in semiconductors, provide useful, but lack surface and element specific information about the electronic structure. Synchrotron radiation has been used to study nanostructures to separately measure occupied states by photoemission spectroscopy (PES) and unoccupied states by core level X-ray absorption spectroscopy. With these techniques we are able to probe the surface region as well as the core structure of Si, Ge and diamond quantum dots. Our experimental results show how the bare nanoparticle surface reconstructs and how passivation of the bare surface will influence the overall electronic properties of these quantum dots. For both Si and Ge nanoparticles unpassivated nanocrystals have shown a disordered surface shell around a crystalline core. For passivated nanocluster we find that the passivating agent alters the electronic structure of the clusters. We also explore how strain in the nanoparticles will influence the overall electronic structure. This work is supported by the US-DOE, BES Material Sciences under contract W-7405-ENG-48, LLNL.

**11:00 AM F8.6**
**Solid Fullerenes for Tetravalent Semiconductors: The Most Atomlike Quantum Dots.** Yufeng Zhao, Yong-Hyun Kim, Mao-Hua Du and Shengbai Zhang; National Renewable Energy Laboratory, Golden, Colorado.

One of the most fascinating properties of carbon is its bistability both in graphite and diamond. One can thus wrap a graphite sheet into the various forms of (hollow) carbon nanotubes and fullerenes with properties distinctly different from those of a diamond. Other tetravalent semiconductors such as Si and Ge, however, do not have such a bistability and are hence lack of such a fascination. For a long time, a fullerene made of Si or Ge has been considered impossible. On the other hand, at the macroscopic scale, one can cut a crystal almost into any arbitrary shapes, for example to a sphere to minimize surface to bulk ratio. However, when the crystal size is reduced to several tens of an atomic layer, the shapes it can take will be much limited, especially for semiconductors with highly unisotropic surface energies. Seeking for an optimal shape that could yield both low facet energies and high sphericity has been a daunting challenge in semiconductor based nanosciences. Here, we show [1] that the two seemingly

unrelated subjects are intimately related. In the size range from upper tens to several thousand atoms, a tetravalent semiconductor quantum dot is neither cluster- nor bulk-like. Instead, a new icosahedral phase emerges, which can be characterized by a reconstructed fullerene core surrounded by a bulk-like outer shell. In analogous to the hollow fullerene, the quantum dot here is a solid fullerene constructed by bending a solid belt, via the formation of stacking faults, to a seamless full enclosure. Because the solid fullerenes apply to all tetravalent elements, this prediction opens up new opportunities for all archetypical semiconductors such as Si and Ge, not just for C. Calculations on hydrogenated Si icosahedral dots reveal significantly increased level spacing and up to fivefold orbital degeneracy. Discrete valence states are also evident. This is because, while a cubic structure has only 48 group operations, an icosahedral quantum dot (IQD) has the Ih symmetry with 120 operations, the highest for any point group. Thus, the IQDs represent the most atomlike quantum dots possible, with superior potentials in achieving longer decoherence for quantum information processing, in hot-carrier solar cells, and for better control of the amplitude and phase of electron wavefunctions. In principle, one can construct semiconductor quasicrystals out of the IQDs. The icosahedral symmetry also provides a natural bridge between the IQDs and capped carbon nanotubes, from which one can build rich nano-architectures including perfect lattices. Experimental feasibility of fabricating the IQDs will also be discussed. [1] Zhao, Kim, Du, and Zhang, Phys. Rev. Lett. (in press).

**11:15 AM F8.7**
**Electron Exchange Interaction in Electronically Confined Si Quantum Dots.** Seungwon Lee[1], Paul von Allmen[1], Susan N. Coppersmith[2] and Mark Friesen[2]; [1]Jet Propulsion Laboratory, California Inistitute of Technology, Pasadena, California; [2]Department of Physics, University of Wisconsin, Madison, Wisconsin.

Electron exchange interactions in electronically confined Si quantum dots are modeled with an sp3d5s* empirical tight-binding model. Previous work has shown that the exchange energies for electrons confined by P donors in bulk Si display a fast oscillatory behavior with respect to the inter-donor distance [1]. This result implies that P donors need to be positioned with atomic-scale precision in order to implement a Si:P based quantum computer architecture. In contrast to the Si:P architecture, electronically confined Si quantum dots show a simple exponential decay of the exchange energies with the increase of the inter-dot distance. The exponential behavior is attributed to tensile biaxial strain in the Si quantum well, which is epitaxially grown on top of a relaxed SixGe1-x layer. The tensile biaxial strain lifts the degeneracy of six valleys in the Si band structure, with the Z valley lower than the X and Y valleys. The lowest electron wave function originates from the Z valley, and hence Bloch oscillations are present in the z direction only. As a result, when the inter-dot distance changes along the x and y directions, the exchange energy, which is determined by the overlap between the two electron wave functions, does not oscillate. [1] B. Koiller, X. Hu, and S. Das Sarma, Phys. Rev. Lett. 88, 27903 (2002).

**11:30 AM F8.8**
**Quasiballistic Electron Emission from Planarized Nano-crystalline-Si Surface Emitting Devices.** Yoshishige Tsuchiya[1], Takuya Nakatsukasa[1], Hiroshi Mizuta[2], Shunri Oda[1,2], Akira Kojima[3] and Nobuyoshi Koshida[3]; [1]Quantum Nanoelectronics Research Center, Tokyo Institute of Technology, Tokyo, Japan; [2]Department of Physical Electronics, Tokyo Institute of Technology, Tokyo, Japan; [3]Department of Electrical and Electronic Engeneering, Tokyo University of Agriculture and Technology, Koganei, Japan.

Planar-type cold cathode surface emitting devices based on Si nano-fabrication technologies attract much attention because they have many advantages such as vacuum tolerance, directional emission, low operation voltage, and easy fabrication. We have developed a cold cathode electron emitter based on nanocrystalline-Si (nc-Si) formed in the gas phase by VHF plasma decomposition of $SiH_4$ and its efficiency has been improved by the planarization of the nc-Si layer by the reflow technique [1]. However, electron transport mechanism through the nc-Si layer is still unclear. In this paper, the transport mechanism through the nc-Si layer in the nc-Si surface emitting devices is discussed based on the results of energy distribution of emitted electrons. Fabrication processes of the nc-Si surface emitting devices are as follows. The nc-Si dots were deposited onto the $n^+$-Si substrates by VHF plasma process. Subsequent oxidation, phosphorus diffusion, and annealing processes cause a planarization of nc-Si layer. An Al ohmic electrode on the backside of the Si substrates and a 20 nm-thick Au film on front surface were formed by evaporation and then the diode structure is completed. Electron emission characteristics are measured in vacuum with a base pressure of $10^{-6}$ Torr. Au electrode is grounded and a negative extraction voltage is applied to the Al electrode. A metal collector plate with the applied voltage of 100 V was placed in front of the surface of the sample, and a distance between the sample and the collector is about 5 mm.

Energy distribution of emitted electrons was measured using a conventional ac-retarding-field analyzer [2]. The emission current was observed around at the external voltage, $V_{ex}$, of 5 V and rapidly increased with applying $V_{ex}$. The energy distribution of emission electrons obtained at $V_{ex} = 30$ V showed that obviously the distribution is not Maxwellian, which was usually obtained at conventional cold cathode devices. The energy that provides maximum number of electrons is higher than the case of Maxwellian. Similar result was obtained in the porous Si diode [2], and according to Ref. [2], this behavior strongly suggests that electrons are emitted quasiballistically from our devices. These results indicate that the planarized nc-Si layer play an important role in this high efficiency cold cathode emitter. [1] K. Nishiguchi, X. Zhao, and S. Oda, J. Appl. Phys. 92, (2002) 2757. [2] T. Komoda, X. Sheng, and N. Koshida, J. Vac. Sci. Technol. B 17, (1999) 1076.

**11:45 AM F8.9**
**Enhancing the Sound Pressure of Thermally Induced Ultrasonic Emitter Based on Nanocrystalline Porous Silicon.** Kenji Tsubaki[1], Takuya Komoda[1] and Nobuyoshi Koshida[2]; [1]Corporate R&D Planning Office, Matsushita Electric Works, Ltd., Osaka, Japan; [2]Graduate School of Eng., Tokyo Univ. of A&T, Tokyo, Japan.

Due to the complete carrier depletion associated with strong quantum confinement, both the thermal conductivity and heat capacity per unit volume of nanocrystalline porous silicon (nc-PS) are extremely low in comparison to those of single-crystalline silicon (c-Si). Previously [1], we reported this high contrast of thermal properties makes it possible to use nc-PS device as a thermally induced ultrasonic emitter (TIUE) by efficient heat transfer at the device surface without any mechanical vibrations. We now report detailed experimental study for intensifying the sound pressure output by the control of nc-PS structure and driving mode. As the sound pressure is proportional to input power, a TIUE device can generate high power of acoustic wave by a temporal burst electrical input. To obtain a large acoustic output, major limiting factors for the electrical input power need to be clarified. Taking into account that the key component of the device is a patterned thin metal electrode deposited onto the nc-PS surface, we can assume that the most important determining factor for a maximum electrical input power is a mechanical stress at the interface induced by a rapid interfacial temperature raise rather than an electromigration inside the thin metal film. To confirm this hypothesis, the maximum acoustic pressures were measured under a pulsed operation at a pulse-width of 16 $\mu$s and a pulse-period 1 s for two devices with different nc-PS layer thicknesses of 2 $\mu$m and 50 $\mu$m. It has been confirmed that the sound pressure of 2-$\mu$m-thick device is enhanced twice compared with that of 50-$\mu$m-thick one at the same input power. The frequency dependence of the acceptable maximum input power also shows the behavior as expected from the theoretical analysis. These are consistent with the result of nano-indentation measurements that the hardness and youngfs modulus of the nc-PS layer are significantly increased with decreasing its thickness. The present result provides useful information for further progress of the nc-PS acoustic device. 1. H. Shinoda, T. Nakajima, K. Ueno, and N. Koshida, Nature 400, 853 (1999).

SESSION F9: Group IV Semiconductor Nanowires
Chairs: Seiji Takeda and P. Yang
Wednesday Afternoon, December 1, 2004
Constitution B (Sheraton)

**1:30 PM *F9.1**
**Formation of Nanocatalysts for the Growth of Silicon Nanowires.** Seiji Takeda, Jun Kikkawa and Hideo Kohno; Department of Physics, Osaka University, Toyonaka, Osaka, Japan.

