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Natalia Lvova, Nano Res Appl 2018, Volume 4
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Adsorption properties of the diamond C(100)-(2×1) surface containing vacancies and nitrogen - vacancy defects

Natalia Lvova
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The nitrogen - vacancy complexes (NV complexes) determine the useful properties of nanodiamond fluorescence [1]. Single nitrogen - vacancy defects in diamond consist of a carbon-substituting nitrogen atom (N) and a vacancy (V) located in the neighboring lattice point [2]. In order to use the NV center, it should be located in a nanometer-size diamond particle. In our recent paper [3], we found that the most stable position of the vacancy in the near-surface layers of the clean surface C(100)-(2×1) is the defect position in the third layer directly under the dimer row of the upper layer, and for the complex defect nitrogen - vacancy is configuration «vacancy in the third layer, nitrogen in the fourth layer» [4]. In this study, the energy characteristics of hydrogen chemisorption on the C(100)-(2×1) diamond surface with vacancy defects and nitrogen - vacancy complexes in singlet and triplet states are investigated using quantum chemistry methods using semi-empirical quantum chemical methods on the C195H112 cluster. Modeling of the hydrogenated surface is traditionally used to determine the overall passivation effect [5]. The main conclusion of this study was shown that the most active centers for hydrogen adsorption are atoms of the surface hexagon, formed from the atoms of the upper and the second layers when a vacancy occurs in a third layer. However, the specific values of the energy characteristics depend on the nature and state of the defect.

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2. Jelezko F., Wrachtrup J. (2006) Single defect centres in diamond: A review. Phys. Stat. Sol.(a) 203:3207
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Biography

Anna Ryazanova has graduated MIPT in 2018 and has defended her master's degree on theoretical study of point defects in diamond. Currently, she continues her study as a PhD student.

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Annenkov Mikhail et al., Nano Res Appl 2018, Volume 4
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Interaction of fluorine with vacancies of graphene

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Chemical modification of graphene is a promising method aimed at changing its electronic properties and creating on its basis quantum structures. Fluorine, as hydrogen, is an element that converts graphene into a semiconductor material. One of the methods is the fluorination of graphene in aqueous solutions of hydrofluoric acid. The aim of the work was to study the interaction of F-, FHF- ions and their associates with water molecules with monovacancy and divacancy defects in graphene by quantum-chemical modeling. The C96H24 cluster modeling ordered graphene had a hexagonal shape with zigzag edges corresponding to the most stable configuration of the graphene sheet. Our model and approximation reproduce well the available literature data of the geometry and relative stability of monovacancies on a pure graphene surface, as well as fluorine adsorption on vacancies. As a result of the investigation, the energy characteristics of the chemisorption of fluorine from the associates of ions with water molecules were determined. It is shown that vacancies influence the chemisorption parameters: the activation energy decreases, the heat of adsorption increases in comparison with the ordered graphene sheet. The dependence of the heat of chemisorption on the degree of coverage by fluorine is studied. The characteristics of the reaction of vacancy defects with F-, FHF- and hydronium ion are compared. The results obtained can be useful for determining the optimum regimes for the synthesis of fluorographene with specified properties under laboratory conditions.

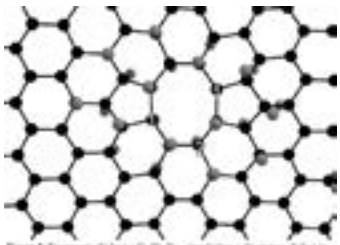

Figure 1: Fragment of cluster $C_{96}H_{24}F_{24}$ simulating a divacancy defect in graphene with 24 chemisorbed fluorine atoms. The most stable centers of adsorption are the marked atoms.

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Biography

Annenkov Mikhail has completed his Graduation at Moscow Institute of Physics and Technology (MIPT), Russia in 2017. Currently, he is pursuing his PhD at MIPT. His research interest includes “Investigation of the diamond surface and two-dimensional structures by the quantum chemistry simulation”.

