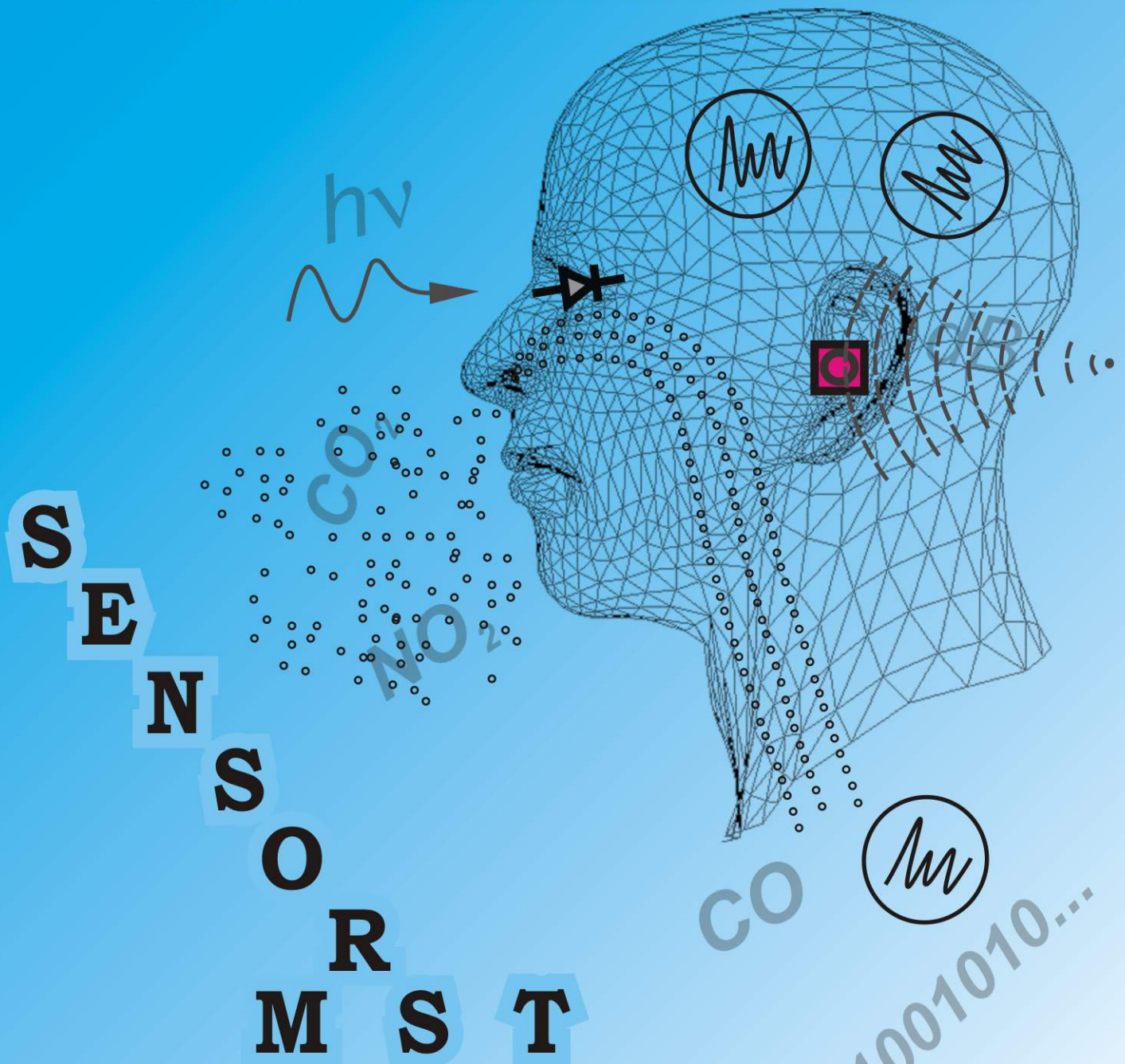


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БУТИ СТВОРЕНІ СЕНСОРИ

PHYSICAL, CHEMICAL AND OTHER PHENOMENA,  
AS THE BASES OF SENSORS

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ПОЛЯРИЗАЦИОННЫЕ ЯВЛЕНИЯ В АЦЕНТРИЧНЫХ КРИСТАЛЛАХ  
В УСЛОВИЯХ НЕОДНОРОДНОГО ТЕМПЕРАТУРНОГО ГРАДИЕНТА

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ПОЛЯРИЗАЦИОННЫЕ ЯВЛЕНИЯ В АЦЕНТРИЧНЫХ КРИСТАЛЛАХ В УСЛОВИЯХ  
НЕОДНОРОДНОГО ТЕМПЕРАТУРНОГО ГРАДИЕНТА

*В. Ф. Косоротов, Л. В. Щедрина*

**Аннотация.** Рассматриваются поляризационные явления в ацентричных кристаллах в условиях пространственно неоднородного температурного градиента. Проведен теоретический анализ различных вкладов в пирозлектрический эффект в термодинамически неравновесных кристаллах. Описано размежевание вторичного и третичного пирозлектрических эффектов в пьезоэлектрических средах при учете различных особенностей проявления неравновесного процесса в кристалле, а также проанализирована роль ложных вкладов в пироотклик в этих условиях, что необходимо на стадии разработки и проектирования принципов построения сенсорных устройств.

**Ключевые слова:** пространственно неоднородный температурный градиент, индуцированная пироактивность, вторичный и третичный пирозлектрический эффекты

ПОЛЯРИЗАЦІЙНІ ЯВИЩА В АЦЕНТРИЧНИХ КРИСТАЛАХ В УМОВАХ НЕОДНОРІДНОГО  
ТЕМПЕРАТУРНОГО ГРАДІЄНТА

*В. П. Косоротов, Л. В. Щедрина*

**Анотація.** Розглядаються поляризаційні явища в ацентричних кристалах в умовах просторово неоднорідного температурного градієнта. Проведено теоретичний аналіз різних внесків в піроелектричний ефект у термодинамічно нерівноважних кристалах. Описано розмежування вторинного й третинного піроелектричних ефектів у п'єзоелектричних середовищах при урахуванні різних особливостей прояву нерівноважного процесу в кристалі, а також проаналізована роль хибних внесків у півовідгук за цих умов, що необхідно на стадії розробки й проектування принципів побудови сенсорних пристроїв.

**Ключові слова:** просторово неоднорідний температурний градієнт, індукована піроактивність, вторинний і третинний піроелектричний ефекти

**POLARIZATION PHENOMENA IN ACENTRIC CRYSTALS UNDER INHOMOGENEOUS  
TEMPERATURE GRADIENT CONDITIONS**

*V. F. Kosorotov, L. V. Shchedrina*

**Abstract.** Polarization phenomena in acentric crystals under the spatially inhomogeneous temperature gradient conditions are investigated. Theoretical analysis of the different contributions to pyroelectric effect in the thermodynamically nonequilibrium crystals is presented. A separation of the secondary and tertiary pyroelectric effects in piezoelectric media taking into account the distinctive features of nonequilibrium process manifestation in a crystal is described. A role of the false contributions to the pyroelectric response under examined conditions is analysed, that is necessary for a design and developing the construction principles of a new class of infrared sensors on the basis of the polarization phenomena under investigation.

**Keywords:** spatially inhomogeneous temperature gradient, induced pyroactivity, secondary and tertiary pyroelectric effects

# ПРОЕКТУВАННЯ І МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ СЕНСОРІВ

## SENSORS DESIGN AND MATHEMATICAL MODELING

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УДК 621.382, PACS 85.45.-W

### ЕЛЕКТРОННО-ОПТИЧНЕ МОДЕЛЮВАННЯ АВТОЕМІСІЙНИХ МІКРОКАТОДІВ

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### ЕЛЕКТРОННО-ОПТИЧНЕ МОДЕЛЮВАННЯ АВТОЕМІСІЙНИХ МІКРОКАТОДІВ

*А. О. Дружинін, В. І. Голота, І. Т. Когут, Ю. М. Ховерко*

**Анотація.** Застосовано комплексний підхід до електронно-оптичного моделювання кремнієвих автоемісійних мікрокатодів. В рівнянні Фаулера-Нордгейма враховано форму потенціального бар'єру для зони провідності і валентної зони. Отримано апроксимацію рівняння Лапласа для розрахунку потенціалів методом скінчених різниць. Показано результат розрахунку потенціалу і електричного поля мікрокатода. Встановлено вплив просторового заряду на рух електронів і показано їх траєкторії. Отримано оцінку чутливості фоторезисту для цифрової літографії

**Ключові слова:** автоемісія, кремнієвий мікрокатод, електронна оптика, траєкторія електронів

### ELECTRON-OPTICAL MODELLING OF FIELD EMISSION MICROCATODES

*A. A. Druzhinin, V. I. Holota, I. T. Kogut, Yu. M. Khoverko*

**Abstract.** The complex approach to electron-optical simulation of silicon field emission microcathodes is applied. In Fowler-Nordheim equation the shape of potential barrier for conductance band and valence band is considered. It is received approximation of Laplace equation for potentials calculation by finite-difference method. The result of calculation of potential and an electric field of the microcathode is shown. Influence of space charge on electron motion is established and their trajectories are shown. It is received an estimation of sensitivity of photoresist for digital lithography.

**Keywords:** field emission, the silicon microcathode, an electron optics, electron trajectory



**ЭЛЕКТРОННО-ОПТИЧЕСКОЕ МОДЕЛИРОВАНИЕ  
АВТОЭМИССИОННЫХ МИКРОКАТОДОВ**

*А. А. Дружинин, В. И. Голота, И. Т. Когут, Ю. М. Ховерко*

**Аннотация.** Применен комплексный подход к электронно-оптическому моделированию кремниевых автоэмиссионных микрокатодов. В уравнении Фаулера-Нордгейма учтена форма потенциального барьера для зоны проводимости и валентной зоны. Получено аппроксимацию уравнения Лапласа для расчета потенциалов методом конечных разностей. Показан результат расчета потенциала и электрического поля микрокатада. Установлено влияние пространственного заряда на движение электронов и показаны их траектории. Получено оценку чувствительности фоторезиста для цифровой литографии.

**Ключевые слова:** автоэмиссия, кремниевый микрокатод, электронная оптика, траектория электронов

## СЕНСОРИ ФІЗИЧНИХ ВЕЛИЧИН

## PHYSICAL SENSORS

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УДК 621.382.28

### ДАТЧИК ТЕМПЕРАТУРЫ НА ОСНОВЕ ОДНОПЕРЕХОДНОГО И ПОЛЕВОГО ТРАНЗИСТОРОВ ПРИ РАДИАЦИОННОМ ВОЗДЕЙСТВИИ

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### ДАТЧИК ТЕМПЕРАТУРЫ НА ОСНОВЕ ОДНОПЕРЕХОДНОГО И ПОЛЕВОГО ТРАНЗИСТОРОВ ПРИ РАДИАЦИОННОМ ВОЗДЕЙСТВИИ

*И. М. Викулин, Ш. Д. Курмашев, И. Е. Майстренко, П. Ю. Марколенко*

**Аннотация.** Разработана схема датчика температуры на основе генератора на однопереходном транзисторе с двумя токозадающими полевыми транзисторами, частота генерации которого линейно растет с увеличением температуры. Экспериментально исследовано воздействие радиации на его работоспособность.

**Ключевые слова:** датчик, однопереходный транзистор, генератор

### ДАТЧИК ТЕМПЕРАТУРИ НА ОСНОВІ ОДНОПЕРЕХІДНОГО І ПОЛЬОВОГО ТРАНЗИСТОРІВ ПРИ ДІЇ РАДІАЦІЇ

*І. М. Вікулін, Ш. Д. Курмашев, І. Е. Майстренко, П. Ю. Марколенко*

**Анотація.** Розроблена схема датчика температури на основі генератора на одноперехідному транзисторі з двома струмозадаючими польовими транзисторами, частота генерації якого лінійно зростає із збільшенням температури. Експериментально досліджена дія радіації на його працездатність.

**Ключові слова:** датчик, одноперехідний транзистор, генератор

### SENSOR OF TEMPERATURE ON THE BASIS OF UNIJUNCTION AND FIELD TRANSISTORS AT THE RADIATION-DAMAGE

*I. V. Vikulin, Sh. D. Kurmashev, A. E. Maistrenko, P. Yu. Markolenko*

**Abstract.** The chart of sensor of temperature is developed on the basis of generator on an unijunction transistor with two current-lead fields transistors, frequency of generation of which linear grows with the increase of temperature. Influence of radiation is experimentally investigational on his capacity.

**Keywords:** sensor, unijunction transistor, generator

ОПТИЧНІ, ОПТОЕЛЕКТРОННІ І РАДІАЦІЙНІ СЕНСОРИ  
OPTICAL, OPTOELECTRONIC AND RADIATION SENSORS

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PACS 61.43.FS, 78.30.LY, 78.90.+T  
УДК 539.216.2

IR OPTICAL PROPERTIES OF  $As_{32}Sb_8S_{60}$  CHALCOGENIDE GLASS  
AND EFFECT OF  $\gamma$ -IRRADIATION

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IR OPTICAL PROPERTIES OF  $As_{32}Sb_8S_{60}$  CHALCOGENIDE GLASS AND EFFECT  
OF  $\gamma$ -IRRADIATION

*T. S. Kavetsky, O. I. Shpotyuk, G. I. Dovbeshko, I. V. Blonsky, V. M. Tsmots*

**Abstract.** In this paper, impact of  $\gamma$ -irradiation on the transmittance of  $As_{32}Sb_8S_{60}$  chalcogenide glass in the near and mid IR spectral range is investigated. The radiation-induced changes in the main IR impurity absorption bands are discussed to be taken into account in IR optical devices based on the glass composition studied to work in the conditions of high energy radiation fields.