Silicon nanowires can be grown spontaneously via nanocatalysts. They usually nucleate at nanocatalysts and then grow in a certain direction under the flow of source gases. Preparing a nanocatalyst of a desired size at the desired site on a substrate before the growth of nanowires, one can simply decide the nucleation site and the radius of a one-dimensional structure artificially. Furthermore, impurities added to nanocatalysts occasionally induce the modulation of diameters of silicon nanowires. It is also known that twins and polytype structures are frequently observed in silicon nanowires, modulating the electronic structures in some extent. Despite of accumulated experimental data, the mechanism of either the formation of nano-catalysts or the early stage in growth of silicon nanowires has not yet been fully described. We have examined the formation process of nanocatalysts by means of ultrahigh vacuum scanning tunneling microscopy and transmission electron microscopy (TEM) at high temperatures. Gold-silicon nanocatalysts that we have examined were thought to form on a hydrogen (H)-terminated (111) silicon surface and to expel silicon nanowires of extremely high aspect-ratio via the vapor-liquid-solid

(VLS) mechanism. We have observed that a nanocatalyst, i.e. a droplet of melted gold-silicon alloy of about 5 nm in diameter, is actually formed in a pit on a H-terminated surface in the narrow temperature range around 500C. Based on the result, we have proposed a method of making a thin template, which facilitates to decide the nucleation sites and the sizes of nanocatalysts, resulting in the precise control of those of silicon nanowires. As is well known, the growth Si nanowires is very fast. We have measured the growth rate of Si nanowires ex-situ by means of TEM. The rate certainly depends on various growth parameters, especially the growth temperatures. We discuss the details on the kinetics of the growth of Si nanowires. A lot of applications are possible of an array of one-dimensional silicon nanostructures whose arrangement, morphology and interior structures is well controlled. For instance, our work can be utilized for fabricating of nano-sensors, microelectronic-mechanical system (MEMS) as well as nanoelectronic devices.

**2:00 PM F9.2**
**Synthesis, Properties, and Applications of Modulation-Doped Silicon Nanowires.** Chen Yang[1], Zhaohui Zhong[1] and Charles M. Lieber[1,2]; [1]Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts; [2]Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts.

Semiconductor nanowires are versatile building blocks for fundamental studies in nanoscience, and have the potential to open up many exciting opportunities in nanoelectronics and nanophotonics in the future. Yet to push these fundamental and application areas forward requires increasing control of, and more generally modulation of the dopant within nanowire structures. To this end we describe the first demonstration of the controlled synthesis of modulation-doped silicon nanowires. The nanowires were prepared using nanoclusters-catalyzed vapor-liquid-solid growth process, where electron microscopy was used to verify that no radial over coating occurred during axial elongation and to determine axial growth rates. Scanning gate microscopy investigations show that modulation-doped nanowires can be differentially gated, where regions with low dopant concentration are turned on/off relative to heavily doped regions. Systematic growth and characterization studies further demonstrate that all key properties of these modulation doped nanowires can be controlled, including the number, size and period of the differentially doped regions. In addition, two applications of these new nanostructures will be described. First, a lithography-free approach for addressing based on modulation doped silicon nanowire field-effect transistor arrays has been developed, and results for the assembly and demonstration of a 2x2 address decoder circuits will be discussed. Second, low temperature transport studies of modulation doped silicon nanowire, where modulation doping is used to define potential barriers, will be discussed. Significantly, these investigations show coulomb blockade/single electron tunneling behavior with quantum structure defined by modulation doped barriers during synthesis. Prospects and future directions will be discussed.

**2:15 PM F9.3**
**Size Control and Phonon Confinement of Silicon Nanowires Synthesized by Laser Ablation.** Naoki Fukata[1,2], Takashi Oshima[1] and Kouichi Murakami[1,2]; [1]Institute of Applied Physics, University of Tsukuba, Tsukuba, Japan; [2]Special Research Project on Nanoscience, University of Tsukuba, Tsukuba, Japan.

Silicon nanowires (SiNWs) have been synthesized by laser ablation method or chemical vapor method. The remarkable point for the former method is that SiNWs can be synthesized in gas phase without forming and putting nano-sized metal catalyst as seeds of SiNWs, which are necessary for the latter method. However, the size control of SiNWs has not yet been investigated in the former method. In order to achieve the size control of SiNWs for laser ablation method, we have synthesized SiNWs under various conditions and investigated the dependence on the content of catalyst, the laser power, the flowing gas pressure, and temperature during laser ablation using a frequency-doubled Nd:YAG laser. SiNWs were synthesized by laser ablation of a target which was placed in a quartz tube heated at 1000-1200°C in a flowing Ar gas. The diameter of SiNWs was found to significantly depend on above-mentioned parameters, i.e., it decreased with decreasing them. Thus, it is found that the diameter of SiNWs can be controlled by the synthesis parameters even for laser ablation method. Furthermore, the effect of phonon confinement depending on the diameter of SiNWs was investigated by micro-Raman measurements. The slight downshift (1-2 cm$^{-1}$) of Si optical phonon and asymmetric broadening were observed in the Raman spectra for SiNWs. The Si optical phonon peak shifted towards lower wavenumber with the decrease in diameter of the SiNWs. The relation between the downshift of the optical phonon peak and the diameter of SiNWs was in accordance with the phonon confinement model. The degree of both the downshift of the optical phonon and the peak broadening is much more dependent on the size of SiNWs with increasing excitation power, which is due to local

heating. This is caused by the difference in the thermal conductivity among SiNWs with different diameters. Hence, it is found that the effect of local heating also gives useful information about SiNWs with different diameters. Electron spin measurements and photoluminescence measurements are in now progress to investigate doping effects of P donor in one-dimensional SiNWs.

**2:30 PM F9.4**
**Ge Nanowire Formation on Si(124) Surface.** Heedon Hwang, Kenji Ohmori, Benjamin Cho, J.A.N.T. Soares, Jian-Guo Wen, Ivan Petrov and J. E. Greene; Department of Materials Science and Materials Research Laboratory, University of Illinois, Urbana, Illinois.

Self organized Ge nanostructures on high index Si substrates have been the subject of intense research because of their promise for novel devices. We have grown Ge layers on Si(124) surfaces, which upon annealing form a surface composed of alternating (113) and (157) facets. This faceting behavior results in an extended and uniform hill-and-valley structure along $[-2 -1 \ 1]$, providing a natural template for nanowire formation. Ge layers were grown at 600 °C by gas-source molecular beam epitaxy (GS-MBE). Surface and cross-sectional morphologies were observed by atomic force microscopy and transmission electron microscopy. Average film thickness of Ge layers was measured by Rutherford backscattering spectroscopy. Initial growth of Ge is faster on (157) resulting in an asymmetric cross-sectional geometry due to differences in the interface energy between Ge and Si on two facets. At a Ge thickness of 8.7 monolayers (MLs), we observe a well-ordered array of Ge nanowires which are nearly symmetric cross section. The Ge nanowires are typically 40 nm wide, 7 nm high, and 1 $\mu$m in length, with a lateral period of 80 nm. After 10 MLs growth, Ge nanowires started to ripen irregularly. The growth rate of Ge on Si(124) was 4.3 times slower than that on Si(001) substrates at 600 °C. Nanowire-related photoluminescence peaks were observed at around 0.83 eV for Si-capped samples. The morphological evolution of Ge nanowires will be discussed along with observed photoluminescence.

**2:45 PM F9.5**
**Complex Diameter Modulations in Silicon Carbide Nanowire Growth.** Hideo Kohno, Hideto Yoshida and Seiji Takeda; Physics, Osaka University, Toyonaka, Osaka, Japan.

Some of semiconductor nanowires grown via self-organized processes exhibit diameter modulations. Not only periodic, but also non-periodic complex modulations have been observed. Nevertheless, such complex diameter modulations have never been investigated from the viewpoint of random walk and fractality so far. In this study we fabricated SiC nanowires with non-periodic diameter modulation and investigated the modulations in terms of scaling. SiC nanowires were grown by heating a Si substrate on which Au of 7.5 nm thick was deposited and a SiC powder in an evacuated silica container at 1200 degree C for 2 hours. Numerous SiC nanowires with diameters of several tens of nanometer were grown on the Si substrate. By processing transmission electron microscopy (TEM) images of the SiC nanowires, the digitized diameter data were obtained. We found that increments of the diameter modulations are power-law distributed. This means that the modulations are not Brownian motion. By calculating height-height correlation functions of the modulations, we found multiaffinity in the modulations. We note that experimental observation of multiaffinity in actual physical systems is very rare. Furthermore, it is interesting that such complex fractality appears in nanometer scale. The growth mechanism and degree of determinism will be also discussed.

**3:15 PM *F9.6**
**Elemental Semiconductor Nanowires and their Thermoelectric Properties.** P. Yang and Rong Fan; University of California-Berkeley, Berkeley, California.

Nanowires are of both fundamental and technological interest. They represent the critical components in the potential nanoscale electronic and photonic device applications. In this regard, heterojunction and superlattice nanowires are especially important. In this talk, we will present our recent work on the growth of elemental semiconductor nanowires and superlattice nanowires. Their precise size, positional and orientational control of these nanowires will be discussed. We will then discuss the interesting thermoelectric properties of these Si/Ge nanowires and their relationship with the phonon confinement.

**3:45 PM F9.7**
**Quantum Confinement and the Vibrational and Electronic Properties of Group IV and III-V Semiconductor Nanowires.** Xinyuan Zhao[1], Li Yang[1], C. M. Wei[1,2] and Mei-Yin Chou[1]; [1]School of Physics, Georgia Institute of Technology, Atlanta, Georgia; [2]Institute of Physics, Academia Sinica, Taipei, Taiwan.

We have investigated the structural, electronic, vibrational, and

optical properties of hydrogen-passivated silicon nanowires along [110] and [111] directions with diameter d up to 4.2 nm from first-principles density-functional calculations. The size and orientation dependence of the band gap is investigated and the local-density gap is corrected with the GW approximation. Quantum confinement becomes significant for d < 2.2 nm, where the dielectric function exhibits strong anisotropy and new low-energy absorption peaks start to appear in the imaginary part of the dielectric function for polarization along the wire axis [1]. Similar studies are also performed for III-V semiconductor nanowires. Lattice vibrations are investigated and the density of vibrational modes at $\Gamma$ is calculated and analyzed for silicon nanowires as a function of diameter. It is discovered that the frequencies of the optical modes are red-shifted as the diameter decreases, while the newly created collective modes are blue-shifted. These features can be understood using simple physical models. The Raman scattering activity of selected wires is also evaluated. [1] X. Zhao, C. M. Wei, L. Yang, and M. Y. Chou, Phys. Rev. Lett. 92, 236805 (2004).