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Notes:

Myung Chul Chang, Nano Res Appl 2018, Volume 4
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Preparation and fabrication studies of three dimensionally ordered nano-, micro- and meso-scale calcium phosphate crystallites scaffold for artificial bone materials (3-DOMm)

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Preparation and fabrication studies of three dimensionally ordered nano-, micro- and meso-scale calcium phosphate crystallites scaffold for artificial bone materials (3-DOMm): In clinical surgeon for humane bone replacement the artificial bone materials have been developed on a basis of biomechanical capability and nontoxic ability. Since 1987 the calcium phoaphte bone materials have been developed, showing proper mechanical strength, bioability and bone regeneration in bone metabolism. From several years ago global companies such as Stryker, ETEX and Biomet-Merck have commercially introduced the calcium phosphate bone products. The structure of humane bone is known to be the nanocomposites between collagen and hydroxyapatite. Biomimetic bone science have studied for the clinically possible surgical application of calcium phosphate bone. The primary study was how to mimic porous bone scaffold in calcium phosphate/collagen matrix. The second issue was how to attain the mechanical property of real humane bone. In first generation of artificial bone development acrylic polymer such as PMMA was mostly used because of the good mechanical strength in spite of serious toxic problem during surgery. Since calcium phosphate cement [CPC] bone has been introduced as bone regeneration, there was a big problem in clinical application because of low mechanical strength. Polymer modification study into CPC cement has been tried. We have focused on the development of pure calcium phosphate products having proper mechanical strength similar to real humane bone. The bioregeneration ability was shown and new syringe design was introduced for the clinical surgeon. We have been keeping the study of calcium phosphate science and engineering technology in bone metabolic condition. All of phosphate research are based on monodispersed control of nano-, micro-, and meso-scale for the bone scaffold application.

Biography

Myung Chul Chang has completed his PhD at Seoul National University and Postdoctoral studies at University Illinois at Urbana Champaign. He is the Director of Biomaterials Lab. He has published more than 50 papers in reputed journals and has been serving as an Editorial Board Member of reputed journals.

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Sergey Mikhailovich Afonin, Nano Res Appl 2018, Volume 4
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Absolute stability of control system with electromagnetoelastic actuator for nanotechnology applications

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The application of the electromagnetoelastic actuator based on the electromagnetoelasticity for the piezoelectric, piezomagnetic, electrostriction, magnetostriction effects is promising in the nanotechnology, the nano-biology, the power engineering, the microelectronics and the adaptive optics equipment. The correcting devices are chosen for providing the high quality of the control systems for the deformation of the piezo actuator. The analytical expressions for the sufficient absolute stability conditions of the system with the hysteresis nonlinearity of the electromagnetoelastic actuators are written using the Yakubovich absolute stability criterion with the condition on the derivative, which is the development of the Popov absolute stability criterion. For the Lyapunov-stable control system, the Yakubovich absolute stability criterion for the systems with the single hysteresis nonlinearity provides the simplest and pictorial representation of results of the investigation of the stability and the possibility of the synthesis of the correcting devices of the system ensuring the stability of the strain control systems with the electromagnetoelastic actuators. The characteristics of the electromagnetoelastic actuators are the alternating-sign hysteresis type for the piezo actuators and the constant-sign butterfly type for the electrostriction actuators. In the magnetostriction and electrostriction actuators their initial operating point is chosen on one wing of the butterfly, for example, in the first quadrant, for the deformation range to be symmetric at both sides of the initial point. For the butterfly characteristic the initial working point displaced by the half deformation range. The values of the tangents of the inclination angles of the tangent line to the hysteresis nonlinearity on the butterfly wing for the electromagnetoelastic actuator are determined similar to the hysteresis characteristic. The stationary set of the control systems is the segment of the straight line. The absolute stability conditions with the condition on the derivative of the control systems with piezo actuator deformation in the case of the longitudinal, transverse and shift piezo effect for the hysteresis characteristic of the deformation of the piezo actuator are obtained. The obtained absolute stability conditions for the control system with the electromagnetoelastic actuator allow one to estimate and calculate the characteristics of the control system for the deformation of the electromagnetoelastic actuator.