**Keywords:** chalcogenide glasses, impurity absorption, radiation modification, IR optics

ВПЛИВ  $\gamma$ -ОПРОМІНЕННЯ НА ІЧ ОПТИЧНІ ВЛАСТИВОСТІ  
ХАЛЬКОГЕНІДНОГО СКЛА  $As_{32}Sb_8S_{60}$

*T. S. Кавецький, О. Й. Шпотюк, Г. І. Довбешко, І. В. Блонський, В. М. Цмоць*

**Анотація.** В статті представлено результати вивчення впливу  $\gamma$ -опромінення на прозорість халькогенідного скла  $As_{32}Sb_8S_{60}$  в ближньому та середньому ІЧ діапазоні спектру. Обговорюються радіаційно-індуковані зміни основних смуг ІЧ домішкового поглинання, які слід врахувати при використанні скла даного хімічного складу в ІЧ оптичному приладобудуванні для роботи в умовах високоенергетичних радіаційних полів.

**Ключові слова:** халькогенідні стекла, домішкове поглинання, радіаційна модифікація, ІЧ оптика

**ВЛИЯНИЕ  $\gamma$ -ОБЛУЧЕНИЯ НА ИК ОПТИЧЕСКИЕ СВОЙСТВА  
ХАЛЬКОГЕНИДНОГО СТЕКЛА  $As_{32}Sb_8S_{60}$**

*Т. С. Кавецкий, О. И. Шпотюк, Г. И. Довбешко, И. В. Блонский, В. М. Цмоць*

**Аннотация.** В статье представлены результаты по изучению влияния  $\gamma$ -облучения на прозрачность халькогенидного стекла  $As_{32}Sb_8S_{60}$  в ближнем и среднем ИК диапазоне спектра. Обсуждаются радиационно-индуцированные изменения основных полос ИК примесного поглощения, которые следует учитывать при использовании стекла данного химического состава в ИК оптическом приборостроении для работы в условиях высокоэнергетических радиационных полей.

**Ключевые слова:** халькогенидные стекла, примесное поглощение, радиационная модификация, ИК оптика

PACS 32.15RM;  
УДК 539.184

## ON SENSING NUCLEI OF THE $^{207}\text{Bi}$ AND $^{207}\text{Pb}$ ISOTOPES BY MEANS OF LASER SPECTROSCOPY OF HYPERFINE STRUCTURE

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### ON SENSING NUCLEI OF THE $^{207}\text{Bi}$ AND $^{207}\text{Pb}$ ISOTOPES BY MEANS OF LASER SPECTROSCOPY OF HYPERFINE STRUCTURE

*O. Yu. Khetselius*

**Abstract.** It is presented the new theoretical scheme for sensing different parameters of nuclei of the Bi, Pb isotopes on the basis of hyperfine structure spectroscopy of the corresponding atoms.

**Keywords:** sensing, laser technology, hyperfine structure, isotopes of Bi, Pb

### О ДЕТЕКТРОВАНИИ ЯДЕР ИЗОТОПОВ $^{207}\text{Bi}$ И $^{207}\text{Pb}$ МЕТОДАМИ ЛАЗЕРНОЙ СПЕКТРОСКОПИИ СВЕРХТОНКОЙ СТРУКТУРЫ

*О. Ю. Хецелиус*

**Аннотация.** Рассмотрена новая теоретическая схема детектирования параметров ядер изотопов Bi, Pb на основе спектроскопии сверхтонкой структуры соответствующих атомов

**Ключевые слова:** детектирование, лазерная технология, теория сверхтонкой структуры, изотопы Bi, Pb

### ПРО ДЕТЕКТУВАННЯ ЯДЕР ІЗОТОПІВ $^{207}\text{Bi}$ ТА $^{207}\text{Pb}$ МЕТОДАМИ ЛАЗЕРНОЇ СПЕКТРОСКОПІЇ НАДТОНКОЇ СТРУКТУРИ

*О. Ю. Хецелиус*

**Анотація.** Розглянута нова теоретична схема детектування параметрів ядер ізотопів Bi, Pb на основі спектроскопії надтонкої структури відповідних атомів.

**Ключові слова:** детектування, лазерна технологія, теорія надтонкої структури, ізотопи Bi, Pb

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UDK 539.184

## ENERGY APPROACH TO ELECTRON CAPTURE AND IONIZATION PROCESSES IN ION-ATOMIC COLLISION SYSTEM

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### ENERGY APPROACH TO ELECTRON CAPTURE AND IONIZATION PROCESSES IN ION-ATOMIC COLLISION SYSTEM

*A. V. Loboda*

**Abstract.** Energy approach is generalized to calculate the electron capture cross sections in the  $H^+ + H(1s)$  collision system. The numerical results are presented for collision energies 10 and 100 keV

**Keywords:** ion-atomic collision system, energy approach

### ЭНЕРГЕТИЧЕСКИЙ ПОДХОД К ИЗУЧЕНИЮ ПРОЦЕССОВ ЗАХВАТА ЭЛЕКТРОНА И ИОНИЗАЦИИ В ИОН-АТОМНОЙ СТОЛКНОВИТЕЛЬНОЙ СИСТЕМЕ

*A. V. Loboda*

**Аннотация.** Энергетический подход обобщен с целью расчета сечения захвата электрона в ион-атомной столкновительной системе  $H^+ + H(1s)$ . Численные оценки получены для энергий столкновения 10 и 100 кэВ.

**Ключевые слова:** ион-атомная столкновительная система, энергетический подход

### ЕНЕРГЕТИЧНИЙ ПІДХІД ДО ВИВЧЕННЯ ПРОЦЕСІВ ЗАХОПЛЕННЯ ЕЛЕКТРОНУ ТА ІОНІЗАЦІЇ В ІОН-АТОМНІЙ СИСТЕМІ ІЗ ЗІТКНЕННЯМ

*A. V. Loboda*

**Анотація.** Енергетичний підхід узагальнено з метою розрахунку перерізу захоплення електрону в іон-атомній системі у стані зіткнення  $H^+ + H(1s)$ . Чисельні оцінки отримані для енергій зіткнення 10 і 100 кеВ.

**Ключові слова:** іон-атомна система із зіткненням, енергетичний підхід

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## АКУСТОЕЛЕКТРОННІ СЕНСОРИ

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## ACOUSTOELECTRONIC SENSORS

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УДК 539.2:539.4

PACS 43.40.LE, 85.30.-Z, 73.40.VZ

### ДИНАМІКА АКУСТИЧНОЇ ЕМІСІЇ У ЛОКАЛЬНО-НЕОДНОРІДНО ТЕРМОНАПРУЖЕНИХ ГЕТЕРОСТРУКТУРАХ

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### ДИНАМІКА АКУСТИЧНОЇ ЕМІСІЇ У ЛОКАЛЬНО-НЕОДНОРІДНО ТЕРМОНАПРУЖЕНИХ ГЕТЕРОСТРУКТУРАХ

*О. В. Ляшенко*

**Анотація.** В роботі проведено аналіз динаміки акустичної емісії, що супроводжує деградацію і локальні процеси релаксації та дефектоутворення в локально-неоднорідно термонапружених гетероструктурах *InGaN/GaN* та *GaAsP/GaP* при покроковому збільшенні прямого постійного струму. Показано, що динаміка АЕ добре узгоджується з основними висловленими припущеннями — АЕ є детермінованим в часі хаотичним релаксаційним процесом, параметри АЕ залежать від величини зміни та швидкості зміни рівня зовнішнього фіксованого навантаження, кількості однотипних джерел АЕ, активованих цим впливом на протязі часу його дії, а також дисперсією деяких параметрів цих джерел АЕ.

**Ключові слова:** динаміка акустичної емісії, гетероструктура, дефект

### THE DYNAMICS OF ACOUSTIC EMISSION IN LOCALLY-IS NON-UNIFORMLY THERMO STRAINED HETEROSTRUCTURES

*O. V. Lyashenko*

**Abstract.** In operation the analysis of dynamics of an acoustic emission that accompanies with degradation and local processes of a relaxation and a defect formation in locally-is non-uniformly thermostained heterostructures *InGaN/GaN* and *GaAsP/GaP* at step-by-step magnification of a direct current is lead. It is shown, that dynamics AE is well coordinated with the basic guesses — AE is the chaotic relaxation process determined in time, parameters AE depend on quantity of change and velocity of change of a level of the exterior fixed loading, quantity of the same sources AE activated by this influence during time of its activity, and also a variance of some parameters of these sources AE

**Keywords:** The dynamics of acoustic emission, heterostructure, defect

**ДИНАМИКА АКУСТИЧЕСКОЙ ЭМИССИИ В ЛОКАЛЬНО-НЕОДНОРОДНО  
ТЕРМОНАПРЯЖЕННЫХ ГЕТЕРОСТРУКТУРАХ**

*О. В. Ляшенко*

**Аннотация.** В работе проведен анализ динамики акустической эмиссии, что сопровождается деградацией и локальные процессы релаксации и дефектообразования в локально-неоднородно термонапряженных гетероструктурах *InGaN/GaN* и *GaAsP/GaP* при пошаговом увеличении прямого постоянного тока. Показано, что динамика АЕ хорошо согласовывается с основными предположениями — АЕ является детерминированным во времени хаотическим релаксационным процессом, параметры АЕ зависят от величины изменения и скорости изменения уровня внешней фиксированной нагрузки, количества однотипных источников АЕ, активированных этим влиянием в течение времени его действия, а также дисперсией некоторых параметров этих источников АЕ

**Ключевые слова:** динамика акустической эмиссии, гетероструктура, дефект



## БІОСЕНСОРИ

## BIOSENSORS

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УДК 616-008.9-073

### ВИКОРИСТАННЯ НАПІВМАГНІТНИХ НАПІВПРОВІДНИКОВИХ НАНОЧАСТИНОК ДЛЯ ВІЗУАЛІЗАЦІЇ СТРУКТУР БІОЛОГІЧНИХ ТКАНИН

*В. І. Федів<sup>1</sup>, І. С. Давиденко<sup>1</sup>, А. Й. Савчук<sup>2</sup>, М. М. Марченко<sup>2</sup>, Т. А. Савчук<sup>2</sup>*

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### ВИКОРИСТАННЯ НАПІВМАГНІТНИХ НАПІВПРОВІДНИКОВИХ НАНОЧАСТИНОК ДЛЯ ВІЗУАЛІЗАЦІЇ СТРУКТУР БІОЛОГІЧНИХ ТКАНИН

*В. І. Федів, І. С. Давиденко, А. Й. Савчук, М. М. Марченко, Т. А. Савчук*

**Анотація.** При оптимальних умовах синтезу отримано комплекс наночастинка напівмагнітного напівпровідника CdMnS — меркаптоетанол. Утворення наночастинок проконтрольовано оптичними методами. Виявлено незалежність розмірів наночастинок від концентрації вихідних компонент у діапазоні  $5 \cdot 10^{-4}$  —  $5 \cdot 10^{-2}$  моль/л. Деякі структури біологічних тканин виявлені селективною люмінесцентною візуалізацією з використанням наночастинок на прикладі досліджень гістологічних зрізів плацентарної тканини.

**Ключові слова:** наночастинка, напівмагнітний напівпровідник, люмінесценція, біологічна тканина, біосенсор

### APPLICATION OF SEMIMAGNETIC SEMICONDUCTOR NANOPARTICLES FOR VISUALISATION OF BIOLOGICAL TISSUE STRUCTURES

*V. I. Fediv, I. S. Davydenko, A. I. Savchuk, M. M. Marchenko, T. A. Savchuk*

**Abstract.** Complex type of semimagnetic semiconductor nanoparticle CdMnS — mercaptoethanol has been obtained at optimum synthesis conditions. Formation of nanoparticles was monitored by optical methods. It is shown independence of the size nanoparticles from concentration initial a component in a range of  $5 \cdot 10^{-4}$  —  $5 \cdot 10^{-2}$  mol/L. Some structures of biological tissue were revealed on selective luminescent visualisation of the synthesized nanoparticles by applying to study of histological section of a placental tissue.

**Keywords:** nanoparticle, semimagnetic semiconductor, luminescence, biological tissue, biosensor

**ИСПОЛЬЗОВАНИЕ ПОЛУМАГНИТНЫХ ПОЛУПРОВОДНИКОВЫХ НАНОЧАСТИЦ  
ДЛЯ ВИЗУАЛИЗАЦИИ СТРУКТУР БИОЛОГИЧЕСКИХ ТКАНЕЙ**

*В. И. Федив, И. С. Давыденко, А. Й. Савчук, М. М. Марченко, Т. А. Савчук*

**Аннотация.** При оптимальных условиях синтеза получено комплекс наночастица полу-магнитного полупроводника CdMnS — меркаптоэтанол. Оптическими методами проконтролировано формирование наночастиц. Показано независимость размеров наночастиц от концентрации исходных компонент в диапазоне  $5 \cdot 10^{-4}$  —  $5 \cdot 10^{-2}$  моль/л. Некоторые структуры биологических тканей выявлены селективной люминесцентной визуализацией с помощью наночастиц, на примере исследований гистологических срезов плацентарной ткани.

**Ключевые слова:** наночастица, полумагнитный полупроводник, люминесценция, биологическая ткань, биосенсор

## МАТЕРІАЛИ ДЛЯ СЕНСОРІВ

## SENSOR MATERIALS

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### КРИСТАЛІЧНА СТРУКТУРА ТА МАГНІТНІ ВЛАСТИВОСТІ СПЛАВІВ ТВЕРДИХ РОЗЧИНІВ У СИСТЕМІ Tm-Ge-Si

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### КРИСТАЛІЧНА СТРУКТУРА ТА МАГНІТНІ ВЛАСТИВОСТІ СПЛАВІВ ТВЕРДИХ РОЗЧИНІВ У СИСТЕМІ Tm-Ge-Si

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**Анотація.** Сплави твердих розчинів у системі Tm-Ge-Si досліджено методами рентгенівської дифракції і магнітної сприйнятливості (МС). Встановлено, що кристалічна структура даних сплавів належить до гексагонального структурного типу  $AlB_2$ , у якій для атомів малого розміру (Si, Ge) характерна тригонально-призматична координація. Результати вимірювань МС в залежності від температури (80-800 К) та напруженості магнітного поля (0,5-4,0 кЕ) свідчать про наявність парамагнітної складової, яка добре описується законом Кюрі-Вейсса і не залежить від напруженості магнітного поля. Також визначені магнітні характеристики досліджуваних матеріалів (параметр Вейсса, ефективний магнітний момент на формульну одиницю і константа Кюрі).