**4:00 PM F9.8**
**Coherent Single Charge Transport in Molecular-Scale Silicon Nanowire Transistors.** Zhaohui Zhong[1], Ying Fang[1], Wei Lu[1] and Charles M. Lieber[1,2]; [1]Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts; [2]Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts.

We have investigated the low-temperature electrical transport properties of single-crystal silicon nanowires with diameters as small as several nanometers. Coulomb blockade oscillations are observed with the periodic addition of single charges over a large gate voltage range. Analysis of data recorded on nanowire devices with varying source-drain separations suggests that nanowires behave as single quantum dots for lengths up to several hundred nanometers. Detailed studies of the conductance vs. source-drain and gate voltages provide evidence for resonant tunneling through individual quantized energy levels of the molecular scale silicon nanowires. These results differ from those obtained for nanofabricated planar silicon devices, which show localization on much shorter length scales, and thus suggest potential for molecular-scale silicon nanowires as building blocks for quantum and conventional electronics.

**4:15 PM F9.9**
**Silicon nanowires: doping-dependent n- and p- channel FET behavior and UV photoresponse.** Kumhyo Byon[1], C. K. W. Adu[2], P. C. Eklund[2] and J. E. Fischer[1]; [1]Materials Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania; [2]Department of Physics, Penn State University, University Park, Pennsylvania.

One-dimensional nanostructures such as silicon nanowires (Sinws) are promising materials for nano-scale sensors and photo-detectors. Moreover, the electrical and optoelectronic properties of silicon nanowires (SiNws) can be tailored by quantum confinements for diameters of order 5nm or less. In this work, we studied the electrical transport properties of Sinws grown by Fe-catalyzed pulsed laser vaporization (R. J. Barsotti, J. E. Fischer, C. H. Lee, J. Mahmood, C. K. W. Adu and P. C. Eklund, Appl. Phys. Letters 81, 2866, 2002). Previous AFM and TEM studies showed that the average diameter is 7 nm including 1-2 nm native oxide. E-beam lithography was used to make 2 and 4 terminal devices with back gate. Two layers of titanium and gold were used as electrodes to give low contact resistance. As-grown devices showed p-type behavior with high resistivity. To modify conductivity and majority carrier type, spin-on glass or FIB (focused ion beam) were used to dope with phosphorous or gallium respectively. I-V and gate response were compared before and after doping; with P-glass we found that the FET behavior changed from p- to n-type. Furthermore, photoresponse of 2-terminal devices was investigated under UV illumination using a low pressure mercury pencil lamp with strong 254 nm emission and 2 mW/cm$^2$ power. We found that the electrical properties of Sinw devices are very sensitive to UV. The conductance increased significantly when Sinws devices were exposed to UV, much more strongly than with room light or 0.5 mW HeNe laser. The possible mechanisms will be discussed.

**4:30 PM F9.10**
**Fabrication and Electrical Characterization of Silicon Nanowire Arrays.** Sarah M. Dilts, Ahmad Mohammad, Kok-Keong Lew, Suzanne E. Mohney and Joan M. Redwing; Department of Materials Science and Engineering, Materials Research Institute, Penn State University, University Park, Pennsylvania.

Resistivity measurements of individual nanowires are challenging, requiring techniques to assemble the nanowires and lithographically define electrical contacts at each end. Furthermore, contact resistance often dominates nanowire resistance measurements carried out using a simple two-point geometry. In this study, resistivity measurements were carried out on high-density vertical arrays of boron-doped silicon

nanowires (SiNWs) synthesized by vapor-liquid-solid growth within the pores of anodized alumina membranes. The membrane provides a support structure for nanowire growth and alignment and also facilities the formation of electrical contacts via the top and bottom membrane surfaces. The alumina membranes used in this study were nominally 60 $\mu$m thick with 200 nm diameter pores. To prepare the nanowire structures, a thin layer of silver was initially sputtered on the back-side of the membrane followed by sequential electrodeposition of 5 $\mu$m of silver, 28-42 $\mu$m of cobalt and 0.25 $\mu$m of gold within the pores. Vapor-liquid-solid growth of SiNWs within the pores was then carried out at 500°C and 13 Torr using SiH4 and trimethylboron (TMB) as the silicon and boron-dopant sources, respectively. Cobalt silicide, which forms during nanowire growth at the cobalt-silicon interface served as the back-side contact to the nanowires. Circular Al dots, deposited by e-beam evaporation, were used to form top-side electrical contacts to the nanowire arrays. For measurements of nanowire resistivity and contact resistance, a series of samples were prepared in which the length of the SiNWs was varied from 13 to 27 $\mu$m using a constant TMB/SiH4 inlet gas phase ratio during growth. The resistance of the SiNW arrays and the average contact resistance were extracted from plots of total resistance versus SiNW length. Preliminary measurements yield an average resistivity of 35 ± 6.14 $\Omega$-cm for the boron-doped SiNWs measured using this technique. The effect of dopant concentration on nanowire resistivity will also be reported.

**4:45 PM** <u>F9.11</u>
**Nano-Bridging: An Effective Solution to Interconnecting Nano-Scale Devices.** <u>M. Saif Islam</u>[1,2], Shashank Sharnma[1], Ted I. Kamins[1] and R. Stanley Williams[1]; [1]Quantum Science Research, Hewlett-Packard Laboratories, Palo Alto, California; [2]Electrical and Computer Engineering, University of California, Davis, California.

Interconnecting nanoscale devices made of one dimensional nanowires (NWs) with other circuit elements has been a challenge since NWs were first contemplated as device components. The research-based approach of sequentially connecting electrodes to individual NWs has contributed to understanding the characteristics of the NWs and exploring novel device applications, but provides no path to mass-fabrication nor to circuit integration. A method for high density integration along with a massively parallel, self-assembly technique for interconnecting these building blocks of nano-electronics is critical for practical application of NWs. We report a novel technique of growing a high density of highly oriented lateral silicon NWs between two electrically isolated Si electrodes defined by conventional optical lithography. A metal-catalyzed chemical vapor deposition (CVD) process was used to grow NWs and form robust "nano-bridges" on a silicon-on-insulator (SOI) substrate. Current-voltage measurements of p-type boron-doped NWs demonstrate highly linear I-V characteristics, confirming excellent ohmic contacts for suitably doped nanowires. An approximate correlation between the resistivity and the dopant gas flow has also been observed. Our VLSI compatible, self-assembly technique of connecting NWs between two electrodes needs only relatively coarse lithography and offers the high surface-to-volume ratio needed for nano-sensor applications. This novel bridging technique has the potential for solving the long-standing issue of interconnecting nanoscale devices in many material systems.

SESSION F10: Poster Session
Chairs: Siegfried Janz and C. Reynaud
Wednesday Evening, December 1, 2004
8:00 PM
Exhibition Hall D (Hynes)

<u>F10.1</u>
**Nanometer scale metal/Si nanowire junctions and aligned silicon quantum dot arrays for nanoelectronics fabricated with self-assembled etch masks.** <u>Regina Ragan</u>[1], Sehun Kim[2] and R. Stanley Williams[1]; [1]Quantum Science Research, Hewlett Packard, Palo Alto, California; [2]Department of Chemistry, Korea Advanced Institute of Science and Technology, Daejon, South Korea.

Research in semiconductor physics is undergoing a paradigm shift. A bottom up or self-assembly approach is being investigated as an alternative to the current top down lithographic approach. Most significantly, the shift from the exclusive use of lithography for device fabrication opens the field to not only novel fabrication schemes but to the incorporation of diverse material systems. Hexagonal rare earth disilicide nanowires self-assemble during epitaxial growth as one-dimensional metallic nanostructures on Si(001) substrates due to an anisotropic lattice mismatch with Si[110]. We have demonstrated that dense arrays of parallel RE disilicide (RE = Er, Dy, Sm, Gd) nanowires exhibiting high aspect ratios, having lengths exceeding 1 micron and widths less than 5 nm can be grown on vicinal Si(001)

substrates with a miscut of 2.5 degree toward the [110] azimuth. We now demonstrate that platinum passivates the Er disilicide nanowire surface and acts as an etch mask during reactive ion etching. Scanning electron microscopy images taken after reactive ion etching (RIE) of these Er disilicide and Pt coated Er disilicide nanostructures shows that nanowires without Pt on the surface are significantly etched whereas the Pt coated nanowires are not. AFM images were obtained both before and after etching the nanowires to measure the change in nanowire feature height. The average feature height changed from 1.0 nm to 7.8 nm for Pt coated nanowires and from 1.0 nm to 5.8 nm for the remaining uncoated Er disilicide nanowires. Er disilicide nanowires are on the order of 1 nm tall; thus these self-assembled nanowires act as an etch mask to define Si nanowires. Furthermore, Er disilicide nanowires with a lower coverage of Pt on the surface formed arrays of quantum dots aligned along Si[110] with a very narrow size distribution after RIE. STM images taken prior to etching show that Pt forms clusters on the nanowire surface when the Pt coverage is incomplete. The cluster size is related to the nanowire width. Thus, the Si quantum dots have a narrow size distribution, a high density, $10\hat{1}0/$ cm$\hat{2}$, and are aligned along the Si[110] direction due to the original template. The Si-quantum dot size is tunable between 1-5nm (depending on the size of the RE disilicide nanowire), the size regime where strong quantum confinement effects are expected. Using scanning tunneling spectroscopy, we measured current rectification at the RE disilicide/ p-type Si junction. Coupled with self-assembled molecular layers, these nanometer scale junctions could have current switching and rectifying behavior and in large arrays may be used for general computing. The achievement of a high density of ordered self-assembled nanostructures is an important precursor to forming sensing, memory and logic devices with density and features sizes not attainable using conventional lithography.

<u>F10.2</u>
**Hydrogen Passivation of Er and Si Nanocrystallites in Er-doped SiO$_2$ - Increase in Photoluminescence-.** <u>Naoki Fukata</u>[1,2], Changqing Li[1], Hiroshi Uematsu[1], Takamichi Arai[1], Tetsuya Makimura[1] and Kouichi Murakami[1,2]; [1]Institute of Applied Physics, University of Tsukuba, Tsukuba, Japan; [2]Special Research Project on Nanoscience, University of Tsukuba, Tsukuba, Japan.