Biography

Sergey Mikhailovich Afonin is an Associate Professor in the Department of Intellectual Technical Systems at National Research University of Electronic Technology (Moscow Institute of Electronic Technology MIET). He/She has completed his/her Graduation in Electronic Technology at the National Research University of MIET in 1976 and a PhD in Electronic Technology Engineering and Control Systems at MIET in 1982. He/She has an Academic title of Senior Researcher received at MIET in 1991. He/She is an Aspirant at MIET from 1976 to 79, Junior Researcher at MIET from 1979 to 82, Senior Researcher at MIET from 1983 to 93, Associate Professor at MIET since 1993. His/Her contributions include more than 200 scientific papers to professional publication and 16 inventions. He/She is the Recipient of a Silver medal VDNKH Russia and two Bronze medals VDNKH Russia.

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Notes:

Veroniki P Vidali et al., Nano Res Appl 2018, Volume 4
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Solution-processable organic semiconductors based on anthracene as main components of active layers in OLEDs: Design, synthesis and application

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Well-defined, low molecular weight amorphous organic materials based on polyaromatic compounds exhibit interesting optical, electronic, and magnetic properties; whereas they can also serve as the basis for developing lithographic materials. Thus, they have been receiving attention for the development of organic devices in the nanoscale with substantially enhanced performance and new functions. Solution processability of such materials is highly desirable, since techniques, such as spin-coating, lower significantly the cost for the fabrication of the devices. Herein, a design strategy and synthesis of solution-processable small molecules, with well-defined monomolecular structures based on anthracene, is presented. Anthracene moieties are combined with other poly-functionalized planar and tetrahedral cores, providing control of physicochemical properties, such as solubility, thermal stability, and Tg. Selected members of this class, provided amorphous homogeneous films which were stable at temperatures up to 150°C. These molecules have been, also, evaluated as main components in the active layer of OLEDs, providing very promising results. Self-patterning was also allowed by incorporation of suitable acid-sensitive functional groups and a photoacid generator. These results demonstrate the potential of these materials to be used in the fabrication of patterned structures for OLEDs. A flexible, efficient and cheap methodology, suitable for the preparation of these anthracene-based molecules in large scale is also described, using representative examples.

Biography

Veroniki P Vidali is an Organic Chemist. She has completed her PhD at Agricultural University of Athens in 2004. She worked as a Post-Doctoral Fellow at Natural Products and Bioorganic Chemistry Laboratory/Institute of Nanoscience and Nanotechnology at NCSR “Demokritos" from 2004 to 2007 and as Scientific Staff from 2007 to 2017, while since 2017 she has been working as a Research Assistant at NCSR “Demokritos". Her main research interests include organic synthesis of bioactive natural products and polyaromatic compounds applied in nanotechnology. She has co-authored 18 peer-reviewed research articles in international journals and one book-chapter.

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Accepted Abstracts

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Heterogeneously integrated micro LEDs for displays and beyond

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As self-emitting devices without the need of back light units, Micro LEDs are suitable for many applications such as novel displays. Micro LED displays have the potential to enhance the capabilities of LCDs and OLED displays with its excellent performance in many different aspects, particularly high LUE, simplicity of optical modules without back light unit, long life time and excellent visibility under bright day light. Our group has been working on micro-LED technologies for more than a decade. We have reported the design and fabrication of high pixel per inch (PPI) micro-LED displays with red, green, blue and UV colors by integrating monolithic LED micro arrays and active matrix substrates using Flip Chip technology. A CMOS active matrix driving scheme was designed to provide sufficient drive capability and individual controllability of each LED pixel. The micro LED displays had 400×240 pixels on a single chip with PPI upto 1700. The emission wavelengths were 630 nm, 535 nm, 445 nm and 380 nm respectively. The red, green and blue micro LED displays can be used to form a novel full color direct view display. The micro LED displays could be used for modulated visible light communication systems or for data modulated photo pumped organic semiconductor devices.