**Ключові слова:** кристалічна структура, твердий розчин, магнітна сприйнятливість, парамагнетизм

### CRYSTAL STRUCTURE AND MAGNETIC PROPERTIES OF SOLID SOLUTIONS IN THE Tm-Ge-Si SYSTEM

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**Abstract.** Solid solutions in the Tm-Ge-Si system have been studied by X-ray diffraction data and magnetic susceptibility (MS) techniques. It was found that the crystal structure of the alloys corre-

sponds to the hexagonal type  $AlB_2$ , in which tri-capped trigonal prism coordination is observed for the small atoms (Si, Ge). The results of MS measurements as a function of temperature (80-800 K) and magnetic field (0.5-4.0 kOe) show the existence of a field-independent paramagnetic component well described by the Curie-Weiss law. The magnetic characteristics of the materials (Weiss parameter, effective magnetic moment per formula unit and Curie constant) were also determined.

**Keywords:** crystal structure, solid solution, magnetic susceptibility, paramagnetism

#### КРИСТАЛЛИЧЕСКАЯ СТРУКТУРА И МАГНИТНЫЕ СВОЙСТВА СПЛАВОВ ТВЕРДЫХ РАСТВОРОВ В СИСТЕМЕ Tm-Ge-Si

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**Аннотация.** Сплавы твердых растворов в системе Tm-Ge-Si исследованы методами рентгеновской дифракции и магнитной восприимчивости (МВ). Обнаружено, что кристаллическая структура данных сплавов принадлежит к гексагональному типу  $AlB_2$ , в которой для атомов малых размеров (Si, Ge) характерна тригонально-призматическая координация. Результаты измерений МВ в зависимости от температуры (80-800 К) и напряженности магнитного поля (0,5-4,0 кЭ) свидетельствуют о наличии парамагнитной составляющей, которая хорошо описывается законом Кюри-Вейсса и не зависит от напряженности магнитного поля. Также определены магнитные характеристики исследованных материалов (параметр Вейсса, эффективный магнитный момент на формульную единицу и константа Кюри).

**Ключевые слова:** кристаллическая структура, твердый раствор, магнитная восприимчивость, парамагнетизм

УДК 537.226.4

## ДОСЛІДЖЕННЯ ТЕМПЕРАТУРНИХ ЗАЛЕЖНОСТЕЙ ЕЛЕКТРИЧНОГО ОПОРУ НАПІВПРОВІДНИКОВИХ СЕГНЕТОЕЛЕКТРИЧНИХ КРИСТАЛІВ $\text{Sn}_2\text{P}_2\text{S}_6$

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### ДОСЛІДЖЕННЯ ТЕМПЕРАТУРНИХ ЗАЛЕЖНОСТЕЙ ЕЛЕКТРИЧНОГО ОПОРУ НАПІВПРОВІДНИКОВИХ СЕГНЕТОЕЛЕКТРИЧНИХ КРИСТАЛІВ $\text{Sn}_2\text{P}_2\text{S}_6$

*Ю. І. Тягур*

**Анотація.** Досліджені залежності електричного опору ( $R$ ), відносного температурного коефіцієнту електричного опору ( $\alpha$ ) від температури для кристалів  $\text{Sn}_2\text{P}_2\text{S}_6$ . Встановлено, що при зростанні температури залежність  $R(T)$  експоненціально зменшується з різними термічними константами ( $B$ ). Визначені константи ( $B$ ) та енергія залягання домішкових рівнів в сегнетоелектричній та параелектричній фазах. Встановлено, що коефіцієнт ( $\alpha$ ) має великі значення в сегнетоелектричній і параелектричній фазах, а також проявляє аномалію в околі точки фазового переходу. Обчислено енергію домішкових рівнів, яка в сегнетофазі є рівною  $E_{1,fe} = 0.12\text{eV}$ ,  $E_{2,fe} = 1.17\text{eV}$ , а в парафазі —  $E_{3,pa} = 0.87\text{eV}$ .

**Ключові слова:** сегнетоелектричні кристали, електричний опір, температура, енергія

### INVESTIGATIONS OF TEMPERATURE DEPENDENCES OF ELECTRICAL RESISTANCE OF $\text{Sn}_2\text{P}_2\text{S}_6$ FERROELECTRIC SEMICONDUCTOR CRYSTALS

*Yu. Tyagur*

**Abstract.** Dependences of electrical resistance ( $R$ ) and relative temperature coefficient of electrical resistance ( $\alpha$ ) versus temperature are investigated for  $\text{Sn}_2\text{P}_2\text{S}_6$  crystals. It is established that with increasing temperature, dependence  $R(T)$  exponentially decreases with different thermal coefficients ( $B$ ). In this work coefficients ( $B$ ) and energy of the doped levels are obtained for ferroelectric and paraelectric phases. It is established, that coefficient ( $\alpha$ ) has high values in both phases and also in the vicinity of the phase transition point the anomaly occurs. The energy of the doped levels is calculated: in ferroelectric phase  $E_{1,fe} = 0.12\text{eV}$ ,  $E_{2,fe} = 1.17\text{eV}$ , and paraelectric phase —  $E_{3,pa} = 0.87\text{eV}$ .

**Keywords:** ferroelectric crystals, electrical resistance, temperature, energy

### ИССЛЕДОВАНИЯ ТЕМПЕРАТУРНЫХ ЗАВИСИМОСТЕЙ ЭЛЕКТРИЧЕСКОГО СОПРОТИВЛЕНИЯ СЕГНЕТОЭЛЕКТРИЧЕСКИХ — ПОЛУПРОВОДНИКОВЫХ КРИСТАЛЛОВ $\text{Sn}_2\text{P}_2\text{S}_6$

*Ю. И. Тягур*

**Аннотация.** Исследованы зависимости электрического сопротивления ( $R$ ), относительного температурного коэффициента электрического сопротивления ( $\alpha$ ) от температуры для кристаллов  $\text{Sn}_2\text{P}_2\text{S}_6$ . Установлено, что при увеличении температуры зависимость  $R(T)$  экспоненциально уменьшается с различными по значению термическими константами

( $B$ ). Определены константы ( $B$ ) и энергия примесных уровней в сегнетоэлектрической и параэлектрической фазах. Установлено, что коэффициент ( $\alpha$ ) имеет большие значения в сегнетоэлектрической и параэлектрической фазах, а также проявляет аномалию в окрестности точки фазового перехода. Рассчитано значение энергии примесных уровней, которая в сегнетофазе равна —  $E_{1,fe} = 0.12эВ$ ,  $E_{2,fe} = 1.17эВ$ , а в парафазе —  $E_{3,pa} = 0.87эВ$ .

**Ключевые слова:** сегнетоэлектрические кристаллы, электрическое сопротивление, температура, энергия

## ТЕХНОЛОГІЯ ВИРОБНИЦТВА СЕНСОРІВ

## SENSORS PRODUCTION TECHNOLOGIES

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УДК 621.315.592

### СТВОРЕННЯ І ВЛАСТИВОСТІ ЕЛЕКТРИЧНИХ КОНТАКТІВ Al I Au НА ТОНКОПЛІВКОВОМУ $Zn_{1-x}Mn_xO$

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### СТВОРЕННЯ І ВЛАСТИВОСТІ ЕЛЕКТРИЧНИХ КОНТАКТІВ Al I Au НА ТОНКОПЛІВКОВОМУ $Zn_{1-x}Mn_xO$

*В. В. Хомяк*

**Анотація.** Досліджено електричні характеристики контактів металів Au і Al нанесених на вирощені ВЧ-магнетронним розпилюванням тонкі плівки  $Zn_{1-x}Mn_xO$ . Встановлено, що хімічна обробка поверхні перед металізацією приводить до зменшення питомого контактного опору за рахунок утворення тонкого приповерхневого збагаченого електронами  $n^+$ -шару, а також за рахунок створення на поверхні більшої густини вакансій кисню.

**Ключові слова:** оксид цинку, тонкі плівки  $Zn_{1-x}Mn_xO$ , електричний контактний опір

### CREATING AND PROPERTIES OF ELECTRICAL CONTACTS OF Al AND Au ON THE $Zn_{1-x}Mn_xO$ THIN FILMS

*V. V. Khomyak*

**Abstract.** Electrical characteristics of Au and Al metal contacts on the  $Zn_{1-x}Mn_xO$  thin films, grown by high-frequency magnetron sputtering have been investigated. It has been established that chemical treatment before metallization leads to the decrease of specific contact resistance because of the creation of thin near-surface  $n^+$ -layer, enriched by electrons as well as because of larger density of oxygen vacancies on the surface.

**Keywords:** zinc oxide,  $Zn_{1-x}Mn_xO$  thin films, electrical contact resistance

СОЗДАНИЕ И СВОЙСТВА ЭЛЕКТРИЧЕСКИХ КОНТАКТОВ Al И Au  
НА ТОНКОПЛЁНОЧНОМ  $Zn_{1-x}Mn_xO$

*В. В. Хомяк*

**Аннотация.** Исследовано электрические характеристики контактов металлов Au и Al нанесенных на выращенные ВЧ-магнетронным распылением тонкие пленки  $Zn_{1-x}Mn_xO$ . Установлено, что химическая обработка поверхности перед металлизацией приводит к уменьшению удельного контактного сопротивления за счет образования тонкого приповерхностного обогащенного электронами  $n^+$ -слоя, а также за счет образования на поверхности большей плотности вакансий кислорода.

**Ключевые слова:** оксид цинка, тонкие пленки  $Zn_{1-x}Mn_xO$ , электрическое контактное сопротивление



УДК 621.383:537.221

## РАЗРАБОТКА ПЛЕНОЧНЫХ СЛОЕВ СУЛЬФИДА КАДМИЯ ДЛЯ ЭКОНОМИЧНЫХ СОЛНЕЧНЫХ ЭЛЕМЕНТОВ

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## РАЗРАБОТКА ПЛЕНОЧНЫХ СЛОЕВ СУЛЬФИДА КАДМИЯ ДЛЯ ЭКОНОМИЧНЫХ СОЛНЕЧНЫХ ЭЛЕМЕНТОВ

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**Аннотация.** Исследованы структурные и оптические свойства пленок сульфида кадмия, полученных методом химического осаждения из раствора. Структурные параметры определены рентгенодифрактометрическим методом, в котором области когерентного рассеивания (о.к.р.) и микродеформации определялись путем аналитической обработки отдельных рентгенодифрактограмм. Проведена математическая обработка спектров пропускания слоев сульфида кадмия. Кристаллическая структура и оптические свойства исследованных пленок CdS определяются толщиной и технологией осаждения слоев CdS.

**Ключевые слова:** химическое осаждение, рентгенодифрактометрический метод, область когерентного рассеивания, микро деформации

## РОЗРОБКА ПЛІВКОВИХ ШАРІВ СУЛЬФІДУ КАДМІЮ ДЛЯ ЕКОНОМІЧНИХ СОНЯЧНИХ ЕЛЕМЕНТІВ

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**Анотація.** Досліджено структурні і оптичні властивості плівок сульфід кадмію, отриманих методом хімічного осадження з розчину. Структурні параметри визначені рентгенодифрактометричним методом, в якому області когерентного розсіяння (о.к.р.) та мікродеформації визначались шляхом аналітичної обробки окремих рентгенодифрактограм. Проведена математична обробка спектрів пропускання шарів сульфід кадмію. Кристалічна структура та оптичні властивості досліджених плівок CdS визначаються товщиною та технологією осадження шарів CdS.

**Ключові слова:** хімічне осадження, рентгенодифрактометричний метод, область когерентного розсіяння, мікродеформації

**FILM LAYER SULFIDE CADMIUM DEVELOPMENT FOR ECONOMIC SOLAR CELLS**

*D. A. Kudiy, N. P. Klochko, G. S. Khrypunov, N. A. Kovtun, K. Y. Krikun, E. K. Belonogov*

**Abstract.** The structural and optical properties CdS films, which received by the chemical deposition from solution, are investigated. The structural parameters are determined by the X-Ray diffractogram method, which the definition of dispersion cogent areas and microdeformations were defined by analytical processing X-Ray diffractogram. The mathematical processing of CdS layers transmission specters are carried out. The crystal structure and optical properties investigated CdS films are defined by the thickness and deposition technology CdS layer.

**Keywords:** Chemical deposition, X-Ray diffractogram method, dispersion cogent area, microdeformations

## ОГЛЯД ПУБЛІКАЦІЙ ЖУРНАЛУ IEEE SENSORS JOURNAL

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### **Electrically Active Magnetic Nanoparticles for Concentrating and Detecting *Bacillus anthracis* Spores in a Direct-Charge Transfer Biosensor**

Pal, S. Settingington, E.B. Alocilja, E.C.