Hydrogen passivation effect of the photoluminescence (PL) from Er ions and Si nanocrystallites (nc-Si) has been investigated in Er-doped SiO$_2$ with nc-Si. Enhancement of the PL at RT from Er ions is one of the main subjects. The relative intensity of PL from Er ions at RT to that at a low temperature was improved by using nc-Si as a host matrix of Er. The crystallinity of nc-Si is important to further enhance the efficiency of the energy transfer from nc-Si to Er ions since residual defects at the interface between nc-Si and the surrounding SiO$_2$ and in the nc-Si act as nonradiative recombination centers, resulting in quenching the PL of both the Er and nc-Si. In order to passivate the residual defects, hydrogen gas treatments were done at 300-500°C for Er-doped SiO$_2$ films with nc-Si fabricated by laser ablation. Enhancement of PL was successfully obtained for Er ions and nc-Si by hydrogen gas treatment. The PL intensities of Er ions and nc-Si increased by a factor of 2-3, respectively, depending on the hydrogenation conditions. Electron spin resonance (ESR) measurements showed a decrease in residual defects performed by hydrogen gas treatment. Based on g-factors of the ESR signal, the temperature dependence of passivation and dissociation of the defects, the defects probably exist at the interface between nc-Si and the surrounding SiO$_2$, namely, $P_b$ type defects. These results strongly indicate that the optical excitation energy of nc-Si is more effectively transferred to Er ions by hydrogen passivation of $P_b$ type defects, which act as nonradiative recombination centers.

<u>F10.3</u>
**Characterization and Modelling of the Emission at 1540 nm from Silicate Glasses Co-doped with Si and Er Ions.** Yousef Lebour[1], <u>Paolo Pellegrino</u>[1], Jose Moreno[1], Cristina Garcia[1], Joan Ramon Morante[1], Blas Garrido[1] and Michel Prassas[2]; [1]Electronics, University of Barcelona, Barcelona, Spain; [2]Fontainebleau Research Centre, Corning S.A., Avon, France.

We have characterized and modelled the mechanism of energy transfer from Si nanoparticles to Er, in different silicate glasses, namely soda-lime and aluminium silicates, in comparison with pure silica. The interest in such composite glasses is their wide optical bandwidth at 1540 nm and large Er solubility. By means of ion implantation and thermal treatment a set of glass wafers have been processed. From a multi-implantation scheme we have prepared a 350 nm thick glass layer with a uniform Si excess (5% or 15% atomic excess) and a Er-rich distribution. Several Er doses were chosen so that the resulting Er peak concentration could vary from 2x10$^{19}$ cm$^{-3}$ up to 6x10$^{20}$ cm$^{-3}$. Fused silica wafers coimplanted in the same conditions were used as a reference material in order to compare the different efficiency and mechanisms of Er emission as the host silicate is changed. Systematic photoluminescence (PL) measurements (both for

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resonant and non resonant Er-excitation) were performed for a comprehensive study of the emission properties around the 1540 nm window. Time-resolved PL characterization was carried out in order to explore the dynamic response of the system. All the measurements have been made as a function of: the matrix composition, the Si and Er content in the implanted layers, the excitation wavelength and the power density. This complete experimental work allows to build up a quantitative model of the interaction between the absorbing Si nanoprecipitates and the emitting Er atoms. As a first approach, the Si clusters- Er system have been aproximated as an effective luminescent medium, whose optical properties can be fully described by a lifetime constant and effective absorption coefficient. From a fitting procedure of the dependence of the PL intensity and lifetime with the incident photon flux and the Er concentration, a more sophisticated description of the system have been built, and second order effects have been revealed, such as energy up-conversion among Er atoms and concentration quenching. This exhaustive model makes use of several physical parameters which describe the PL process and which have been experimentally determined for each kind of host glass: lifetime at 1540 nm (from 3 to 12 ms, depending on the Er dose), effective absorption coefficient (of the order of $1x10^{-17}$ cm$^2$), radiative transition rate at 1540 nm, concentration quencing and up-conversion coefficients, coupling constant between Er and Si clusters. Finally, the dependence of the optical behaviour of the different processed glasses and the comparison with the structural characterization will be discussed.

## F10.4
**Luminescence of Rare Earth Doped Si/Al/SiO$_2$ Co-sputtered Films.** Luis F. Fonseca, <u>Carlos Rozo</u>, Oscar Resto and S. Zvi Weisz; Physics, University of Puerto Rico, San Juan, Puerto Rico.

Er$^{3+}$ and Nd$^{3+}$ doped Si/Al/SiO$_2$ thin films have been prepared by rf co-sputtering. Some of these films were annealed to 700$^\circ$C. Erbium doped Si/Al/SiO$_2$ films were prepared with two different sputtering configurations: one configuration with a large quantity of Al and a second configuration with a smaller quantity of Al. The configuration with large quantity of Al shows a diminished luminescence at 1.53 $\mu$m, but this emission is increased by substrate heating. The configuration with smaller quantity of Al shows emission at 1.53 $\mu$m similar in intensity to the Er-doped Si/SiO$_2$. The spectral shape for the $^4I_{13/2} \rightarrow ^4I_{15/2}$ emission is broader than for an analogous Er$^{3+}$ doped Si/SiO$_2$. The smaller quantity of Al configuration increases the solubility of Nd$^{3+}$ (and luminescence for high Nd$^{3+}$ concentration) in Si/SiO$_2$ films and changes the spectral shape of the $^4F_{3/2}$ emission with respect to the Nd$^{3+}$ doped Si/SiO$_2$ films.

## F10.5
**Optical activation of Erbium by Si nanowires using sol-gel derived Er-doped silica.** <u>Kiseok Suh</u>[1], Jung H. Shin[1], Oun-Ho Park[2], Byeong-Soo Bae[2], Heon-Jin Choi[3] and Jung-Chul Lee[3]; [1]Physics, KAIST, Daejeon, South Korea; [2]Materials Science and Engineering, KAIST, Daejeon, South Korea; [3]Materials Science and Technology Division, KIST, Seoul, South Korea.

Efficient Si-based light emitting material has been attracting much interest because of its potential application in photonics with Si technology. In particular, Er-doping of Si material has great importance due to their Er$^{3+}$ intra-4f emission at 1.54$\mu$m, a standard wavelength for telecommunications. Er-doped Si light emitting diodes (LED) operated at room temperature were demonstrated with good electrical properties. However, the luminescence efficiencies were quite poor due to their intrinsic Auger- and temperature quenching of Er$^{3+}$ luminescence. On the other hand, excellent optical properties were obtained by using silicon-rich-silicon-oxide (SRSO), which consists of nanocluster Si (nc-Si) embedded inside an SiO$_2$ matrix. Although optical gain as well as efficient LED have been demonstrated, SiO$_2$ matrix makes current injection difficult, resulting in requirement high voltages or thin SRSO layers to operate LEDs. Such problems may be solved by using Si nanowires (Si-NWs) instead. we report in the results of such optical activation of Si-NWs using sol-gel derived Er-doped silica. Silicon nanowires (Si-NWs) were grown by typical VLS method using SiCl$_4$ as a source gas. The diameter of Si-NWs is about 100nm and the length is 10$\mu$m. Er doped silica film was spin coated on Si-NWs. The starting solution was prepared by hydrolyzing tetraethoxysilane (TEOS) in 0.05 M HCl aqueous solution with ethanol as a cosolvent and adding the ErCl$_3$·6H$_2$O to the solution. The mixture was then stirred at RT for 1 day and spin coated on Si-NWs and annealed at 450$^\circ$C for 7h, 950$^\circ$C for 5min in a flowing N$_2$/O$_2$ environment. For comparison, Er doped silica film was coated on pure Si wafer without Si-NWs. We measured the Er$^{3+}$ photoluminescence (PL) properties of Er-doped silica with Si-NWs and pure Er-doped silica. The PL intensity of the pure Er-doped silica pumped with the wavelength of 473 nm is feeble since the photon cannot excite the Er3+ ions resonantly. However, that of the Er-doped silica with Si-NWs pumped with the wavelength of 473 nm

is enhanced by an order of magnitude. The enhanced PL is caused by an generated carriers in Si-NWs which can transfer their energy to Er$^{3+}$ ions. Also, the temperature dependence of integrated PL and Er$^{3+}$ lifetime (6.9 msec at RT) of Er-doped silica with Si-NWs shows complete suppression of thermal quenching which means good luminescence efficiency comparable to pure Er-doped silica. The electronic devices using Si-NWs operating voltages of less than 5V were demonstrated already. Therefore, easy current injection and efficient Er$^{3+}$ luminescence can be acquired by sol-gel derived Er-doped silica with Si-NWs.

## F10.6
**Abstract Withdrawn**

## F10.7
**Abstract Withdrawn**

## F10.8
**Anisotropically Nanostructured Silicon: A First-Principle Approach.** Yuri Bonder and <u>Chumin Wang</u>; Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, Mexico D.F., Mexico.

Porous silicon (PSi), obtained from an electrochemical etching of crystalline silicon (c-Si), has efficient photo- and electro-luminescences in the visible at room temperature. Since the beginnings of the last decade it was well established that the pores grow preferentially along the [100] crystallographic directions [1]. During the last years, samples obtained form etching (110)-oriented c-Si, called birefringent PSi, have demonstrated to possess a strong anisotropic structure that provides a sensitive tool to analyze atoms and molecules adsorption in negligible quantities [2]. Furthermore, stacks of birefringent porous silicon layers, alternating their porosity and thickness, act as dichroic microcavities with a transmission dependent on the polarization direction of the incident light [3]. In this work, the density-functional theory (DFT) is utilized to study structural and optical anisotropy in birefringent PSi. The DFT within the local density approximation (LDA) is perhaps the most used ab-initio method to calculate ground-state properties of semiconductors. Unfortunately, this approach underestimates the band gaps which can be overcome by shifting the DFT-LDA conduction-band spectrum to higher energies via a scissors operator. The birefringent PSi is modelled starting from a (110)-oriented c-Si supercell and columns of Si atoms are removed along [100] and [010] crystallographic directions. All the dangling bonds are saturated by hydrogen atoms, as done in Ref. [4]. Firstly, a full geometry optimization is carried out using Car and Parrinello's method to find the structural ground state. Then, optical properties are obtained through Fermi's Golden Rule and Kramers-Kronig transformation [5]. A scissors operator of 0.7 eV is included in order to reproduce the experimental value of the c-Si electronic band gap. In particular, for a [110] incident light, polarized along [1-10] and [001] directions, we observe that the difference of refractive index between this two polarizations decay exponentially with the light wavelength, in good agreement with the experimental data of Ref. [6]. Furthermore, the theoretical absorption spectra follow the same photon-energy dependence as the experimental results [1] for each polarization. [1] V.Yu. Timoshenko, et al., Phys. Rev. B 67, 113405 (2003). [2] E. Gross, et al., J. Appl. Phys. 90, 3529 (2001). [3] J. Diener, et al., J. Appl. Phys. 91, 6704 (2002). [4] E. Vazquez, et al., J. Appl. Phys. 91, 3085 (2002). [5] M. Cruz, et al., Phys. Rev. B 59, 15381 (1999). [6] D. Kovalev, et al., Appl. Phys. Lett. 78, 916 (2001).