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Enhanced metallized nano-porous aluminum oxide films: Principles of obtaining main results and applications

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Exploring the emerging trends in the realm of nano scale electrochemistry in particular the creation of nano porous aluminum oxide (NAO) is a topical problem of modern material engineering. For example NAO films with a high and average density of pores can be used in micro/nanoscale lasers with indirect electrical pumping by laser diodes. Metallized NAO films with ultrahigh density of pores are preferable for optical interferometric chemical sensors. Films with low density of pores are used in the selective interference coloration of the metal surface improving of the corrosion resistance of the metal. Determination of the optimal conditions of the aluminum electrochemical anodization and electrochemical and chemical metallization for each particular case is important task. This work was aimed at obtaining optimal conditions of the metallized NAO films with ultrahigh, average and low density of pores and the study of its applications. In the present study, the optimal conditions of the aluminum electrochemical anodization and electrochemical and chemical metallization were determined. Metallized NAO films with ultrahigh, average and low density of pores were obtained using the optimal conditions and were further characterized using high resolution scanning electron microscopy and the reflective interference spectra (RIFS) in a wavelength range of 235–735 nm at different angles.

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Controlled CVD growth of graphene and it electronic properties

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Graphene is a perfect two-dimensional atomic crystal. It has attracted considerable attention due to its unusual mechanical, optical and electronic properties. Chemical vapor deposition (CVD) is an effective way to prepare large area and high quality graphene because of its ultra-low cost, high controllability and high scalability. In order to enhance electronic properties of graphene based devices, we fabricated graphene single crystals with a variety of shapes using CVD method. The twelve pointed graphene grains were controllably synthesized. Self-aligned single crystal graphene grains were precisely grown controllably on liquid Cu surface by ambient pressure CVD. Meanwhile, we used an in situ etching method to fabricate large scale graphene arrays with control over the size, shape and location. On the other hand, hierarchical graphene architectures with a layer stacking growth were also fabricated by CVD method. The growth mechanism of graphene and its electrical properties were investigated.

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Polymer particles with tunable shapes and internal structures

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Block copolymer assemblies have attracted great attention due to their potential applications in the fields of drug delivery, targeting therapy, medical diagnosing and imaging. Three dimensional (3D) confinements, which can break the symmetry of a structure, have proven to be a powerful route to tailor the morphologies of block copolymer particles. Particle shape and internal structure can thus be tuned by using the supramolecular strategy or tailoring the interfacial interaction of the particles with the dispersed medium. Herein, we will introduce the generation of the block copolymer assemblies with well tunable shapes and structures by taking advantage of 3D confined assembly, supramolecular chemistry and interfacial manipulation. Particles with various overall shapes and internal structures can be obtained due to the 3D soft confinement in emulsion droplets. Moreover, we will show that selective disassembly of the structured particles will give rise to mesoporous particles or nano objects with unique shapes. The block copolymer assemblies with tunable shapes, internal structures and built in functionalities will find applications in controlled drug/gene delivery, catalysis, bioimaging and optical/electronic devices.

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Ionizing radiation sensors based on carbon nanotubes

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Carbon nanotubes (CNTs) are attracting much attention as promising materials for application in nanodevices due to their excellent electrical conductivity, optical, thermal and mechanical properties arising from their quasi-one-dimensional structure. Among these potential applications, the use of SWNTs as ionization radiation sensors is particularly of relevant interest. One of the key features of SWNTs for electronic and optoelectronic applications are that their metallic or semiconductive character depends on the chirality. The presence of a defect in the nanotube walls, i.e. a single atom missing, can result, locally, in the change of the chirality, thus into the variation of the nanotube electronic characteristics (semiconductor-metal junction) within a structure that is only a few nanometers wide. Variations of these electrical properties may be measured and, from these results, a clear correlation with the dose of radiation generated by the local defect in the nanotube can be established. In this investigation, we have deposited CNTs using an inter-digitalized growth pattern (see Figure), which has been connected to two gold electrodes. The morphological and structural properties of the CNTs before and after exposure to ion implantation were characterized by SEM, TEM, and Raman. The conductivity measured by this device was evaluated before and after being exposed to different doses of ion implantation, using an Ar+ gun. The results obtained clearly show a continuous decrease in conductivity, as the time of ion implantation increases. These results open a wide range of applications of these materials in the development of radiation sensors.