On page(s): 647-654

#### **Abstract**

*Bacillus anthracis*, the causative agent of anthrax, is considered as one of the most important pathogens in the list of bioterrorism threats. This paper describes the synthesis of electrically active magnetic (EAM) nanoparticles and their application in a direct-charge transfer biosensor for detecting *B. anthracis* Sterne endospores. These EAM nanoparticles were synthesized from aniline monomer made electrically active by acid doping and gamma iron (III) oxide nanoparticles resulting in nanomaterials with diameters ranging from 50 to 200 nm. Room temperature hysteresis measurements of the synthesized nanomaterials using a quantum design MPMS SQUID magnetometer showed that their saturation magnetization values were between 61.1 and 33.5 emu/gm. The structural morphology of the nanomaterial was studied using transmission electron microscopy and the electronic diffraction patterns were observed to determine their crystalline nature. The EAM nanoparticles were coated with antibodies specific to *B. anthracis* Sterne endospores and used to capture the target antigen from varying spore concentrations ( to ) by applying a magnetic field. The immunomagnetically captured spores were then applied to a direct-charge transfer biosensor having a dimension of 5 mm × 60 mm. The detection of the spores was based on the capillary flow of the captured spores aided by a direct-charge transfer of the EAM nanoparticle. The electric signal generated was recorded for 6 min in a reagentless process. The biosensor was able to detect the presence of *B. anthracis* spores at a concentration of  $4.2 \times 10^2$  spores/ml. Specificity studies were also carried out to determine the biosensor responses in the presence of nontarget antigens. This study shows the novel application of EAM nanoparticles both as an immunomagnetic concentrator and a transducer in a portable, easy to use, biosensor that has the potential to be used as a rapid detection device for defense and biosecurity.

### **A Versatile Biomolecular Charge-Based Sensor Using Oxide-Gated Carbon Nanotube Transistor Arrays**

Pandana, H. Aschenbach, K.H. Lenski, D.R. Fuhrer, M.S. Khan, J. Gomez, R.D.

On page(s): 655-660

#### **Abstract**

Label-free deoxyribonucleic acid (DNA) hybridization detection using carbon nanotube transistor (CNT) arrays is demonstrated. The present scheme is distinguished from other CNT sensing methods as it uses a gate oxide overlayer on top of the carbon nanotubes, which function solely as charge sensors but are not participants in the chemical binding process. Because it involves DNA probe attachment on the gate oxide rather than on the CNT, this approach allows the use of conventional DNA functionalization and bioassay protocols, and is less prone to false positives. The signal sought is a few tens of millivolts in threshold voltage shift due to the increase of surface charges after target hybridization. The hybridization detection is shown to be highly specific and sensitive to a minimum concentration of about 30 nM of 61-mer DNA. Despite differences in the transistor properties due to the spread in the CNT parameters during fabrication, the yields are very high and the sensing characteristics are uniformly consistent in nearly all transistors.

### **Systematic Aptamer-Gold Nanoparticle Colorimetry for Protein Detection: Thrombin**

Pandana, H. Aschenbach, K.H. Gomez, R.D.

On page(s): 661-666

#### **Abstract**

Gold nanoparticle colorimetry assay using aptamers is a low cost and a highly effective means for detecting a wide range of biomolecular targets. In this work, this technique is used to detect the protein thrombin as a model system for understanding the relationship between the aptamer-target binding properties and the optical colorimetric response, as well as to gain insight on the secondary structures of the aptamers. The two known aptamers for thrombin, the 15-mer Bock and the 29-mer Tasset aptamer were conjugated to gold nanoparticles to form complexes that bind to thrombin upon contact. The Bock aptamer causes the aggregation of the nanoparticles and the concomitant reduction of the plasmon resonance peak, whereas the 29-mer Tasset aptamer, despite higher affinity, does not cause a spectral change. The data is understood on the basis of the difference in the number

of binding sites available on thrombin for the respective aptamers. Additional results on single base substitutions suggest that the G-quadruplex secondary structure in the Bock aptamer is intermolecular and comprises of at least two interacting aptamer molecules. An estimate of the dissociation constant, derived from thrombin titration, is comparable to values reported in the literature.

### **The Effect of Frequency Sweeping and Fluid Flow on Particle Trajectories in Ultrasonic Standing Waves**

Lipkens, B. Costolo, M. Rietman, E.

On page(s): 667-677

#### **Abstract**

Particle concentration and separation in ultrasonic standing waves through the action of the acoustic radiation force on suspended particles are discussed. The acoustic radiation force is a function of the density and compressibility of the fluid and the suspended particles. A two-dimensional theoretical model is developed for particle trajectory calculations. An electroacoustic model is used to predict the acoustic field in a resonator, driven by a piezoelectric transducer. Second, the results of the linear acoustic model are used to calculate the acoustic radiation force acting on a particle suspended in the resonator. Third, a particle trajectory model is developed that integrates the equation of motion of a particle subjected to a buoyancy force, a fluid drag force, and the acoustic radiation force. Computational fluid dynamics calculations are performed to calculate the velocity field that is subsequently used to calculate fluid drag. For a fixed frequency excitation, the particles are concentrated along the stable node locations of the acoustic radiation force. Through a periodic sweeping of the excitation frequency particle translation is achieved. Two types of frequency sweeps are considered, a ramp approach and a step-change method. Numerical results of particle trajectory calculations are presented for two configurations of flow-through resonators and for two types of frequency sweeping. It is shown that most effective particle separation occurs when the fluid drag force is orthogonal to the acoustic radiation force.

### **Hybrid Micropower Source for Wireless Sensor Network**

Yanqiu Li Hongyun Yu Bo Su Yonghong Shang

On page(s): 678-681

#### **Abstract**

Wireless sensor networks have become a very significant enabling technology in many applications and the use of environmental energy is a feasible source for low-power wireless sensor networks. The challenges of developing a power supply including generation or conversion, storage, and power management are manifold to extend

the lifetime of a wireless sensor network. The objective of this research is to develop an intelligent hybrid power system to realize a self-sustaining wireless sensor node. The photovoltaic and thermoelectric generators are adopted as energy converters. The lithium ion battery and ultracapacitor are used as reservoirs. An intelligent power management system has been developed to control the power distribution. The design data and experimental results show that the hybrid micropower source can extend the lifetime of a sensor network.

### **Sensor Support Systems for Asymmetric Threat Countermeasures**

Chung-Ching Shen Kupershtok, R. Adl, S. Bhattacharyya, S.S. Goldsman, N. Peckerar, M.

On page(s): 682-692

#### **Abstract**

In the past, primary focus has been given to novel sensor elements for deployment against urban terrorists and in limited force engagements. The issue explored in this paper is the adequacy of electronic system support for these new sensing elements. For example, ad hoc distributed networks must lie dormant for long periods of time and "come alive" when threats are nearby. This presents a unique challenge in the storage, generation, and management of power. In this paper, we demonstrate designs of processor algorithms and telecommunication protocols that alleviate current power-system shortcomings for these stationary networks. These advances include: 1) low-power protocols for data fusion and fault tolerance and 2) system-level energy modeling and analysis. As a concrete example, we define a distributed sensor support system for line crossing recognition. We demonstrate that threat detection is a system-level problem. Single elements of the system chain individually have small impact on overall performance. Through the development of a preamplifier/amplifier chain for optimum signal-to-noise (S/N) ratio, we show the degree to which system-level architecture can improve reliable detection. Specifically, the use of sensor redundancy to improve performance is analyzed from a statistical basis.

### **Electrospun Conducting Polymer-Based Sensors for Advanced Pathogen Detection**

Haynes, A.S. Gouma, P.I.

On page(s): 701-705

#### **Abstract**

This paper focuses on the development of conducting polymer hybrid sensors for pathogen detection for advanced medical diagnostics. Using the electrospinning technique, polyaniline hybrids were developed for the detection of gas and for pH monitoring to determine

the suitability of these sensors for exhaled human breath analyses. Results show that electrospun hybrids based on leucoemeraldine based polyaniline exhibit sensitivity to down to 1 ppm and for the first time, using emeraldine salt polyaniline, demonstrate a conductimetric response to changes in the headspace of aqueous solutions of varying pH. This manuscript discusses the response of these hybrid systems to varying concentrations of pH and NO<sub>2</sub>.

#### **Advanced Agent Identification With Fluctuation-Enhanced Sensing**

Kwan, C. Schmera, G. Smulko, J.M. Kish, L.B. Heszler, P. Granqvist, C.-G.

On page(s): 706-713

##### **Abstract**

Conventional agent sensing methods normally use the steady state sensor values for agent classification. Many sensing elements (Hines, 1999; Ryan, 2004; Young, 2003; Qian, 2004; Qian, 2006; Carmel, 2003) are needed in order to correctly classify multiple agents in mixtures. Fluctuation-enhanced sensing (FES) looks beyond the steady-state values and extracts agent information from spectra and bispectra. As a result, it is possible to use a single sensor to perform multiple agent classification. This paper summarizes the application of some advanced algorithms that can classify and estimate concentrations of different chemical agents. Our tool involves two steps. First, spectral and bispectral features will be extracted from the sensor signals. The features contain unique agent characteristics. Second, the features are fed into a hyperspectral signal processing algorithm for agent classification and concentration estimation. The basic idea here is to use the spectral/bispectral shape information to perform agent classification. Extensive simulations have been performed by using simulated nanosensor data, as well as actual experimental data using commercial sensor (Taguchi). It was observed that our algorithms are able to accurately classify different agents, and also can estimate the concentration of the agents. Bispectra contain more information than spectra at the expense of high-computational costs. Specific nanostructured sensor model data yielded excellent performance because the agent responses are additive with this type of sensor. Moreover, for measured conventional sensor outputs, our algorithms also showed reasonable performance in terms of agent classification.

#### **Fluctuation-Enhanced Sensing: Status and Perspectives**

Schmera, G. Chiman Kwan Ajayan, P. Vajtai, R. Kish, L.B.

On page(s): 714-719

##### **Abstract**

Both selectivity and sensitivity of chemical sensors can be considerably improved by exploiting the information contained in microfluctuations present in the sensor system. We call our collection of methods and algorithms to extract information from these microfluctuations, fluctuation enhanced sensing. In this paper, we present a short survey of results with Taguchi sensors, surface acoustic wave devices, MOSFET-based sensors, and nanosensors.

#### **Nanomonitors: Protein Biosensors for Rapid Analyte Analysis**

Reddy, R.K. Bothara, M.G. Barrett, T.W. Carruthers, J. Prasad, S.

On page(s): 720-723

##### **Abstract**

A technology for electrical detection of proteins has been developed using electrical conductance measurements. It is based on developing high density, low-volume multiwell plate devices. The scientific core of this technology lies in integrating nanoporous membranes with microfabricated chip platforms. This results in the conversion of individual pores into wells of picoliter volume. Specific antibodies are localized and isolated into individual wells. The formation of the antibody-antigen binding complex occurs in individual wells. The membrane allows for robust separation among individual wells. This technology has the capability to achieve near real-time detection with improved sensitivity and selectivity.

#### **III-Nitride Heterostructure Layered Tunnel Barriers For a Tunable Hyperspectral Detector**

Bell, L.D. Tripathi, N. Grandusky, J.R. Jindal, V. Shahedipour-Sandvik, F.S.

On page(s): 724-729

##### **Abstract**

We report on the fabrication and characterization of III-nitride layered tunnel barriers with applications for a new type of tunable hyperspectral imaging detector with intrinsically hyperspectral pixels. This would enable each pixel to be individually tunable in real-time through a range of wavelengths, with the number and width of spectral channels being dynamically adjustable. Shape-engineered electron barriers fabricated from III-nitride heterostructures allow barrier height to be varied by application of a voltage. A spectroscopy of photon

wavelength is enabled via the collection of photoexcited electrons across this barrier. The device is envisioned for tunable detection of ultraviolet through infrared wavelengths.

#### **Synthesis of Ru-Ni Core-Shell Nanoparticles for Potential Sensor Applications**

Shuguang Deng Pingali, K.C. Rockstraw, D.A.

On page(s): 730-734

##### **Abstract**

Nanoparticles of Ru-Ni with a core-and-shell structure were synthesized as potential sensors in a single-step spray-pyrolysis process at 700-1000. The majority of the core consists of ruthenium, while the shell is predominantly composed of nickel. An aqueous precursor containing ruthenium chloride and nickel chloride was nebulized by an ultrasonic atomizer to generate an aerosol. The aerosol droplets were subsequently decomposed to form uniformly distributed Ru-Ni bimetallic nanoparticles. Atomic fractions of precursors, solvent type and process temperature play crucial roles in the formation of core-and-shell structures.

#### **Metal Oxide Nanowire and Thin-Film-Based Gas Sensors for Chemical Warfare Simulants Detection**

Ponzoni, A. Baratto, C. Bianchi, S. Comini, E. Ferroni, M. Pardo, M. Vezzoli, M. Vomiero, A. Faglia, G. Sberveglieri, G.

On page(s): 735-742

##### **Abstract**

This work concerns with metal oxide (MOX) gas sensors based on nanowires and thin films. We focus on chemical warfare agents (CWAs) detection to compare these materials from the functional point-of-view. We work with different chemicals including simulants for Sarin nerve agents, vesicant gases, cyanide agents, and analytes such as ethanol, acetone, ammonia, and carbon monoxide that can be produced by everyday activities causing false alarms. Explorative data analysis has been used to demonstrate the different sensing performances of nanowires and thin films. Within the chosen application, our analysis reveal that the introduction of nanowires inside the array composed by thin films can improve its sensing capability. Cyanide simulants have been detected at concentrations close to 1 ppm, lower than the Immediately Dangerous for Life and Health (IDLH) value of the respective warfare agent. Higher sensitivity has been obtained to simulants for Sarin and vesicant gases, which have been detected at concentrations close or even lower than 100 ppb. Results demonstrate the suitability of the proposed array to selectively detect CWA simulants with respect to some compounds produced by everyday activities.

#### **Optoelectronic Signatures of Biomolecules Including Hybrid Nanostructure-DNA Ensembles**

Vasudev, M. Yamanaka, T. Jianyong Yang Ramadurai, D. Stroschio, M.A. Globus, T. Khromova, T. Dutta, M.