## F10.9
**Generation of Singlet Oxygen at Room Temperature Mediated by Energy Transfer from Si Nanocrystals.** <u>Minoru Fujii</u>[1], Shingo Minobe[1], Shinji Hayashi[1], Egon Gross[2], Joachim Diener[2] and Dmitri Kovalev[2]; [1]Department of Electrical & Electronics Engineering, Kobe University, Kobe, Japan; [2]Physik Department, Technische Universitaet Muenchen, Muenchen, Germany.

The molecule-like electronic structure of Si nanocrystals provides them with nobel functions which have been realized so far by organic molecules. Very recently, Si nanocrystal assemblies are found to be an efficient photosensitizer for the formation of singlet oxygen ($^1O_2$). Singlet oxygen representing electrically excited states of an oxygen molecule is a very important material in biology and chemistry because it mediates important processes in modification of biological structures. Formation of $^1O_2$ requires the presence of light-absorbing photosensitizer with subsequent energy transfer of electronic excitation to molecular oxygen. For efficient energy transfer photosensitizers must have spin-triplet excited states to satisfy the spin-conservation rule during the energy transfer process. Furthermore, the lifetime of the excited triplet state should be long to enhance the probability of energy exchange. Si nanocrystals satisfy all these criteria and triplet excitons in Si nanocrystals plays the same role as a triplet-excited state of dye molecules. The formation of $^1O_2$ is evidenced by photoluminescence (PL) measurements in the

near-infrared spectral region where a narrow line due to radiative relaxation of the lowest excited singlet state to the ground triplet state of oxygen molecules is detected. However, because of the restriction of spin and angular momentum conservation rules, the oscillator strength of the transition is extremely small; the intrinsic lifetime of the state is very long ($2.7 \times 10^3$s) resulting in very weak PL intensity. The emission was so far detected only at very low temperatures when oxygen molecules are condensed on the surface of Si nanocrystals. Although the intrinsic lifetime is extremely long, intermolecular interactions lead to an enhancement of the transition rate. The radiative transition rate is three to four orders of magnitude larger in solution than in diluted gas phase. However, in most solvents, deactivation of $^1O_2$ is radiationless by collisional electronic to vibrational energy transfer from $^1O_2$ to a solvent molecule. Therefore, to obtain reliable luminescence data, solvents consisting of poor quenchers should be chosen. The second important requirement on the solvent is that it should not quench luminescence of Si nanocrystals. As a solvent which satisfies these requirements, we employed hexafluorobenzene ($C_6F_6$). The singlet oxygen lifetime in the solution is about 25 msec, which is about three orders of magnitude longer than that in benzene ($C_6H_6$). In this work, we study PL from porous Si powder dispersed in $C_6F_6$. From the PL studies, we demonstrate that singlet oxygen can be generated by the energy transfer from Si nanocrystals at room temperature.

## F10.10
**Control of Photoluminescence Properties of Si Nanocrystals by Simultaneously Doping n and p Type Impurities.**
Minoru Fujii, Yasuhiro Yamaguchi, Keiichi Ninomiya and Shinji Hayashi; Department of Electrical & Electronics Engineering, Kobe University, Kobe, Japan.

Si nanocrystals (nc-Si) show strong luminescence in the visible range. The luminescence is considered to arise from the recombination of excitons across the widened bandgap of nc-Si. The luminescence property is expected to be modified by controlling impurities in nc-Si. However, shallow impurity doping in nc-Si results in radiationless Auger recombination, in which the energy released by the recombination of an exciton is consumed by giving kinetic energy to an electron (hole) supplied by doping. The Auger recombination could be avoided if isoelectronic impurities are doped or carriers in nc-Si are perfectly compensated by simultaneously doping n and p type impurities. In nc-Si, an exciton is confined in a space comparable to or smaller than the Bohr radius, and the wavefunction of excitons as well as shallow impurities are extended in a whole nanocrystal. If for example one P atom and one B atom are doped simultaneously in a nanocrystal a few nanometer in diameter, it could be treated as a perfectly compensated single system with no excess carriers, and thus the exciton could enjoy the enhancement of oscillator strength due to further localization by impurity doping without being afraid of the Auger recombination. Therefore, impurity control of nc-Si may add new optical properties on nc-Si which can not be realized by pure nc-Si. In this work, we have prepared B and/or P doped nc-Si embedded in glass matrices by controlling B and P concentrations in a wide range, and studied the PL properties. We will demonstrate that proper control of shallow impurities allow us to extend the tunable range of luminescence energy at room temperature below the bulk bandgap (till 0.9 eV) without losing intensity so much. The near-infrared luminescence at room temperature may open up new application of nc-Si based materials on an optical telecommunication field.

## F10.11
**Pump-probe experiments on low loss silica waveguides containing Si nanocrystals.** Daniel Navarro[1], Nicola Daldosso[1], Mirko Melchiorri[1], Lorenzo Pavesi[1], Cristina Garcia[2], Paolo Pellegrino[2], Blas Garrido[2], J.R. Morante[2], E. Scheid[3] and G. Sarrabayrouse[3]; [1]Physics, University of Trento, Povo (Trento), Italy; [2]Electronica, Universitat de Barcelona, Barcelona, Spain; [3]Laboratory for Analysis and Architecture of Systems of C.N.R.S., Touluse, France.

Rib-loaded silica waveguides containing Si nanocrystals were grown by quadruple implantation of Si ions into a 2 $\mu$m-thick thermally-grown $SiO_2$ layer. The thickness of the resulting flat-profile active region was about 300 nm, with Si excess ranging from 7% to 13% (determined by X-ray photoelectron spectroscopy). Complete phase separation and nanocrystal formation was assured by annealing at 1100 °C, and studied by means of optical tools such as Raman, optical absorption and luminescence. The rib-loaded structure of the waveguides was fabricated by photolithographic and reactive ion etching processes, with patterned rib widths ranging from 1 to 8 $\mu$m. Efficient light propagation was observed when end-fire coupling a probe signal both at 633 nm and 780 nm into the waveguides, with attenuation losses as low as 11 dB/cm in the red. An increase of losses has been observed and explained as a function of the rib width and the mechanisms involved in these losses (scattering and absorption) have been evaluated and discussed. Pump and probe experiments under CW and time resolved conditions at 780 nm are under-way to look for optical gain in these structures. The results of the experiments will be presented and discussed at the conference.

## F10.12
**Multi-color Luminescence from nanocrystalline silicon.**
Hiroshi Kunii[1], Keisuke Sato[1], Kenji Hirakuri[1] and Tomio Izumi[2]; [1]Electronic and Computer Engineering, Tokyo Denki University, Hatoyama, Saitama, Japan; [2]Electronics, Tokai University, Hiratsuka, Kanagawa, Japan.

The nanocrystalline silicon (nc-Si) is extremely attractive material for luminescent color. Luminescent color from the nc-Si shifts from red light to blue light by varying the size. We previously studied that the size was dependent on quantity of Si atoms introduced into amorphous $SiO_x$ (a-$SiO_x$) film. In this study, we report the correlation between the luminescent color and the Si concentration in the a-$SiO_x$ film. The a-$SiO_x$ film including the Si atoms was prepared by sputtering method. The Si concentration of the a-$SiO_x$ films tuned by changing the sputtering condition. The nc-Si was formed by the coagulation of Si atoms at annealing temperature of about 1000°C. The Si concentration and the luminescent properties were estimated by using X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), and photoluminescence (PL) measurements. Red luminescent was obtained from the nc-Si formed at the Si concentration of 9%. When the Si concentration was decreased from 9% to 2%, the luminescent color blue-shifted from red to blue light, because the decrease of the Si concentration leads to the reduction of the size. Moreover, the intensity of their luminescence was very strong.

## F10.13
**Improvement of Operating Voltage and Luminescent Properties in Nanocrystalline Silicon Electroluminescent Device.** Keisuke Sato[1,2], Kenji Hirakuri[1], Mitsuo Iwase[3] and Tomio Izumi[4]; [1]Dept. of Electronic and Computer Engineering, Tokyo Denki University, Saitama, Japan; [2]Dept. of Applied Science, Tokai University, Hiratsuka, Japan; [3]Dept. of Materials Science, Tokai University, Hiratsuka, Japan; [4]Dept. of Electronics, Tokai University, Hiratsuka, Japan.

Nanocrystalline silicon (nc-Si) is useful candidate materials for development of new flat panel displays including electroluminescent (EL) display and field emission display. However, the EL device using nc-Si has a poor performance under luminance and operating voltage. In this paper, we fabricate the EL device using hydrofluoric acid (HF) treated nc-Si to realize high brightness and low operating voltage. Moreover, we report luminescence and electrical properties from the EL device. The luminous layer was prepared on p-type Si wafer. The nc-Si, which used for the luminous layer, was formed in a silicon dioxide ($SiO_2$) layer by co-sputtering of Si/$SiO_2$ targets and subsequently annealing at high temperature. The nc-Si, then, were dispersed uniformly onto the p-type Si wafer with the removal of $SiO_2$ layer by treating in HF solution. And the electrode was formed at top and bottom of the luminous layer. The top and the bottom electrodes were used an indium tin oxide (ITO) and aluminum (Al), respectively. The EL device using nc-Si with the $SiO_2$ layer showed red luminescence with a peak of 650 nm by applying the operating voltage above 5.0 V. When the $SiO_2$ layer in the EL device was removed by the HF treatment, the operating voltage decreased from 5.0 V to 2.5 V. Moreover, the luminance of the EL device was also increased more than one order of magnitude by the HF treatment, because the carrier was efficiently injected into the nc-Si by the removal of $SiO_2$ layer. The red luminescence from the EL device could be seen with naked eye under room illumination at the operating voltage of 3.0 V.

## F10.14
**Photoluminescence from Crystalline Silicon Quantum Dots Embedded in Silicon Nitrides.** Tae Wook Kim[1], Baek Hyun Kim[1], Chang Hee Cho[1], Seong Ju Park[1], Nae Man Park[2] and Gun Yung Sung[2]; [1]Material Science and Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea; [2]Basic Research Laboratory, Electronics and Telecommunications Research Institute, Daejeon, South Korea.