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Electron dynamic in DNA based nano wires

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Dynamical properties of electron motion in polynucleotide wire are considered. The charge motion is described in terms of quantum mechanics. Whereas, vibrational degrees of freedom are treated both classically and quantum mechanically. A typical charge transfer/transport pattern can physically be viewed as a polaron and/or soliton. A closed analytical expression for charge carrier velocity dependence on electric field has been derived and analyzed in detail. Special attention is given to: dynamical behavior of electrons in rigid chains, band structure of regular polynucleotide chains, dynamics of polaron states formation in Holstein chain, polaron motion in an electric field, the role of dispersion, Bloch oscillations and breather states.

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Development of mineral-filled polymeric membranes obtained by extrusion to implement in separation by MEAUS procedure

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Microporous membranes are commonly used in separation processes such as battery separators and medical applications to control the permeation rate of chemical components. Due to the wide range of chemical structures, optimum physical properties, and low cost of polymers and polymer blends, these materials are known as the best candidates for the fabrication of microporous membranes. The two main techniques to develop polymeric membranes are: solution casting and extrusion followed by stretching. High cost and solvent contamination are the main drawbacks of the solution technique. Techniques to make porous membranes from polymers without using any solvent were developed in the seventies of the last century for some applications, but most of the information on these processes remains proprietary to the companies' and are not available to the scientific community. One of the techniques is MEAUS (melt extrusion annealing uniaxial strain). It is based on the stretching of a polymer film containing a row-nucleated lamellar structure. Then, three consecutive stages are carried out to obtain porous membranes: creating a precursor film having a row-nucleated lamellar structure by mechanisms of shear and elongation-induced crystallization; annealing the precursor film at temperatures near the melting point of the resin to remove imperfections in the crystalline phase and to increase lamellae thickness, and; stretching at low and high temperatures to create and enlarge pores, respectively. In fact, in this process the material variables as well as the applied processing conditions are key parameters that control the structure and the final properties of the fabricated microporous membranes. The material variables include molecular weight, molecular weight distribution and chain structure of the polymer. These factors mainly influence the row-nucleated structure in the precursor films at the first step of the formation of microporous membranes. Among a wide range of resins, polypropylene (PP) is a well-known semi-crystalline polymer and, in comparison with polyethylene, have higher melting point, lower density, higher chemical resistance, and better mechanical properties, which make it useful for many industrial applications.

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Design of bulk nanostructured materials for superior multifunctional properties

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Multiple studies in recent years have proved severe plastic deformation (SPD) techniques as a very efficient way to produce nanostructured metals and alloys with significantly improved mechanical and functional properties, the latter affected by several factors, including ultrafine grains and also the atomic structure of boundaries in resulting nanomaterials. This report presents the results of complex studies of the formation of different grain boundaries (low angle and high angle ones, special and random, equilibrium and non-equilibrium with strain-distorted structure as well as with the presence of grain boundary segregations and precipitations) in nanostructured materials processed using SPD with various regimes and routes. This entails the materials with superior multifunctional properties, i.e., the combination of high mechanical and functional properties (corrosion and radiation resistance, electrical conductivity, etc.) that are induced by grain boundary design. Particular emphasis is laid on the physical nature and the use of multifunctional nanomaterials for their innovative applications in medicine and engineering.

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Some modern ideas of circuit diagnostics theory in the nanotechnology age

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Miniaturization of chips increases the problem of their diagnostics, and here it is necessary to be taken into account a number of factors. Tendencies in reducing accessibility for electrical connections and increasing the number of elements in the volume of the chip contradict each other. The problems intensify the need for additional theoretical studies on circuit diagnostics. The circuit diagnosis in common case can be defined as identification of the unknown element parameters by using test influences form current and voltage sources and by using acceptable current and voltage measurements. The analytical description of the problem solving has an important value. Complex application of several ideas permits to create a new line of circuit diagnostic models. These ideas are a conception of three different types of nodes for connecting sources and measurements, a conception of two sets of circuit elements with known and unknown parameters and idea of special matrix constructions. On the basis of this it was managed to create circuit diagnostic models taking into consideration a number of practically important features of the diagnostic process. Some of them are enumerated. Variations of external passive parameters, short circuits and breaks can be considered as test influences on the circuit. Some of the unknown parameters subsets may correlate each other with (linear) known ratios and this feature may be an important factor. It is managed to find some analytical solutions in theory of circuit diagnosis in the frequency domain.