On page(s): 743-749

##### **Abstract**

Biological macromolecules such as DNA, proteins, and polysaccharides often display unique absorptive signatures in the THz region, useful in their identification and imaging through Raman and Fourier transform transmission spectroscopy. The optoelectronic properties of nanostructure-DNA complexes immobilized on transparent, semi-rigid substrates such as polymethyl methacrylate (PMMA) have been studied. By chemically modifying the PMMA substrates with amine terminal groups and using suitable linking agents, amine terminated DNA can be localized on these substrates. THz Fourier transform transmission spectroscopy was used to detect low-frequency vibrational modes ( $10\text{-}25\text{ cm}^{-1}$ ) within single- and double-stranded DNA molecules immobilized on PMMA attached to  $\text{TiO}_2$  nanoparticles. Additionally, DNA strands end terminated with  $\text{TiO}_2$  nanoparticles are used in this study to cleave the DNA at guanine (G) rich sites due to trapping of photo-induced charge carriers from the  $\text{TiO}_2$  at these sites. Theoretical modeling of charge transport through DNA via polaron transport is discussed in detail. By examining the vibrational modes of DNA, as well as the transport of charge in DNA this study underlies potential applications involving DNA micro-arrays, DNA-based sensors, and DNA-based THz devices.

#### **High- $T_c$ Josephson Square-Law Detectors and Hilbert Spectroscopy for Security Applications**

Divin, Y. Poppe, U. Gubankov, V.N. Urban, K.

On page(s): 750-757

##### **Abstract**

Among various discussed ways of explosive detection, the techniques using electromagnetic radiation are considered as having great potential and research activities are recommended in this field. To identify new threats, like liquid explosives, with low rate of false alarms, fast spectral measurements are required in a broad frequency range from microwave to terahertz. We attract attention to a great potential of high- $T_c$  Josephson technology in security applications and present our results in developing high- $T_c$  Josephson junctions for Hilbert spectroscopy and detector arrays.

**Organizational Structure and Electronic Decoupling of Surface Bound Chiral Domains and Biomolecules**

Santagata, N.M. Pengshun Luo Lakhani, A.M. DeWitt, D.J. Day, B.S. Norton, M.L. Pearl, T.P.

On page(s): 758-766

**Abstract**

For the development of reagentless biological and chemical species detection at the single molecule level using external fields, including terahertz radiation, it is paramount to study model systems that uncover how intermolecular and molecule-surface interactions dictate monolayer ordering and electronic properties. This paper addresses two types of molecule-surface interactions and two distinct molecular systems, both of which impact our fundamental understanding of confined molecular domains and single molecule detection. We will first discuss the ordering and electronic characteristics of a chiral molecule, tartaric acid, weakly bound to an achiral metal surface, Ag(111), as studied with low temperature scanning tunneling microscopy (STM). This particular molecule-surface system contains many key elements, including hydrogen bonding interactions and stereochemical features, that would be common to other functional detection schemes. This paper will also treat the characterization of isolated, thiolated DNA molecules chemically bound to Au(111) terraces. Ambient STM and atomic force microscopy (AFM) measurements of both short and long DNA structures in both single and double strand configurations will be discussed with particular attention paid to imaging mechanisms involved. These results are particularly relevant to systems involving biomolecules anchored to inert metal surfaces, such as those used in external field-based assays.

**Diffusive Transport in Graphene**

Liu, S.Y. Lei, X.L. Horing, N.J.M.

On page(s): 767-770

**Abstract**

Recently, a single-layer of carbon atoms, termed graphene, has attracted a great deal of interest due to its great potential for application in electronics. In experiments involving graphene, a finite residual conductivity was found at zero gate voltage in the density dependence of conductivity. However, the theoretical explanation of this observation has been confused, with derivations predicting differing values of residual conductivity. In this paper, considering electron-impurity scattering, we present a kinetic equation approach to investigate transport in graphene. The effect of interband polarization on conductivity is taken into account. We find that, in the density dependence of conductivity, there is a minimum (rather than residual) conductivity sensitively dependent on the carrier-impurity scattering potential. For higher

electron density, the conductivity varies almost linearly with the electron density.

**Radiative Plasmonic-Polariton Dispersion Relation for a Thin Metallic Foil With Interband Damping Transitions**

Horing, N.J.M.

On page(s): 771-774

**Abstract**

Plasmons in a thin metallic foil are of two types: (Ritchie, 1957; Ando, 1982; Stratton, 1941) 1) a two-dimensional plasmon (Ritchie, 1957) whose electrostatic dispersion relation has its frequency proportional to the square root of wave number, which propagates along the surface of the foil and 2) a plasmon constituted of collective electron density oscillations across the foil in the nature of capacitor-like discharges perpendicular to the surfaces of the foil (Ando, 1982). The latter (type 2) occur at the bulk plasma frequency and it has long been known that they produce electromagnetic (EM) radiation (Ferrell, 1958) (whereas type 1 plasmons do not radiate). The object of this research is to carefully examine the coupling of both these plasmon modes to the EM field in producing radiative polaritons. We carry this out using a complex dielectric function approach embodying both types of plasmons in the context of an exact analytic solution for the dyadic EM field Green's function describing radiative plasmonic-polariton propagation for a thin metallic foil (Horing, et al.), including the role of interband damping transitions. In particular, we will formulate and examine the dispersion relation for such polaritons, which is significantly modified from Stern's result (Stern, 1967) by the radiative type 2 plasmon described above and interband damping. The complex dielectric function embodying both type 1 and type 2 plasmons and interband damping involves a frequency dependent imaginary part and is expected to exhibit interesting radiative plasmonic-polariton phenomenology. This expectation is based on a recent calculation we have carried out (Horing) using a generic dielectric function of the Lorentzian type, which produced inhomogeneous (Jackson, 1975) plane wave radiation from excitation of the foil modes. Such inhomogeneous plane waves, which grow locally as a function of distance away from the foil (without violating the causality principle), have been known to occur previously and are discussed in the literature (Stratton, 1941). This local growth of the EM field may contribute to enhanced focusing properties of an array of nanoholes in the foil.

**Characterization of Nanoporous Silicon-Based DNA Biosensor for the Detection of Salmonella Enteritidis**

Deng Zhang Alocilja, E.C.

On page(s): 775-780

**Abstract**

A biosensor for the detection of food-borne pathogens (*Salmonella Enteritidis*) was fabricated based on nanoporous silicon (NPS). P-type silicon wafers (100, 0.01  $\mu\text{m}$ ) were anodized electrochemically in an electrochemical Teflon cell, containing ethanoic hydrofluoric acid solution to produce the porous layer on the silicon surface. The porous silicon surface was functionalized with DNA probes specific to the insertion element (Iel) gene of *Salmonella Enteritidis*. A biotin-streptavidin system was utilized to characterize the availability of the nanopores and the specificity of the DNA probe. Based on the electrical property of DNA, redox indicators and cyclic voltammetry were used for the characterization of the biosensor. Results showed that the DNA probe was specific to the target DNA, and the porous silicon-based biosensor had more active surface area and higher sensitivity (1 ng/mL) than the planar silicon-based biosensor. This simple, label-free porous silicon-based biosensor has potential applications in high-throughput detection of pathogens.

**THz Characterization of All-Trans and 9-cis Retinal, Experiment, and Modeling**

Wright, T.J. Ying Luo Globus, T. Gelmont, B. Khromova, T. Swami, N. Isin, A.

On page(s): 781-785

**Abstract**

Two conformations of the retinal molecule have been studied in order to characterize the molecule's THz transmission spectra in both the ground and metastable states. When subjected to an adequate external excitation the retinal molecule can experience a change in conformation and associated THz transmission spectra. In an attempt to accomplish this characterization, the FTIR system was modified to include a simple off axis excitation source inside of the systems sample chamber. Measurements were made of the retinal molecule's THz spectra both with and without external excitation of the molecule. The results gathered were then compared with the results obtained from simulation. Data obtained from two retinal isomers reveal more spectral features at frequencies  $\sim 11 - 15 \text{ cm}^{-1}$  than were predicted for these conformations. The most likely explanation for this is that the material is actually a mixture of several metastable conformations. There is correlation between simulated and measured THz spectra in the ground state at a frequency of  $14 \text{ cm}^{-1}$  for all-trans retinal. The strongest vibrational mode frequency predicted for the 9-cis conformation through modeling was  $22 \text{ cm}^{-1}$ , which corre-

lates quite well with the experimental line at  $21.3 \text{ cm}^{-1}$  in the ground state. When the 9-cis samples were exposed to UV illumination there was a noticeable change in the absorption spectra and this line at  $21.3 \text{ cm}^{-1}$  almost disappeared which can be related to the transformation of a 9-cis into a more stable all-trans retinal. The absorption spectra of all-trans retinal that is the most stable conformation showed very weak features in experimental spectra, with some of them changing under illumination.

**Noise Spectroscopy of Gas Sensors**

Aroutiounian, V.M. Mkhitarian, Z.H. Shatveryan, A.A. Gasparyan, F.V. Ghulinyan, M.Zh. Pavesi, L. Kish, L.B. Granqvist, C.-G.

On page(s): 786-790

**Abstract**

We study current-voltages and low-frequency noise characteristics of the metal-porous silicon-silicon single crystal-metal structure with 50% and 73% porosity of porous silicon. The study is performed in dry air and in a mix of dry air with carbon monoxide of different concentrations. The Hooge noise parameter and the parameter in the frequency dependence of the noise voltage spectral density were determined from experimental data. High sensitivity of spectral dependence of noise to gas concentration allows offering powerful method for determination of gas concentration in the air or environment.

**Terahertz (THz) Electromagnetic Field Enhancement in Periodic Subwavelength Structures**

Gelmont, B. Parthasarathy, R. Globus, T. Bykhovski, A. Swami, N.

On page(s): 791-796

**Abstract**

In this paper, we show that periodic arrays of rectangular slots with subwavelength width provide for local electromagnetic field enhancements due to edge effects in low-frequency range,  $10-25 \text{ cm}^{-1}$ . Periodic structures of Au, doped Si, and InSb with subwavelength thickness were studied. The half power enhancement width is  $\sim 500 \text{ nm}$  and less around the slot edges in all cases, thereby possibly bringing terahertz (THz) sensing to the nanoscale. InSb is confirmed to offer the best results with the local power enhancements on the order of 1100 at frequency  $14 \text{ cm}^{-1}$ . InSb and Si have large skin depths in the frequency range of interest and so the analysis of their structures was done through the Fourier expansion method of field diffracted from gratings. Au, however, has small skin depths at these frequencies compared with the thickness. Surface impedance boundary conditions were employed to model the Au structure, for which the Fourier expansion method was unsuitable owing to the huge magnitude



of Au permittivity at these frequencies. The applications possibly include development of novel biosensors, with the strongly enhanced local electromagnetic fields leading to increased detection sensitivity, and monitoring biophysical processes such as DNA denaturation.

#### **Single Electron Transistor-Based Gas Sensing With Tungsten Nanoparticles at Room Temperature**

Karre, P.S.K. Acharya, M. Knudsen, W.R. Bergstrom, P.L.

On page(s): 797-802

##### **Abstract**

Single electron transistor (SET)-based gas sensors utilizing tungsten nanoparticles as conducting islands and operating at room temperature have been fabricated. Electrical characterization showed a strong correlation between the drain current of the SET device and the concentration of gas. The reversible exposure to gas resulted in reduction of both the Coulomb blockade voltage and the drain current. The reduction in the drain current shows an oscillatory behavior, with the variation on the gate bias. The sensitivity of the gas sensor can be tuned by controlling the charge on the gate electrode. Relaxation times of 400 ms for a concentration of 36% of gas in were achieved. Although the SET sensor has not been demonstrated with sensitivities in the few tens of ppm compared with existing technologies, the response is very fast and the sensitivity can be tuned by modulating the gate bias. The sensor demonstrates the possibility of gas sensing using SET devices as sensitive electrometers. The sensitivity of the SET gas sensor is higher at lower concentrations.

#### **A DNA Sensor for Sequencing and Mismatches Based on Electron Transport Through Watson-Crick and Non-Watson-Crick Base Pairs**

Jauregui, L.A. Seminario, J.M.

On page(s): 803-814

##### **Abstract**

A combined density functional theory and Green's function procedure is used to calculate the electrical characteristics of Watson-Crick and non-Watson-Crick base pairs; calculations are performed to determine: the molecular orbitals that participate in the electron-transfer process, junction current-voltage characteristics, density of states, transmission function, and molecular electrostatic potentials. The distinct current-voltage features of base pairs can be used for detecting and sequencing DNA, as well as for detecting DNA base-pair mismatches by passing the double strand through two perpendicular metallic electrodes to the DNA, or by scanning the double strand with conducting probes. We find in the range

from 1 to 1 V for the Watson-Crick pairs that the CG is a better electron conductor than the AT and, on the other hand, the best and worst conductors are the non-Watson-Crick mismatches CT and AA, respectively.

#### **Selective Chemical Sensing Using Structurally Colored Core-Shell Colloidal Crystal Films**

Potyrailo, R.A. Zhebo Ding Butts, M.D. Genovese, S.E. Tao Deng

On page(s): 815-822

##### **Abstract**

We demonstrate for the first time selective sensing of multiple vapors at low concentrations based on the structurally colored colloidal crystal film formed from composite core/shell nanospheres. Since color changes of sensing colloidal crystal films are negligible at relatively low vapor partial pressures ( $P/P_0 < 0.1$ ), a straightforward detection of color changes cannot be applied. To overcome this limitation, we apply a differential spectroscopy measurement approach coupled with the multivariate analysis of differential reflectance spectra. The vapor-sensing selectivity is provided by the combination of the composite nature of the colloidal nanospheres in the film with the multivariate analysis of the spectral changes of the film reflectivity upon exposure to different vapors. The multianalyte sensing was demonstrated using a colloidal crystal film comprised of 326-nm diameter core polystyrene nanospheres coated with a 20-nm thick sol-gel shell. Discrimination of water, acetonitrile, toluene, and dichloromethane vapors using a single sensing colloidal crystal film was evaluated applying principal components analysis (PCA) of the reflectivity spectra. The polar and nonpolar vapors at different relative vapor partial pressures were well separated in PCA space. The best selectivity was obtained between toluene and dichloromethane vapors, while water and acetonitrile vapors were almost unresolved. Achieved detection limits were within the range of interest or better than those needed for determinations of these vapors for industrial applications.