Even though the electronic and optical properties of silicon quantum dots are expected to be very different from those of bulk material, very few experimental evidences have been reported. In this study, we report on the growth of silicon quantum dots and structural and optical properties of silicon quantum dots which can be used for various silicon optoelectronic devices. Well-defined crystalline silicon quantum dots(c-Si QDs) embedded in silicon nitride films was grown by plasma enhanced chemical vapor deposition (PECVD) without post annealing. The wavelength of photoluminescence peak of sample was decreased from 697nm(1.78eV) to 454nm(2.73eV) with decreasing the dot size. High resolution transmission electron microscopy (HRTEM) analysis showed that the average size of Si QDs was in a range from 4.9 to 2.9nm. In addition, the ring pattern in transmission

electron diffraction (TED) data is consistent with the formation of c-Si QDs in silicon nitride matrix. Especially, the crystalline plane of the Si QDs was observed in HRTEM image suggesting an excellent crystallinity of Si QDs in silicon nitride matrix. This result suggests that the size of c-Si QDs can be controlled in a silicon nitride film using PECVD without post annealing. An effective mass theory with an assumption of an infinite potential barrier predicts that band gap of c-Si QDs is very different from that of amorphous silicon quantum dots(a-Si QDs). It has been reported that the quantum confinement effect is less remarkable in a-Si QDs than that of c-Si QDs [1, 2]. This study showed that the quantum confinement parameter of c-Si QDs is larger than that of a-Si QDs, indicating that c-Si QDs have strong quantum confinement effect compared to a-Si QDs. 1. N.-M. Park, C.-J. Choi, T.-Y. Sung, and S.-J. Park, Phys. Rev. Lett. 86, 1355(2001) 2. K. Nishio, J.Koga, T. Yamaguchi, and F. Yonezawa, Phys. Rev. B 67 195304(2003) * sjpark@gist.ac.kr

### F10.15
**Soft X-ray Spectroscopy of Dopant Atoms in Semiconductor Nanocrystals.** R. W. Meulenberg, Anthony van Buuren, Trevor Willey and Louis Terminello; LLNL, Livermore, California.

Understanding the confinement and surface physics of doped and undoped nanocrystals is currently an important field of research. Quantum confinement effects as well as the impact of surface termination are critical to the design and future utilization of these novel materials in devices. We use soft x-ray probes such as x-ray absorption spectroscopy (XAS), photoelectron spectroscopy (PES), and soft x-ray fluorescence (SXF) experiments to determine the electronic structure of a variety of nanostructured materials. We report the changes in the band edge shifts and effect of surface termination of group IV nanocrystals as the particle shape is changed (i.e. from a sphere to a rod). Finally, we will show that synchrotron radiation techniques are an ideal tool to study the chemical environments of transition metal dopants in Si nanocrystals. This work was supported by the Division of Materials Sciences, Office of Basic Energy Science, and performed under the auspices of the U. S. DOE by LLNL under contract No. W-7405-ENG-48. Part W of program listing

### F10.16
**Structural, Electronic and Defect Properties of Chemically Modified Silicon Nanoparticles.** Andrea Baumer[1], Martin Stephan Brandt[1], Martin Stutzmann[1], Claudia Dahmen[2], Joerg Auernheimer[2], Horst Kessler[2], H. Wiggers[3], P. Roth[3], M. Pridoehl[4] and F. M. Petrat[4]; [1]Walter Schottky Institut, TU Muenchen, Garching, Germany; [2]Institut fuer Organische Chemie und Biochemie, TU Muenchen, Garching, Germany; [3]Institut fuer Verbrennung und Gasdynamik, Universitaet Duisburg-Essen, Duisburg, Germany; [4]Creavis Technology and Innovation, Degussa AG, Marl, Germany.

The surfaces of the nanoparticles are decisive for the properties of electronic devices made from nanocrystals. In this work, we present an investigation of the influence of different chemical surface modifications (as-grown oxide, H-termination and organic functionalization) of silicon nanoparticles produced in hot wall and microwave reactors on the structural, electronic and defect properties. The surface area, size and morphology is determined by high resolution transmission electron microscopy and nitrogen adsorption at 77 K. On the as-grown nanoparticles, partially oxidized and hydrogenated surfaces are observed with the help of Fourier transform infrared spectroscopy (FTIR) and nuclear magnetic resonance (NMR). By etching with hydrofluoric acid (HF), most of the oxide can be removed and Si-H and Si-H2 bonds are generated. Using thermally induced hydrosilylation, alkyl chains can be attached to these H-terminated nanoparticles, forming direct covalent Si-C bonds. Information on the nature and density of electronic defects on the surface-modified silicon nanoparticles are obtained by electron spin resonance (ESR). The as-grown particles show a broad Gaussian line with gdb = 2.0052 superimposed by a powder pattern with gpar = 2.0018 and gperp = 2.0091. We attribute the powder pattern to Pb-like centers located mainly at the surface of the nanoparticles, since these defects can be passivated with H by HF etching while the broad resonance stays almost unaltered. The defect density of the as-grown particles of ?1018 cm-3 can be reduced by about one order of magnitude by HF etching. The alkyl-terminated nanoparticles show an intermediate defect density of 4?1017 cm-3. The stability of the surface modifications against oxidation is crucial for their applicability for device fabrication at ambient atmosphere. Successive FTIR and ESR measurements show that the H-termination of the silicon nanoparticles is stable in ambient atmosphere for several hours. Alkyl-termination improves the resistance against oxidation by about a factor of four.

### F10.17
**Preparation of the atomically straight step-edge Si (111) substrates as templates for nanostructure formation.**

Shunji Yoshida, Takeharu Sekiguchi and Kohei M. Itoh; Dept. of Applied Physics and CREST-JST, Keio university, Yokohama, Japan.

We report on the successful fabrication of the atomically straight step-edge structures on the surface of the Si (111) wafers with the intentional miscut of about 1 degree towards [-1-12] direction. High resolution STM shows clearly that a series of parallel single atomic step-edges with the average separation distance of 10nm are formed along [-1-12] direction. Each step edge is completely straight (without any atomic kinks) for about 10^4 Si atoms and has the identical atomic structures, in which this step edge structure is classified as U(2,0) [W.Shimada and H.Tochihara, Surf. Sci. 311, 107(1994) ]. The method to prepare such structures developed in this study is an extension of the one developed by the Himpsel's group [Lin et al., J. Appl. Phys. 84, 255 (1998) and J.Viernow et al, Appl. Phys. Lett. 72, 948(1998) ]. The differences are the cooling procedures and new discovery of the importance of the current direction during annealing. Even after a rapid quenching process from 1250°C to 830°C within 3 seconds as developed by the Himpsel's group, there exists a number of kinks along the [-1-12] step-edges due to a slight azimuthal misorientation of the slope direction from [-1-12]. In order to transport these kinks from the template area to the other, we perform annealing at 800°C for 10 hours with the current direction parallel to the step-edges. Here we find that the dc current direction climbing up the kinks straightens the step-edge more efficiently than the opposite going-down direction. With the climbing-up direction, the kinks are transported away and concentrate at a certain part of the sample. We propose a mechanism in current direction dependent re-distribution of kinks in analogy of step-bunching phenomena [K.Yagi et al., Surf. Sci. Rep. 43, 57(2001) ]. We also find that a long annealing duration of at least 10 hours is important to form step edges of a perfectly straight and unique atomic configuration even for samples with the azimuthal misorientation of 1 degree and less. At the conference, we present high-resolution STM images around the steps and discuss the their structures. The knowledge of these structures will provide ideas of how deposited atoms and/or molecules stick to the step-edges, when these straight edged Si steps are employed as templates for nanostructure formation.

### F10.18
**Surface Cusp Formation in Si Homoepitaxy.**
Jean-Marc Baribeau[1], Nelson L. Rowell[2], Xiaohua Wu[1], David J. Lockwood[1] and Michel Beaulieu[1]; [1]Institute for Microstructural Sciences, National Research Council Canada, Ottawa, Ontario, Canada; [2]Institute for National Measurements Standards, National Reasearch Council Canada, Ottawa, Ontario, Canada.

There is currently a broad interest in the development of deposition of group IV semiconductor nanostructures for selective growth of quantum dots and for surface functionalization. In silicon homoepitaxy, lowering the growth temperature results in breakdown of single crystal growth at a limiting thickness that decreases with decreasing temperature. The loss of crystallinity may initially involve point defect formation or surface roughening, followed by twinning, polycrystalline and finally amorphous growth. We have also observed that for relatively high growth temperatures (400-450 °C) the epitaxy breakdown can be very sluggish and proceed via columnar growth in which surface cusps are formed in the early stage of epitaxy breakdown. We have used atomic force microscopy to study the shape, size and distribution of those surface cusps. Surface cusps are generally of square shape with sides predominantly oriented along [110] directions and are typically 50 nm in size and at least 5 nm deep. The cusps can be very regular in size and their surface density is typically of the order of 10^10 cm^{-2}. The dimensions and distribution of the cusps is comparable to that of self-assembled Ge dots on Si and thus these features may be of interest for tailoring dot synthesis. We have observed that Ge self-assembled dots can be grown on cusped surfaces and that dot nucleation is enhanced in the vicinity of surface cusps. Large area AFM reveals that surface cusps are //decorated// by clusters of large dome-like Ge dots, while a lower density of smaller dome and pyramid shape islands is seen away from the dots. These results are suggestive of preferential nucleation and enhanced mass transport in the vicinity of cusps. The structural and optical properties of dots grown on flat and cusped surfaces will be compared.

### F10.19
**Synthesis of Microcrystalline Silicon Films by Low Energy Electron-Beam-Induced Deposition at Cryogenic Temperature.** Tetsuya Sato[1], Kiyokazu Nakagawa[2], Yutaka Aoki[3] and Shouji Sato[3]; [1]Clean Energy Research Center, University of Yamanashi, Kofu, Yamanashi, Japan; [2]Center for Crystal Science and Technology, University of Yamanashi, Kofu, Yamanashi, Japan; [3]Miyatsu Co.,LTD., Uenohara, Yamanashi, Japan.

[Introduction] We have proposed an advanced method for synthesis of semiconductor thin films at substrates temperatures lower than room temperature. This is based on the technique of the electron-beam-induced deposition (EBID) combined with vacuum

vapor deposition. Source gases and low-energy electrons generated by grow discharge of He gas were sprayed onto substrates (glass, organic films and Si wafer) at cryogenic temperature (6-200 K). We have successfully demonstrated that hydrogenated amorphous Si (a-Si:H) films and microcrystalline Si ($\mu$c-Si) films are synthesized at cryogenic temperature via non-thermal process. In this presentation, we focus on the characterization of morphology, the structure and chemical composition of a-Si:H and $\mu$c-Si films grown by EBID of monosilane and disilane. [Experimental] Monosilane (SiH$_4$ /He = 0.25) and disilane (Si$_2$H$_6$/ H$_2$ = 0.25) molecules were deposited on the quartz substrates (0.5 mm thickness, 4 inch) which were clamped to the cold head of the cryocooler. The thin films of these molecules were irradiated with low-energy electrons and metastable helium (He$^*$) which were produced by the DC glow discharge of He gas. The electron energy was distributed in the range of 0-200 eV (peak energy $\fallingdotseq$ 100eV) and current density was about 0.1 mA/cm$^2$. The substrate temperature during electron irradiation was changed in the ranges of 10-45 K in the case of SiH$_4$ and 10-95 K in the case of Si$_2$H$_6$. The real-time and in situ observation of the solid-phase reactions was made by the spectroscopic ellipsometory (SE) and Fourier transform-infrared (FT-IR) spectroscopy. [Results] We have studied the temperature dependence on the growth rate, hydrogen content (C$_H$), and morphology of silicon films. The values of C$_H$ and growth rate were decreased with increase of temperature (Table 1). On the other hand, the ratio [$\mu$c-Si/a-Si:H] increases with increase of temperature. The evolution of the crystalline phase with film growth was examined by SE. The crystallinity of these films was estimated by Raman scattering (peak of TO phonon mode : $\fallingdotseq$ 509 cm$^{-1}$, on Al substrate) and X-ray diffraction (XRD) measurements (peak: $2\theta$= 44.3$^\circ$). In this presentation, the mechanism of growth process of silicon thin films and nucleation of $\mu$c-Si by low energy EBID are discussed.

### F10.20
### Abstract Withdrawn

### F10.21
### Self-Limiting Photo-Assisted Synthesis of Silicon Nanocrystals.
C.Y. Chen[1,2], S. Kimura[1], S. Sen[1], Shinji Nozaki[1,2], H. Ono[1,2], K. Uchida[1] and H. Morisaki[1]; [1]Department of Electronics Engineering, University of Electro-communications, Tokyo 182-8585, Japan; [2]The 21st Century COE Program: Coherent Optical Science, University of Electro-communications, Tokyo 182-8585, Japan.

Anomalous growth of silicon nanocrystals was observed during the Raman scattering measurements of the nanosilica SiO$_x$ powder with an average diameter of 40 nm, which was fabricated using SiH$_4$ and O$_2$. Although there was no Raman peak to suggest presence of silicon nanocrystals initially in the nanosilica powder, the intensity of the peak around 500 cm$^{-1}$ increased with the laser-exposure time. For a laser power density of 1.5 W/cm$^2$, the nanocrystals started to be seen after 5 sec and their average size increased to 5 nm after 60 sec. The further increase of the laser-exposure time did not increase the size. This suggests the self-limiting growth of silicon nanocrystals, and the final size increased with increasing the laser power. The effect of the laser exposure on the nanosilica powder could be thermal. It has been reported that the thermal decomposition of the SiO$_x$ thin film into Si and SiO$_2$ results in formation of silicon nanocrystals. However, the lowest temperature required for the growth of silicon nanocrystals from the nanosilica powder was experimentally found to be 600 $^\circ$C, and it is unlikely for the temperature of the nanosilica powder to increase to such a high temperature by laser exposure. Furthermore, the size obtained by thermal annealing in nitrogen atmosphere at 600 $^\circ$C for 30 min was 3 nm, smaller than the final size obtained by the laser exposure for much shorter time. Therefore, the laser exposure seems to more effectively decompose SiO$_x$ into Si and SiO$_2$ and form silicon nanocrystals than the thermal annealing. In summary the photo-assisted synthesis is a new technique to form the nanocrystals with a narrow size distribution and possible controlled positioning at room temperature.

SESSION F11: Rare-Earth Doped Group V
Semiconductor Nanostructures
Chairs: Tom Gregorkiewicz and Paolo Pellegrino
Thursday Morning, December 2, 2004
Constitution B (Sheraton)

### 8:30 AM *F11.1
### Photoluminescence Properties of Er and/or Shallow Impurity Doped Silicon Nanocrystals.
Minoru Fujii, Department of Electrical & Electronics Engineering, Kobe University, Kobe, Japan.

The electronic states of Si nanocrystals are strongly modified from that of a bulk silicon crystal due to the confinement of electrons and holes in a space smaller than the exciton Bohr radius of bulk Si

crystals. One consequence of the quantum confinement effects is efficient visible photoluminescence (PL) at room temperature. The strong confinement also modifies the behavior of impurity atoms doped into (or on the surface of) Si nanocrystals, and provides nanocrystals with new functions. One example is that Er ions existing nearby Si nanocrystals can efficiently be excited by the energy transfer from nanocrystals and show temperature-independent PL at 1.54 micrometer. Similar below bulk-bandgap PL can be realized by controlling shallow impurities in Si nanocrystals without doping optically active materials. Simultaneous doping of n- and p-type impurities into Si nanocrystals results in the recombination of electrons and holes via impurity states; for relatively large Si nanocrystals, strong PL is observed at around 0.9 eV at room temperature. The simultaneous doping improves PL intensity of nc-Si due to the relaxation of momentum conservation rule during the optical transition and due to the smaller probability of the impurity-related Auger recombination compared to either n- or p-type impurity doped nc-Si.

### 9:00 AM F11.2
### Energy Transfer from Si Nanocrystals to Er Ions - Different Mechanisms Depending on Er Concentration.
Kenji Imakita, Yasuhiro Yamaguchi, Minoru Fujii and Shinji Hayashi; Kobe University, Kobe, Japan.

Silicon nanocrystals (nc-Si) act as an efficient photo-sensitizer for erbium ions (Er$^{3+}$). The presence of nc-Si in Er-doped SiO$_2$ enhances the effective absorption cross section of Er$^{3+}$ by more than four orders of magnitudes. This enhancement is due to the efficient energy transfer from nc-Si. Since the absorption band of nc-Si covers all the visible range, Er$^{3+}$ can be excited by white light. Furthermore, luminescence from Er$^{3+}$ in this system shows almost no temperature quenching. Due to these features, this system is considered to be a key component to realize planar waveguide type compact optical amplifier operating at 1.54$\mu$m. In our previous work on SiO$_2$ thin films containing nc-Si and Er$^{3+}$ (Er:nc-Si:SiO$_2$), we studied the mechanism of energy transfer from nc-Si to Er$^{3+}$ by analyzing the time transient of Er$^{3+}$ photoluminescence (PL) at 1.54$\mu$m just after pulsed excitation. The analysis revealed that there are two energy transfer processes occurring simultaneously, i.e., fast and slow processes, and that the ratio of the fast to slow processes increases with increasing the size of nc-Si. This suggests that the mechanism of the fast process is essentially the same as that in Er-doped bulk-Si; an excited electron is trapped to Er$^{3+}$ related center in the bandgap, and then the recombination energy of a bound exciton is transferred to Er$^{3+}$ by an Auger-like process. In this mechanism, Er$^{3+}$ should be located inside nc-Si or very close to the surface of nc-Si. On the other hands, the slow process is a characteristic process occurring only in Er:nc-Si:SiO$_2$. This is probably the Förster type Coulombic interaction between Er$^{3+}$ and free-excitons in nc-Si, and is considered to occur even if Er$^{3+}$ are located relatively far from nc-Si. In this work, the time transient of Er$^{3+}$ PL is studied as a function of Er concentration. It is shown that the ratio of the fast to slow process increases with increasing Er concentration. In order to analyze quantitatively the observed Er concentration dependence, we introduce a simple model in which Er$^{3+}$ is categorized into three groups depending on the location relative to nc-Si. We consider three spherical fields around a nanocrystal. Er$^{3+}$ located in the first field which is the closest to nc-Si is excited by the fast process, and that in the second field by the slow process. Er$^{3+}$ located outside the second field do not interact with nc-Si. Under the assumption that Er$^{3+}$ is uniformly distributed in a whole film, the observed Er concentration dependence is well fitted by the model. The fitting reveals that Er$^{3+}$ located within about 1nm from nc-Si surface is excited by the fast process and those located within about 2nm by slow process. Similar values are obtained by fitting the nc-Si size dependence of the ratio with the same model.

### 9:15 AM F11.3
### Pump-probe experiments on Er coupled Si-nanocrystals rib-loaded waveguides.
Nicola Daldosso[1], Daniel Navarro[1], Mirko Melchiorri[1], Lorenzo Pavesi[1], Fabrice Gourbilleau[2], Marzia Carrada[2], Richard Rizk[2], Cristina Garcia[3], Paolo Pellegrino[3], Blas Garrido[3] and Livio Cognolato[4]; [1]Physics, University of Trento, Povo (Trento), Italy; [2]LERMAT-ISMRA, Caen, France; [3]Electronica, Universitat de Barcelona, Barcelona, Spain; [4]Agilent Technologies, Torino, Italy.

Rib-loaded silica waveguides containing Er ions and Si nanoclusters were grown by reactive sputtering on a 10 $\mu$m-thick SiO$_2$ layer deposited on a Si wafer. The rib-loaded structure of the waveguides was fabricated by photolithographic and reactive ion etching processes, with patterned rib widths ranging from 1 to 8 $\mu$m. Time resolved experiments on the Er luminescence have allowed to measure an excitation cross section of Er through the Si nanocrystals of about 10$^{-16}$ cm$^2$ at low flux at 488 nm. A significant reduction down to 10$^{-18}$ cm$^2$ is observed for high pumping rates at 365 nm. Er luminescence lifetime of 3 ms was measured independent on the

pumping rates. Efficient light propagation was observed when end-fire coupling a probe signal in the rib waveguide both at 1310 nm and 1550 nm, with attenuation losses as low as 2 dB/cm at 1600 nm. Insertion losses measurement as a function of wavelength in the Er absorption region has permitted to estimate an Er absorption cross section at 1535 nm of $6x10^{-21}$ $cm^2$. Pump and probe experiments at 1310 nm show an increased absorption as the pump power is increased due to excited state absorption of the Si nanoclusters. Pump and probe experiments at 1535 nm show two regimes: at intermediate power the excited state absorption of the Si nanoclusters is observed that is overcome at high pumping rate by signal amplification, in fact an internal gain of 0.5 dB/cm was observed for a waveguide 1 cm long. A discussion of these results in terms of direct and indirect excitation of Er and a comparison with results reported in the literature will be presented at the conference. This work was supported by EC through the SINERGIA project.