#### **Defect-Tolerant CMOL Cell Assignment via Satisfiability**

Hung, W.N.N. Changjian Gao Xiaoyu  
Song Hammerstrom, D.

On page(s): 823-830

##### **Abstract**

We present a novel CAD approach to cell assignment of CMOL, a hybrid CMOS/molecular circuit architecture. Our method transforms any logically synthesized circuit based on AND/OR/NOT gates to a NOR gate circuit and maps the NOR gates to CMOL. We encode the CMOL cell assignment problem as Boolean condi-

tions. The Boolean constraints are satisfiable if and only if there exists a solution to map all the NOR gates to the CMOL cells. We further investigate various types of static defects for the CMOL architecture and propose a reconfiguration technique that can deal with these defects. We introduce a new CMOL static defect model and provide an automated solution for CMOL cell assignment. Experiments show that our approach can result in smaller area (CMOL cell usage) and better timing delay than prior approach.

#### **Effect of Sol Strength on Growth, Faceting and Orientation of Sol-Gel Derived ZnO Nanostructures**

Bahadur, H. Srivastava, A.K. Rashmi Chandra, S.

On page(s): 831-836

##### **Abstract**

ZnO thin films are used for a number of MEMS-based sensors because of the piezoelectric and semiconducting properties. In certain class of devices, especially those using surface acoustic wave (SAW) technology on a layered substrate (such as ZnO on Si), it is a requirement to grow several micron thick ZnO layer which must be highly c axis oriented. In this attempt, we have deposited ZnO films by sol-gel spin process and using three different concentrations of 10%, 12.5%, and 25% of sol using zinc acetate as the precursor material and characterized for their thickness and other associated characteristics. The XRD pattern showed diffraction peaks of the hexagonal ZnO phase. The intensity of the 002 peak was much low for low-strength sols indicating substantial preferred orientation of the crystallites perpendicular to the sample surface. The crystallite size was estimated to be about 45 nm from the 100 diffraction peak. For the sample with 25% strength of the sol, the XRD pattern showed diffraction peaks of the hexagonal ZnO phase. The crystallite size was estimated as about 60 nm from the 100 peak and about 145 nm from the 002 peak. The TEM results showed fine nanoparticles with hexagonal ZnO crystal structure and morphology dependence upon the sol strength. Faceted morphology of hexagonal ZnO nanostructures has been obtained. The results would find application in nanoelectronic piezoelectric sensors.

#### **Dissociation Chemistry of Gas Molecules on Carbon Nanotubes—Applications to Chemical Sensing**

Govind, N. Andzelm, J. Maiti, A.

On page(s): 837-841

##### **Abstract**

It is well known in the literature that carbon nanotubes (CNTs) interact weakly with many gas molecules like H<sub>2</sub>O, O<sub>2</sub>, CO, NH<sub>3</sub>, H<sub>2</sub> and NO<sub>2</sub>, to name a few. Exposure to NO<sub>2</sub>, O<sub>2</sub> and NH<sub>3</sub> significantly affects the electrical

conductance of a single wall nanotube (SWNT). These can be explained using a simple charge transfer picture, which results in the observed changes in the hole conduction of the tubes. It is also known that pure SWNTs only weakly interact with these molecules. We have recently investigated (Andzelm, 2006) how common defects in CNTs [Stone-Wales (SW), monovacancy, and interstitial] influence the chemisorption of NH<sub>3</sub>. This paper is a continuation of our previous work. Here, we further investigate, via density functional theory (DFT) calculations, the effects of SW defects on the adsorption/dissociation of O<sub>2</sub> and H<sub>2</sub>O. We also study the diffusion of adsorbed oxygen atoms on the nanotube surface in the vicinity of the SW defect, as well as the dissociation of in the presence of adsorbed oxygen atoms.

#### **Widely Separate Spectral Sensitivity Quantum Well Infrared Photodetector Using Interband and Intersubband Transitions**

Alves, F.D.P. Santos, R.A.T. Amorim, J. Issmael, A.K. Karunasiri, G.

On page(s): 842-848

##### **Abstract**

Recent commercial and military infrared sensors have demanded multispectral capabilities, high sensitivity and high selectivity, usually found in quantum well infrared photodetectors (QWIPs). This paper presents the design and characterization of a three-band QWIP capable to detect simultaneously near infrared (NIR), mid-wavelength infrared (MWIR), and long-wavelength infrared (LWIR), using interband and intersubband transitions. Separate readouts provide the flexibility to optimize each band detection by allowing the application of different bias voltages. The quantum well structure was designed using a computational tool developed to solve self-consistently the Schrodinger-Poisson equation with the help of the shooting method. The detector comprises of three different stacks of uncoupled (wide barriers) quantum wells that combine AlGaAs, GaAs, and InGaAs, separated by contact layers, grown by molecular beam epitaxy (MBE) on a GaAs substrate. The spectral responses in all three bands were measured using a standard photocurrent spectroscopy setup with light coupling via a 45 facet. The measured photoresponse showed peaks at 0.84, 5.0, and 8.5 wavelengths with approximately 0.8, 0.03, and 0.12 A/W peak responsivities for NIR, MWIR, and LWIR bands, respectively. A good agreement between the measured and simulated figures of merit shows the possibility to improve and tailor the detector for several applications with low computational effort. Finally, this work has demonstrated the possibility of detection of widely separated wavelength bands using interband and intersubband transitions in quantum wells.

### **Temperature and Chemical Sensors Based on FIB-Written Carbon Nanowires**

Zaitsev, A.M. Levine, A.M. Zaidi, S.H.

On page(s): 849-856

#### **Abstract**

Carbon nanowires written by focused ion beam on diamond surface are novel nanostructures with interesting electronic properties. In this communication, carbon nanowire structures working as temperature and chemical sensors are reported. The sensor structures were made as arrays of carbon nanowires written by a 30 keV Ga<sup>+</sup> focused ion beam on polycrystalline CVD diamond films. The electronic structure of a carbon nanowire array is discussed as multiple unipolar heterodiodes graphite-diamond-graphite (G-D-G). The energy barrier of the G-D-G diodes has been found of a value 0.25 eV. The structures exhibited changes in conductance when measured at different temperatures or when put in proximity of some volatile liquids. This temperature and chemical sensitivity is explained by the activation of the charge carrier flow over the G-D barrier caused by temperature or by the charge of the analyte molecules adsorbed on the surface of the structure. The temperature response of the sensors in the range from 40 to 140 °C is exponential at a rate of 0.11 dB/°C. The chemical sensitivity has been found selective and particularly pronounced for water vapor. The advantages of the novel carbon nanowire sensors are their blindness to visible light, compatibility with carbon nanotechnology, simplicity and reproducibility of fabrication. The all-carbon nature of the sensors implies their applicability in medicine and biology.

### **Modeling Electrostatic and Quantum Detection of Molecules**

Vasudevan, S. Walczak, K. Kapur, N. Neurock, M. Ghosh, A.W.

On page(s): 857-862

#### **Abstract**

We describe two different modes for electronically detecting an adsorbed molecule using a nanoscale transistor. The attachment of an ionic molecular target shifts the threshold voltage through modulation of the depletion layer electrostatics. A stronger bonding between the molecule and the channel, involving actual overlap of their quantum mechanical wavefunctions, leads to scattering by the molecular traps that creates characteristic fingerprints when scanned with a backgate. We describe a theoretical approach to model these transport characteristics.

### **Infectious Agent Detection With SERS-Active Silver Nanorod Arrays Prepared by Oblique Angle Deposition**

Driskell, J.D. Shanmukh, S. Yong-Jun Liu Hennigan, S. Jones, L. Yi-Ping Zhao Dluhy, R.A. Krause, D.C. Tripp, R.A.

On page(s): 863-870

#### **Abstract**

The aligned silver nanorod array substrates prepared by the oblique angle deposition method are capable of providing extremely high enhancement factors ( $\sim 5 \times 10^8$ ) at near-infrared wavelengths (785 nm) for a standard reporter molecule 1,2 trans-(bis)pyridyl-ethene (BPE). The enhancement factor depends strongly on the length of the Ag nanorods, the substrate coating, the polarization of the excitation light, as well as the incident angle. With the current optimum structure, we demonstrate that the detection limit for BPE can be lower than 0.1 fM. We also show that this surface-enhanced Raman spectroscopy (SERS)-active substrate can serve as a sensor to detect and differentiate the molecular fingerprints of several important human pathogens, particularly, respiratory syncytial virus, human immunodeficiency virus, rotavirus, and the bacterium *Mycoplasma pneumoniae*. Utilizing chemometric methods, SERS nanorod array data can be used to sensitively detect and to classify viruses at the strain level. These results suggest that the SERS Ag nanorod array is a powerful technique for direct, rapid, and sensitive detection of infectious agents.

### **Ferrocenedimethanol Transport in Thin Films Consisting of Laponite and Hydrogel**

Smith, O. Seo, S.S.

On page(s): 871-873

#### **Abstract**

The development of multifunctional materials, which exhibit properties suitable for the development of advanced optical, electrochemical, and other such sensors have been at the forefront of many scientific research. In remaining consistent with this trend, this work presents a methodology for characterizing clay-hydrogel thin films by monitoring the transport of 1,1-ferrocenedimethanol (Fc(MeOH)<sub>2</sub>) via cyclic voltammetry techniques. Multilayer thin films were prepared by alternate layer deposition of poly(N-isopropylacrylamide-co-acrylic acid) hydrogel and laponite clay on regular glass carbon electrode. The ratio of the current intensity at the modified electrode compared with that at the bare electrode was used to provide information about the permeation of the electroactive species through the thin films. The current was also plotted as a function of the various layers to determine how permeation changes with increasing layers. The results procured thus far suggest the possible incorporation of these thin films in sensor development.

However, further work, such as the determination of the responsiveness of the thin films to environmental stimuli (temperature, pH, etc.) must be done in order to optimize the technology.

#### **Arrays of Nanoarrays: Elements of Binding**

Norton, M.L. Day, B.S. Huan Cao Rahman, M. Gin, A.

On page(s): 874-879

#### **Abstract**

The development of strategies for the robust attachment of organized patterns of nanostructures to a variety of surfaces has been a major objective of this laboratory. One of the significant impediments to single molecule, as opposed to multiple molecule, attachment arises from the size gap or intrinsic mismatch between the size of readily obtainable "downward" nanostructures and the native size scale of the molecules of interest. Although binding structures of diameter significantly less than 100 nm can certainly be fabricated, the techniques required to generate them are not widely available to researchers and the failure rate for the production of such structures is relatively high. These concerns have motivated this laboratory to instead pursue the synthesis of adapter structures which bridge, or partially bridge, this size gap by increasing the effective footprint of a single DNA molecule. Although several different approaches to the generation of adapter structures are under parallel development in the laboratory, one is based on a totally synthetic polydentate macromolecule. In this paper, the merits of this multithiol system will be presented. The development of an experimental platform for the characterization of attachment sites and adapter structure/attachment site interactions will also be described. These platforms are compatible with a wide range of characterization methods, including scanning electron microscopy, atomic force microscopy, laser scanning confocal microscopy, scanning tunneling electron microscopy and near field scanning optical microscopy, which can be used to evaluate these structures over the macro/micro/nano size range.

#### **Large-Area Well-Ordered Nanodot Array Pattern Fabricated With Self-Assembled Nanosphere Template**

Huaqing Li Low, J. Brown, K.S. Nianqiang Wu

On page(s): 880-884

#### **Abstract**

This paper has demonstrated a simple method to fabricate a large-area ( $\sim 1 \text{ cm}^2$ ) well-ordered gold nanodot array pattern with high throughput at low cost. At first, self-assembled polystyrene (PS) spheres are closely packed on a water surface, and then transferred from the

water surface to a solid substrate by dip coating. This results in a large-area defect-free close-packed PS sphere monolayer template on the solid substrate. It is worthy noting that the large-area close-packed PS sphere template can be transferred to the surfaces of various solids including silicon, oxides and metals, offering great flexibility. Furthermore, the close-packed PS monolayer can be tailored to a loose-packed sphere array template by reactive ion etching (RIE) technique. The sphere size is reduced upon etching but the spacing between spheres retains unchanged. By utilizing the PS sphere template, gold nanodot arrays with feature size down to 30 nm have been fabricated.

#### **Robust Negative Differential Conductance and Enhanced Shot Noise in Transport Through a Molecular Transistor With Vibration Assistance**

Bing Dong Lei, X.L. Horing, N.J.M.

On page(s): 885-890

#### **Abstract**

In this paper, we analyze vibration-assisted sequential tunneling (including current-voltage characteristics and zero-frequency shot noise) through a molecular quantum dot with two electronic orbitals asymmetrically coupled to the internal vibration. We employ rate equations for the case of equilibrated phonons, and strong Coulomb blockade. We find that a system with a strongly phonon-coupled ground state orbital and weakly phonon-coupled excited state orbital exhibits strong negative differential conductance; and it also shows super-Poissonian current noise. We discuss in detail the reasons and conditions for the appearance of negative differential conductance.

#### **Label-Free DNA Sensor on Nanoporous Silicon-Polypyrrole Chip for Monitoring Salmonella Species**

Joon-Hyung Jin Deng Zhang Alcolija, E.C. Grooms, D.L.