### 9:30 AM *F11.4
### Location of Er Atoms with Respect to Si Nanoclusters in Luminescent Er and Si Co-implanted Silicates.

Paolo Pellegrino[1], Youcef Lebour[1], Cristina Garcia[1], Jordi Arbiol[1], Joan Ramon Morante[1], Blas Garrido[1] and Michel Prassas[2]; [1]Electronics, University of Barcelona, Barcelona, Spain; [2]Fontainebleau Research Centre, Corning S.A., Avon.

The formation of Er and Si clusters doped silica films has been shown as one of the most promising approaches for emission and optical amplification in the infrared. In this contribution we explore the structural properties of different silicate glasses co-implanted with silicon and Er ions to various doses, and see how they affect the emission properties around 1540 nm. We have used silica, soda-lime and aluminum silicates as substrates. A Si multi-implantation scheme has been adopted, in order to provide a uniform Si excess background to the subsequently implanted Er atoms. Si excess is ranging from 5 to 15 atomic percent while Er concentration has been varied between $2x10^{19}$ to $6x10^{20}$ $cm^{-3}$. By isochronal annealing experiments the best conditions have been investigated in order to precipitate the excess Si and activate the Er atoms. Different optimal annealing temperatures have been found in the range of 500-600 C depending on the particular composition of the original glass substrate. The structural analysis of the resulting structures have been performed by means of SIMS, XPS, Raman, FTIR and EFTEM and ensures that the best photoluminescence (PL) emission properties are the ones for which a phase separation between the implanted Si and the matrix occurs, even without the formation of nanocrystalline aggregates. A detailed structural study has been performed by using EFTEM coupled with PEELS and a Gatan image filter, which allows subnanometer resolution. For the best performing samples, HREM does not show any crystalline precipitates while EFTEM shows clearly the presence of Si amorphous nanoclusters in the samples. The average diameter of the nanocluster depends on the glass but always ranges between 3-6 nm. By analysing the images by HAADF in z-contrast we have been able to determine the location of Er atoms relative to the Si nanoclusters for the first time to our knowledge. The Er atoms are always located outside the Si nanoclusters and at the peak of the Er implantation a reduction in the density of Si nanoclusters is observed. This strongly suggests a modification of the Si coordination at high Er concentrations. Concurrently, and mainly in samples with Er concentration higher than $10^{20}$ $cm^{-3}$, the Er atoms are not randomly dispersed in the matrix, but somehow aggregated, forming small clusters. This correlates with the fact that concentration quenching of the Er PL starts to appear at concentrations around $2x10^{20}$ $cm^{-3}$. A detailed modelling of these effects and its implications will be presented and discussed.

### 10:15 AM *F11.5
### Self-Organized Formation of Erbium-Silicon-Oxide Superlattice.

Hideo Isshiki[1,2], Albert Polman[2] and Tadamasa Kimura[1]; [1]University of Electro-communications, Tokyo, Japan; [2]FOM Institute for Atomic and Molecular Physics, Amsterdam, Netherlands.

An entirely new method to fabricate optically active and electrically excitable erbium complexes on silicon is presented. The Er-Si-O compounds are formed by spin-coating a Si(100) substrate with an ErCl3 solution, followed by a rapid thermal oxidation and annealing sequence. This process leads to the formation of a self-organized Er-Si-O crystalline superlattice, epitaxially aligned with facets on the (100) surface. The superlattice period is 0.9 nm, as determined by high-resolution TEM imaging and diffraction, and the Er content is very high: 10-20 at. %. Intense room-temperature 1528 nm luminescence is observed from the Er-Si-O superlattice, with a line width as narrow as 4 meV at room temperature. From the Stark splitting, it is estimated that Er is encapsulated in six-fold-coordinated Er-O6 octahedra, with a size of 0.45 nm, corresponding to one half-period of the superlattice. The PL excitation spectrum has a cutoff at 1.22 eV, well above the bandgap

of bulk Si, suggesting that quantum confinement effects play a role in the excitation process. The results suggest that this new material is composed of a superlattice of alternating layers of Si and Er-doped octahedra. Strong coupling is then achieved between the extended electronic states in the superlattice and the Er intra-4f states.

### 10:45 AM *F11.6
### Si/Si:Er Multi-Nanolayers for Silicon Photonics.

N. Q. Vinh[1], M. A.J. Klik[1], B. A. Andreev[2] and Tom Gregorkiewicz[1]; [1]Van der Waals-Zeeman Institute, University of Amsterdam, Amsterdam, Netherlands; [2]Institute for Physics of Microstructures, Russian Academy of Sciences, Nizhny Novgorod, Russian Federation.

Si/Si:Er multi-nanolayer structures grown by sublimation MBE technique exhibit unusual optical properties which make them very interesting for photonic applications. In particular, our recent investigations have proven that a particular type of an Er-related optically active center is preferentially formed in this material. The microscopic structure of this center (labeled Er-1) is characterized by high symmetry type (orthorhombic) and comprises a single Er3+ ion most and multiple oxygen ligands, most likely in its direct surrounding. Consequently, emission from that center does not suffer from inhomogeneous broadening typical for Si:Er materials prepared by ion implantation, and exhibits an low temperature characterized an ultra-narrow linewidth of ?E ? 10 ?eV (at T = 4.2 K). This makes Si/Si:Er multi-nanolayers attractive for Si photonics. In the contribution, we will review properties of Er-related optical centers formed in the multi-nanolayer structures as revealed by high-resolution time-resolved photoluminescence, excitation and magneto-optical spectroscopies. In particular, the following issues will be addressed: - Details of microscopic structure of the Er-1 center - Excitation cross-section and its variation upon excitation wavelength (band-to-band vs. subbandgap pumping) and mode (cw vs. pulsed) - The percentage of optically active Er-related centers in comparison to the total concentration of Er atoms. - Fast components appearing in the decay kinetics at high pumping rate and Auger quenching Based on the experimental findings, potential of Si/Si:Er nanolayers for silicon photonics will be discussed. [1] N.Q. Vinh et al. Phys. Rev. Lett. 90, 066401 (2003). [2] M.A.J. Klik et al. submitted for publication

### 11:15 AM F11.7
### Three-dimensional Confocal Microscopy of Ultra-High Q Toroidal Microcavities on Silicon Doped with Er and Si Nanocrystals.

Anna Tchebotareva[1], Jeroen Kalkman[1], Tobias J. Kippenberg[2], Kerry J. Vahala[2] and Albert Polman[1]; [1]Optoelectronic Materials Group, FOM-Institute AMOLF, Amsterdam, Netherlands; [2]Department of Applied Physics, California Institute of Technology, Pasadena, California.

It has been recently demonstrated that $CO_2$ laser annealing enables the fabrication of ultra-high quality-factor silica-based toroidal microresonators on a Si chip [1]. Erbium ions inside such a microtoroid provide the gain medium to fabricate a microcavity-based laser emitting at 1.5 $\mu m$ [2]. In a similar way, Si nanocrystals embedded in ultra-high-Q microcavities could serve to test models of optical gain in Si nanocrystals in the visible or near-infrared. Alternatively, Si nanocrystals may serve as sensitizer for erbium. Here, we present the first results of direct imaging of photoluminescence of Er ions and Si nanocrystals inside a laser-annealed toroidal microcavity. Two- and three-dimensional images are obtained with a sub-micron resolution using confocal photoluminescence (PL) spectroscopy. We demonstrate that, after laser annealing, both Er and Si nanocrystals exhibit intense PL in the toroidal microcavities, and allow to determine the 3 dimensional spatial distribution of both Si nanocrystals and Er within the microcavity. $SiO_2$ films on Si were first doped with Er ions and/or Si nanocrystals by ion implantation. Toroidal microcavities were subsequently fabricated by a combination of photolithography and selective wet and dry etching followed by laser annealing for different times [1]. The quality factor of such microcavities was found to be of $10^7$. Laser anneal times above 3 s lead to the highest Er PL intensity, while for Si nanocrystal emission short anneal times (< 100 ms) are favorable. The laser annealing is observed to lead to a blue shift in the nanocrystal PL, suggesting melting and recrystallization kinetics that leads to a reduction in average nanocrystal size. In addition, experimental results will be presented on the study of energy transfer between Si nanocrystals and Er inside microcavities, as well as effects of the cavity modes on the Si quantum dot spontaneous emission spectrum. 1. D. Armani et al., Nature 421, 507 (2003) 2. A. Polman et al., Appl. Phys Lett. 84, 1037 (2004)

### 11:30 AM F11.8
### CMOS Compatible Erbium Coupled Si Nanocrystal Thin Films for Microphotonics.

Michael A. Stolfi[1], Luca Dal Negro[1], Jurgen Michel[1], Xiaoman Duan[1], John Le Blanc[2], John Haavisto[2] and Lionel C. Kimerling[1]; [1]Materials Science and Engineering, MIT, Cambridge, Massachusetts; [2]Charles Stark Draper Laboratory,

Cambridge, Massachusetts.

We have deposited Erbium (Er) doped Silicon-rich $SiO_2$ films where Er emission is activated at low temperatures enabling the fabrication of compact planar light sources and amplifiers with a low thermal budget for integration with standard Si CMOS processes. Silicon-rich $SiO_2$ films containing Er were deposited through reactive rf magnetron co-sputtering and subjected to a single annealing step to simultaneously form Silicon nanocrystals (Si-nc/s) and activate the Er emission. We studied, in detail, the fabrication parameters of Si content, annealing temperature and annealing time to investigate the role of Si-nc density, morphology and crystalline/amorphous quality on the Er energy transfer mechanism. For comparison, Si-nc/s were fabricated in $SiO_2$ through furnace annealing from Silicon-rich oxide films deposited through reactive rf magnetron sputtering. Near infrared emission from the Si-nc/s was optimized by controlling the Si content, annealing temperature and annealing time. By comparing Si-nc and Er coupled Si-nc samples, obtained in a wide range of fabrication parameters, we found that the Er emission enhancement due to the presence of the Si-nc/s increases for samples annealed at temperatures well below the annealing temperature that optimizes the Si-nc emission. In particular, maximum room temperature photoluminescence at 1535 nm has been measured for annealing temperatures between 600 °C and 800 °C and a factor of almost $10^3$ increase in the Er excitation cross section has been measured for samples containing Si-nc relative to the Er excitation cross section in $SiO_2$. In addition, preliminary Variable Stripe Length (VSL) gain measurements show the presence of optical gain in the films. The Er emission cross section derived from the gain measurements is comparable with the cross section of Er in $SiO_2$ and is not affected by the presence of the Si-nc/s.