On page(s): 891-895

#### **Abstract**

Label-free DNA sensors based on nanoporous silicon (nPS) substrate were fabricated and electrochemically characterized. A low resistivity ( $0.01\text{-}0.02 \Omega \cdot \text{cm}$ ) p-type silicon wafer (100 orientation) was electrochemically anodized in an ethanoic hydrofluoric acid (HF) solution containing ethanol to construct the nPS layer with pore diameter of about 10 nm. This nano structure is compatible with organic polymeric conductors. Polypyrrole (PPy) film was directly electropolymerized on the nPS substrate without pre-deposition of any metallic thin-film underlayer. The rough surface of the nPS layer was favorable for strong adsorption of the PPy film. The intrinsic negative charge of the DNA backbone was ex-

ploited to adsorb 26 base pairs of probe DNA (pDNA) into the PPy film by applying positive bias forming the nPS/PPy+pDNA layer. DNA from salmonella enterica serovar enteritidis (tDNA) was extracted using standard protocol and, subsequently, amplified by polymerase chain reaction (PCR). Salmonella species are classified as bioterrorism threat agents by the centers for disease control and prevention (CDC). Results from the scanning electron microscopy (SEM) image of the cross section of the nPS/PPy multilayered film shows successful direct electropolymerization of PPy on the nPS substrate. Results also show that the tDNA concentration is inversely related to the peak current ( $i_p$ ) at 0.2 V versus Ag/AgCl. The plot of  $i_p$  versus incubation time showed that current density ( $J$ ) decreases by  $29 \mu\text{A} \cdot \text{cm}^{-2}$  per hour. The sensitivity obtained from the plot of  $i_p$  versus tDNA concentration is  $-166.6 \mu\text{A} \cdot \text{cm}^{-2} \cdot \mu\text{M}^{-1}$ . Current density decreases with increasing incubation time and tDNA concentration. These results demonstrate that the nPS substrate with PPy+pDNA+tDNA film has been successfully developed for a label-free DNA sensor in rapidly and specifically detecting select and threat agents.

#### **Ferromagnetic Resonance Detection for Magnetic Microbead Sensors**

Ghionea, S. Dhagat, P. Jander, A.

On page(s): 896-902

##### **Abstract**

This paper presents a novel detection scheme for magnetic beads used to label target molecules in immunoassay based sensors. The beads are detected inductively using a microwave circuit consisting of a slotline and coplanar waveguide (CPW) fabricated in a single metal layer. The waveguides are terminated at a short-circuited junction that serves as the active sensor area. When the slotline is excited by an input radio frequency (RF) signal, ac magnetic fields are generated at the junction. These fields are orthogonal to the propagation mode allowed in CPWs. As a result, the signal from the slotline does not nominally couple into the CPW. In the presence of a bead immobilized at the junction, fields from the slotline are distorted and the signal is coupled to the output at the CPW. The output signal is further enhanced by exciting ferromagnetic resonance in the bead. Simulation results indicate a single bead to be detectable with a sensitivity of 1-10  $\mu\text{V}/\text{V}$  depending on its location in the active sensor area and the waveguide geometry. The distinctive advantages of this detection technique are ease of implementation, requiring simple and inexpensive fabrication processes; and suitability for integration in lab-on-a-chip systems.

#### **Thermodynamic and Kinetic Analysis of Hydrogen Sensing in Pt/AlGaN/GaN Schottky Diodes at High Temperatures**

Junghui Song Wu Lu

On page(s): 903-909

##### **Abstract**

Schottky diodes on AlGaN/GaN heterostructures with Pt catalytic metal are fabricated and characterized for hydrogen sensing at a wide range of temperature and hydrogen concentration. The thermodynamic and kinetic processes of hydrogen adsorption/desorption at Pt/AlGaN are analyzed based on their steady and transient state sensing characteristics. The devices have great hydrogen detection capability even at sub-ppm level reliably at temperatures up to 800°C. Both forward and reverse currents of Schottky diodes increase with exposure to containing ambient, which is attributed to the reduction of Schottky barrier heights resulted by hydrogen adsorption at Pt/AlGaN. As temperature increases, the device sensitivity ( $S$ ) is improved due to the more effective dissociation, but starts saturating from 600°C. The coverage of hydrogen at the Pt/AlGaN interface exhibits the same trend as  $\Delta\Phi_B$  and  $S$ . The thermodynamic process of hydrogen adsorption in Pt/AlGaN is endothermic with an adsorption enthalpy of  $21 \text{ kJ} \cdot \text{mole}^{-1}$ . The adsorption time constant shortens as the temperature or the concentration increases. On the other hand, the desorption time constant exhibits opposite trend on the temperature and concentration. The absolute magnitudes of the activation energies for hydrogen adsorption/desorption at Pt/AlGaN increase with the  $\text{H}_2$  concentration.

#### **Realistic Nanotube-Metal Contact Configuration for Molecular Electronics Applications**

Andriotis, A. Menon, M. Gibson, H.

On page(s): 910-913

##### **Abstract**

A realistic single-wall carbon nanotube (SWCN)-metal contact configuration is obtained using a tight-binding molecular dynamics method incorporating full consideration of s, p, and d basis sets for carbon and metal atoms. The full structural relaxation of the combined SWCN and metal system is found to be essential for realistic characterization of conductivity. More importantly, convergence with respect to the number of the metal lead (ML) atoms in contact with the SWCN is found to be even more critical. Our results indicate that, in order to maximize device efficiency, one needs to use ML-SWCN systems with a minimal ML-SWCN contact-width to SWCN-length ratio.

**Magneto-Transport Physics in Superlattices With Staggered-Bandgap Structure**

Weidong Zhang Woolard, D.L.

On page(s): 914-921

**Abstract**

Physical models are presented to describe magneto-transport within double-barrier structure with staggered-band lineups. Here, a special case, where the magnetic field is perpendicular to the heterolayers, is considered and the conduction-band electron current is calculated. In addition, the spatial charge transfer due to the heavyhole (HH) interband tunneling is also studied. The interband tunneling probability is related to the Landau index number, which characterizes the quantization of in-plane electron motions. As a consequence, the inversion of hole populations between Landau levels is shown to occur which is a new phenomenon that has relevance for millimeterwave amplification.

**Controlled Growth of Carbon, Boron Nitride, and Zinc Oxide Nanotubes**

Moscatello, J.P. Jiesheng Wang Ulmen, B. Mensah, S.L. Ming Xie Shun Wu Pandey, A. Chee Huei Lee Prasad, A. Kayastha, V.K. Yoke Khin Yap

On page(s): 922-929

**Abstract**

Nanotubes represent a unique class of materials in which all atoms are located near the surface. Since electrons flowing through nanotubes are confined near the surface, nanotubes are attractive for sensing biological and chemical molecules. In addition, their tubular structures enable nanofluidic devices that are useful for novel sensing applications. In this paper, we will discuss current applications and the latest advancements on the growth of carbon nanotubes (CNTs), boron nitride nanotubes (BNNTs), and ZnO nanotubes (ZnONTs). First, CNT growth is highly controlled by regulating the effective catalysts and the dissociative adsorption of the hydrocarbon molecules during chemical-vapor deposition growth. Second, we have achieved low temperature growth of vertically aligned BNNTs at 600 °C, the first success of growing pure BNNTs directly on substrates at temperatures about half of those reported so far. Finally, we have developed an original approach for growing ZnONTs without catalyst or template. Robust, controllable growth techniques for nanotubes are necessary in order to fully realize their sensing potential.

**Gas Sensing With Mats of Gold-Nanoparticle Decorated GaN Nanowires**

Berven, C.A. Dobrokhotov, V. McIlroy, D.N. Chava, S. Abdelrahman, R. Heieren, A. Dick, J. Barredo, W.

On page(s): 930-935

**Abstract**

We report on the use of mats of gold nanoparticle decorated GaN nanowires as gas sensors. The sensing was by the repeated and reversible measurement of changes in the current-voltage characteristics of the mat of nanowires. The nanowires had diameters of about 200 nm and were many microns long. The mat was grown on a 1-cm diameter sapphire disk and was about 10 thick. The selectivity mechanism is attributed to the details of the surface morphology of the gold nanoparticles decorating the surface of the nanowires. The changes in the currents are attributed to a depletion mechanism in the nanowires due to the formation of a Schottky barrier due to the presence of the gold on the inherently n-type GaN. We were able to detect CO, CH<sub>4</sub>, CO<sub>2</sub>, H<sub>2</sub>, and observed possible evidence of creation of the by-products of the water-gas shift reaction.

**InP-Based Quantum-Dot Infrared Photodetectors With High Quantum Efficiency and High-Temperature Imaging**

Tsao, S. Hochul Lim Hosung Seo Wei Zhang Rzeghi, M.

On page(s): 936-941

**Abstract**

We report a room temperature operating InAs quantum-dot infrared photodetector grown on InP substrate. The self-assembled InAs quantum dots and the device structure were grown by low-pressure metalorganic chemical vapor deposition. The detectivity was  $6 \times 10^{10}$  cm Hz<sup>1/2</sup>/W at 150 K and a bias of 5 V with a peak detection wavelength around 4.0 μm and a quantum efficiency of 48%. Due to the low dark current and high responsivity, a clear photoresponse has been observed at room temperature. A 320 × 256 middle wavelength infrared focal plane array operating at temperatures up to 200 K was also demonstrated. The focal plane array had 34 mA/W responsivity, 1.1% conversion efficiency, and noise equivalent temperature difference of 344 mK at 120 K operating temperature.

**Plasmonic Structures Based on Subwavelength Apertures for Chemical and Biological Sensing Applications**

Dhawan, A. Gerhold, M.D. Muth, J.F.

On page(s): 942-950

**Abstract**

Periodic arrays of apertures with subwavelength dimensions and submicron periodicity were fabricated on gold-coated tips of silica optical fibers using focused ion beam (FIB) milling. Interaction of light with subwavelength structures such as an array of nanoapertures in an optically thick metallic film leads to the excitation of surface plasmon waves at the interfaces of the metallic film and the surrounding media, thereby leading to a significant enhancement of light at certain wavelengths. The spectral position and magnitude of the peaks in the transmission spectra depend on the refractive index of the media surrounding metallic film containing the nanohole array. This lays the foundation for the development of fiber-optic chemical and biological sensors that sense the change in refractive index of the medium around the metallic film. This is demonstrated by testing the sensors with solutions of alcohols with different refractive indices and by the attachment of biomolecules to the sensor surface. The bulk refractive index sensitivity of these nanoaperture array-based sensors is shown to be higher than what has been typically reported for metallic nanoparticle-based plasmonic sensors.

**Using Electrospinning for the Fabrication of Rapid Response Gas Sensors Based on Conducting Polymer Nanowires**

Rojas, R. Pinto, N.J.

On page(s): 951-953

**Abstract**

Early detection of trace amounts of toxic gases in an open environment is vital for any successful attempt to contain subsequent damage. The sensors used must respond quickly and reliably in such a situation. A typical method to increase sensitivity is to use sensors that have a large exposed area. It is also desirable for the sensor to be small in size and to consume low power. These characteristics can easily be achieved via the use of conducting polymer nanowires. Polyaniline is such a conducting polymer whose conductivity can be tuned to any desirable value in the range  $10^{-8}$  S/cm<sup>-10</sup> S/cm. We have prepared nanowires of this polymer in air and within seconds of using the electrospinning technique and used them in the fabrication of gas sensors. Due to the large surface-to-volume ratio and small amount of active material used, these sensors are faster and more reliable than conventional sensors based on thin films. While several methods exist to prepare polymer nanowires, most yield short (typically a few microns long) nanowires with te-

dious methods of isolating a single one. Electrospinning is a simple technique for making long (typically several centimeters long) nanowires that can easily be isolated and therefore is a promising method for the fabrication of low cost rapid response sensors.

**Adsorption Equilibrium and Kinetics of Microorganisms on Single-Wall Carbon Nanotubes**

Shuguang Deng Upadhyayula, V.K.K. Smith, G.B. Mitchell, M.C.

On page(s): 954-962

**Abstract**

Adsorption equilibrium and kinetics of pure and mixed cultures of *Escherichia coli* and *Staphylococcus aureus* on single-walled carbon nanotubes (CNT) aggregates were studied in an effort to develop CNT-based biosensors for quick detection of these bacteria in water. Batch experiments were carried out to measure the adsorption kinetics and equilibrium of pure and mixed culture of *E. coli* and *S. aureus* on the CNT aggregates at ambient temperature and various culture concentrations. The CNT aggregates can adsorb significant amounts of *E. coli* and *S. aureus* bacteria with different size and shape characteristics. The smaller size *S. aureus* has a five to ten times faster diffusion rate than *E. coli* and about 100 times higher adsorption affinity with the carbon nanotube aggregates. Freundlich adsorption model correlates well both the pure component and mixture adsorption equilibrium data. It is quite possible the CNT aggregates have separate adsorption sites for both *E. coli* and *S. aureus*. The combined high adsorption affinity and fast adsorption kinetics for *S. aureus* suggest that even unmodified single-wall carbon nanotubes can selectively differentiate *S. aureus* and *E. coli* in water. Transmission electron microscopic analysis qualitatively confirmed the adsorption results and provides direct visualization of the adsorbed bacteria on carbon nanotube aggregates. Both bacteria form biofilms on carbon nanotube aggregates and have a strong tendency to connect with each other rather than with the carbon surface.

**Nanotechnology-Based Detection of Explosives and Biological Agents Simulants**

Primera-Pedrozo, O.M. Jerez-Rozo, J.I. De La Cruz-Montoya, E. Luna-Pineda, T. Pacheco-Londono, L.C. Hernandez-Rivera, S.P.

On page(s): 963-973

**Abstract**

Nanotechnology based detection of threat agents, such as explosives and biological agents, has been a top research priority at the Center for Chemical Sensors Development at the Department of Chemistry of the University

of Puerto Rico-Mayaguez (UPRM). Nanoparticles are of fundamental interest since they possess unique size-dependent properties quite different from the bulk state. When a bulk metal is reduced in size, its properties begin to change dramatically because the constituent electrons begin to suffer the effects of quantum confinement. One of these important properties deals with the extraordinary enhancement of the intensities of Raman scattering events in chemical systems called surface enhanced Raman scattering (SERS). Until very recently, only aromatic moieties containing strong chromophores or highly delocalized  $\pi$  electrons would experience such an enhancement, when in close proximity to a silver or gold nanometallic assembly. In other cases, this SERS condition was not sufficient to satisfy the enhanced Raman scattering requirements because of Coulombic repulsions do not allow an intimate contact with the colloidal suspension of nanoparticles. Recent work in the research group includes optimization of particle size, agglomeration rate and ionic strength of the SERS active aqueous colloidal metallic suspensions. Results have led to extend existing benchmarks limits of detection of  $10^{-7}$  M to  $10^{-8}$  M ( $10^{-15}$  g) in DNT and to  $10^{-12}$  M ( $10^{-19}$  g) in the case of TNT. Other works include preparation and testing of bimetallic nano-interalloys: Au/Ag and metallic-semiconductor SERS active colloidal substrates: Ag/TiO<sub>2</sub>. Group members have prepared silver and gold nanorods and nanolayers in an effort to change the sensing platform: from aqueous media to solventless detection.

#### **Enhanced Raman Scattering of 2,4,6-TNT Using Metallic Colloids**

Jerez-Rozo, J.I. Primera-Pedrozo, O.M. Barreto-Caban, M.A. Hernandez-Rivera, S.P.

On page(s): 974-982

#### **Abstract**

Surface-enhanced Raman scattering (SERS) combines extremely high sensitivity, due to enhanced Raman cross sections comparable or even better than fluorescence emission. The observation of vibrational spectra of adsorbed species on nanoparticles, provides one of the most incisive analytical methods for chemical and biochemical detection and analysis. Nanoparticles are of fundamental interest since they possess unique size-dependent properties (optical, electrical, mechanical, chemical, magnetic, etc.), which are quite different from the bulk and the atomic state. Bimetallic nanoparticles are of particular interest since they combine the advantages of the individual monometallic counterparts. Metal colloids have become the most commonly used nanostructures for SERS. The present study focuses on the use of metallic nanoparticles, with a particle size of 35-80 nm for detecting TNT in solution. Gold, silver, and Au/Ag col-

loids were synthesized by chemical reduction methods, and used for detecting TNT in solution with high sensitivity and molecular specificity. The nanoparticles were characterized with UV-VIS spectroscopy, Scanning and Transmission Electron Microscopies and Raman Spectroscopy. The detection of TNT was conducted via an indirect method that involved the alkaline hydrolysis of TNT in the presence of a strong base. This method offered the advantage of generating reaction products that provided enhanced detection in the SERS experiments. The spectra were obtained in the 100-3500 cm<sup>-1</sup> range. The results revealed an increase in the intensity of the vibrational signals, attributed to the SERS spectra of TNT degradation products. Bands associated with out-of-plane bending modes centered at 820 and 850 cm<sup>-1</sup> and NO<sub>2</sub> symmetric and asymmetric stretching modes were detected.

#### **Gas Sensing Based on Inelastic Electron Tunneling Spectroscopy**

Bommisetty, V. Bhandari, S. Karmacharya, R.L. Rislov, D.A. Mileham, R.D. Galipeau, D. Galipeau, D.W.

On page(s): 983-988

#### **Abstract**

Odor detection with high reliability and selectivity is increasingly in demand in several fields, including defense, homeland security, clinical diagnosis, and air monitoring. Poor selectivity and reliability of existing gas sensor technology has been a major impediment in the development of a versatile odor detector. This work describes a new gas sensor technology based on inelastic electron tunneling spectroscopy (IETS) that may be able to identify gas molecules based on chemical bonds. The IETS responses of metal-insulator-metal tunnel junctions were measured at 77 and 300 K and the results suggest the potential of gas detection with ppm sensitivity. Despite thermal broadening, IETS peaks can be analyzed for room temperature gas identification.

#### **Fabrication of Heteronanorod Structures by Dynamic Shadowing Growth**

Junxue-X Fu Yuping-P He Yiping-P Zhao

On page(s): 989-997

#### **Abstract**

Multilayered heterogeneous one-dimensional (1-D) nanostructures are important building blocks for nanodevice applications. A practical nanofabrication technique to produce heterogeneous nanostructures with arbitrary materials must have the ability to control the dimensions and uniformity, to control the alignment, and to control the interfacial properties of the heterogeneous nanostructures. In this paper, we demonstrate a simple but



versatile method to fabricate three-dimensional (3-D) heterogeneous nanorod structures by multilayer dynamic shadowing growth (DSG). DSG is a process based on the geometric shadowing effect and substrate rotation in a physical vapor deposition system. By combining DSG and the sputtering technique, we successfully fabricated Au/Si matchstick nanorods which can further be developed as a novel biosensor for Respiratory Syncytial Virus (RSV) detection. By changing the source materials during the deposition, we demonstrate that complicated heterostructured nanorod arrays, such as Si/Ni multilayer nanosprings, can be easily produced, and they exhibit particular magnetic anisotropic behavior. We also use the DSG technique to coat a thin catalyst layer asymmetrically on the side of a nanorod backbone, and therefore design catalytic nanomotors with a variety of geometries capable of performing multiple desired motions in a fuel solution. This fabrication method reveals an optimistic step towards complex heteronanorod array design and fabrication.

#### **Influence of Base-Pair Interaction on Vibrational Spectrum of a Poly-dG Molecule Bonded to Si Substrates**

Peiji Zhao Woolard, B.

On page(s): 998-1003

##### **Abstract**

A theoretical investigation is presented that characterizes the interaction dynamics of a double deoxyguanosine molecular system, where two guanine bases are coupled via a sugar-phosphate backbone that is bound to the surface of silicon. Molecular dynamical simulations show that the influence of the coupling between the guanine bases (i.e., as compared with individual deoxyguanosine molecules) leads to a significant increase of the absorption intensity from microwave to infrared (IR) frequencies. Furthermore, these results show that the strong coupling between the guanine bases leads to a much larger number of distinguishable vibrational modes at frequency below the IR at  $\sim 1350 \text{ cm}^{-1}$ . These effects also produce double-peak features in the Far-IR absorption intensity, which represent a splitting of the individual peaks associated with a single deoxyguanosine molecule. Guanine base coupling also leads to a general shifting of all the absorption peaks towards the terahertz frequency regime (i.e.,  $\sim 10 \text{ THz}$  and below), which is also accompanied by a reduction of the absorption intensity as one progresses to longer wavelengths. Most importantly, this interaction phenomenon creates additional spectral features, which may be useful in a long-wavelength optics-based technique for DNA sequencing.

#### **Magnetic Field Control of THz Relaxation Oscillations in RTDs With Diluted Magnetic Semiconductor Layers**

Grubin, H.L.

On page(s): 1004-1010

##### **Abstract**

This discussion concentrates on novel semiconductor quantum barrier/well devices that utilize spin-control mechanisms available in diluted magnetic materials for achieving higher-level functionality (e.g., transistor action) at very high switching speeds and frequencies. The potential simplicity in the design of DMS devices compared with standard three terminal transistors with gate controlled I-V characteristics, is that for DMS structures, no more than two terminals are required, as the magnetic field in controlling the output of the DMS device functions as a controlling third contact. Indeed, properly designed, the magnetic field can transform a passive device into an active device, tune the output of a resonant tunneling device (RTD) fabricated with DMS layers and modify the logic state of a device.

#### **Towards De Novo Design of Deoxyribozyme Biosensors for GMO Detection**

May, E.E. Dolan, P.L. Crozier, P.S. Brozik, S. Manginell, M.

On page(s): 1011-1019

##### **Abstract**

Hybrid systems that provide a seamless interface between nanoscale molecular events and microsystem technologies enable the development of complex biological sensor systems that not only detect biomolecular threats, but also are able to determine and execute a programmed response to such threats. The challenge is to move beyond the current paradigm of compartmentalizing detection, analysis, and interpretation into separate steps. We present methods that will enable the de novo design and development of customizable biosensors that can exploit deoxyribozyme computing (Stojanovic and Stefanovic, 2003) to concurrently perform in vitro target detection, genetically modified organism detection, and classification.

#### **Quantum 1/f Biochemical Detection Limits in THz Signatures Revealed by Scanning Tunneling Microscopy Currents**

Truong, A.M. Handel, P.H. Fraundorf, P.

On page(s): 1020-1027

##### **Abstract**

It may be possible to amplify the characteristic THz frequency oscillations of chemical and biological agents that contaminate surfaces or samples examined with the

scanning tunneling microscope (STM). This THz spectral signature of the biochemical molecules competes with the frequency fluctuations introduced as phase noise close to the examined THz frequency by the  $1/f$  fluctuations of the tunneling resistance, of the resistance of the STM tip, and of the spreading resistance in the sample. Indeed, as we show below, the achievable spectral sensing resolution is  $\Delta\omega/\omega = [2 C \ln 2]^{1/2} = [2 \ln 2 (fS_R/R^2)/4Q_t^4]^{1/2} = [1.66 \cdot 10^{-12}]^{1/2} = 1.3 \cdot 10^{-6}$ . Therefore, we have calculated the quantum  $1/f$  noise of STMs for the first time, also determining the STM image resolution limits, including both the conventional and coherent quantum  $1/f$  ( $Q1/f$ ) effects. The main contributions are found to be quantum  $1/f$  tunneling current noise, and quantum  $1/f$  effect in the piezoelectric transducers in the feedback loop that controls the position of the needle above the sample. The results are compared with experimental data on STM resolution.

#### Sensitivity of Carbon Nanotube Transistors to a Charged Dielectric Coating

Pennington, G. Ervin, M.H. Wickenden, A.E.

On page(s): 1028-1035

##### Abstract

This paper investigates the electronic properties of single-walled carbon nanotube field-effect transistors (SWCNT-FETs) in which the SWCNT element is coated with a charged dielectric. The presence of remote charge on the surface of the dielectric is considered to effect carrier transport in the nanotube as a result of both carrier-scattering and gate screening. Nanotube device characteristics are simulated using the multi-subband Boltzmann transport method incorporating scattering from both phonons and remote charges. This allows assessment of the sensitivity of a nanotube FET to the presence of a charged dielectric coating during room temperature operation. Results show remote charge scattering affects the diameter ( $d$ ) dependence of the peak conductance and peak field-effect mobility of carbon nanotube devices. Under phonon-limited transport conditions, these peak values increase as  $\sim d$  and  $\sim d^2$ , respectively. When remote charge scattering is significant, peak values cease to vary with diameter once a critical diameter reached. Charge scattering is found to particularly degrade device current at gate voltages that allow carriers scattering into or out of a subband minimum. Furthermore, simulations show that intersubband scattering resulting from asymmetry in the circumferential remote charge density becomes increasingly important as the nanotube length decreases. The authors propose that remote charge scattering effects may be applicable in sensing devices allowing for the identification of the charge on a functionalized CNT coating.

#### Guided Self-Assembly of Silsesquioxane Nanocubes: Two Lessons From DNA

Toth-Fejel, T.T.

On page(s): 1036-1040

##### Abstract

The most promising approach to molecular assembly consists of manipulating and connecting chemically synthesized nanoscale building blocks, of which the geometrically most favorable are nanocubes. Silsesquioxanes are a promising set of such nanocubes-cubic cages of silica ( $\sim 1$  nm) with organic groups on each of the eight corners. Silsesquioxanes could be synthesized into larger, easier-to-manipulate multicage nanocubes (3-10 nm), which have the advantage of presenting additional face-bonding opportunities in a larger, easier-to-manipulate molecule. The highest value products that nanocube assembly will manufacture are fully 3-D electronic circuits with 5 nm features. Such integrated circuits would consist of nanocubes with electron-donating or electron-accepting semiconducting moieties in their intracube and intercube links. The synthesized nanocubes must be positioned with high precision and reliability so that they could be connected into NAND gates, billions at a time. Two different approaches are available: (1) Wang cube self-assembly and (2) pixilated DNA origami templating. Wang nanocubes are complex heterogeneous 3-D nanocubes with precisely controlled anisotropy. Their self-assembly would be similar to the sequential solid-phase synthesis process used to make DNA oligomers, and amino and bis-amino acid polypeptides, except that instead of building 1-D linear chain molecules that need additional weak-force self-folding and/or processing to form 3-D nanostructures, Wang nanocubes could form arbitrary 3-D nanostructures directly. Their existence depends on the synthesis of complex enantioselective multicage nanocubes with six independent face-connection chemistries with controlled orientation. In pixilated DNA origami templating, higher order silsesquioxane nanocubes would be attached (via amines, thiols, etc.) to one of hundreds of custom-sequence helper strands. Then, the molecular recognition of subsequences of a long single-stranded scaffold connect via Watson-Crick binding to the matching helper strand/nanocube complex, thereby making many arbitrary nanostructures possible.

**Continuum Theory of Amorphous Carbon Nanostructures**

Umantsev, A. Akkerman, Z.

On page(s): 1041-1046

**Abstract**

Carbon is often considered to be silicon of the future because of the unique properties resulting from the variety of possible structural forms. A wide range of electronic properties of carbon yields many possible applications. Classical thermodynamics successfully describes bulk equilibrium of the diamond-graphite system in a wide range of temperatures and pressures. Equilibrium in the carbon system at nanoscale, however, has not been clarified despite the significance of this information for numerous existing and possible applications of carbon in nanoelectronics. In the present paper, we analyze the transition between diamond and graphite phases using the continuum Landau theory. The theory sheds light

on the details of such transitions, and more importantly, predicts a new stable phase at nanoscale that can be used in carbon-based nanodevices. We find that the transition state of a system capable of undergoing a graphite/diamond phase transition gains thermodynamic stability against the bulk phases under the conditions of a limited volume if the barrier height of the transition is below the critical value. In a large-size closed system, a heterogeneous mixture of the graphite and diamond phases is the most stable state. In a small system (below the critical size), the heterogeneous mixture is not possible and the transition state becomes the globally stable state—a phase. Based on the present analysis, we hypothesize that the transition state is associated with the amorphous phase of carbon observed experimentally. The theoretical results allow us to interpret the experiments on focused  $\text{Ga}^+$  ion beam scanning irradiation of single crystal CVD diamond films, which produce highly conductive regions on the diamond surface.

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