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Advanced ultrafast laser based methods for material micro/nano-structuring and time-resolved studies of nanostructures and reduced dimensionality systems

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Novel laser based methods are currently a hot subject of research as an alternative path towards development of nanostructures in bulk materials and on surfaces of materials. The subject of the ongoing research is the phenomena taking place during laser surface interaction and the potential in creating structures which may give additional functionalities to the material surface. The use of ultra fast lasers with temporally shaped pulses has been a novel methodology in the exploration of the potential in creating novel nano structures that could not have been accessed with traditional laser irradiation of surfaces. In this presentation, author will review the work of his group where he has demonstrated the employment of temporally shaped laser pulses to finely tune tweak the surface morphology (i.e., the grown nanostructures and their characteristics) through a non standard interaction of the incident laser pulses with the irradiated surface. This is a result of numerous fundamental physical processes ranging from the femtosecond to the nanosecond temporal window and are triggered by the temporal regulation of the energy deposition of the laser energy onto the under study surface. The manifestation through the creation of laser induced periodic surface nano-structures and the tuning of their morphological characteristics, e.g., spatial frequency and contrast will be the central part of the discussion. Further, he reviews work on applying time resolved pump prove laser spectroscopy in order to characterize and study the modified ultra fast electronic phenomena and interactions that take place on nano structured surfaces, reduced dimensionality quasi two dimensinal systems and more complex three dimensional metallic nanostructures.

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Gallium nitride metasurfaces: Innovative perspectives and industrially relevant manufacturing processes

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The common way to manipulate light consists of using classical optical elements such as lenses and mirrors. Since few years, a new way to manipulate light with two dimensional optical components (metasurfaces) have been exploited to control light propagation using local phase discontinuities. Abrupt modifications of the fields across an interface can be engineered by depositing an array of sub-wavelength resonators specifically tailored to address local amplitude, phase and polarization changes. Metasurfaces have been implemented to obtain various sorts of optical functionalities, ranging from the basic control of the transmission and reflection of light, to the control of the radiation patterns for comprehensive wave front engineering and holography. In this presentation, we will review the recent works in this field and explain the physical mechanisms utilized for designing efficient planar optical components. We will also talk about our recent results on free-standing dielectric metasurfaces and introduce the concept of conformal boundary optics. As a conclusion, we will present innovative semiconductor based metasurfaces and discuss GaN-metasurfaces manufacturing processes relevant for electronics and optoelectronics industrial applications, e.g. light-emitting diode (LED) and/or augmented reality devices.

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Complexity and multi-functionality of superconducting meta-materials

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Super conducting meta-materials are ultralow loss, artificial, man-made media which are designed to achieve properties not available in natural materials. SQUID (Super conducting Quantum Interference Device) based metamaterials have additional functionality and control properties with exciting new collective properties both in the classical and quantum realms. A SQUID is a unique non-linear oscillator that can be manipulated through multiple external means. This domain flexibility is retained by SQUID based metamaterials and meta-surfaces i.e., extended units that contain a large arrangement of SQUIDs in various interaction configurations. Such units are essentially assemblies of weakly coupled nonlinear oscillators where numerous, classical as well as quantum complex, spatio temporal phenomena may be explored. In this presentation we will focus on SQUID based metamaterials and present basic properties related to their individual and collective responses to external drives. We will show that a SQUID based system acts as a genuine meta material with right as well as left handed properties; demonstrate that Josephson nonlinearity leads to wide band tunability, intrinsic nonlinear as well as flat band localization. We will further present exciting dynamical response properties such as multi stability and self-organization and the emergence of counter intuitive chimera states of selective, partial organization. In the truly quantum regime we will explore the interaction of electromagnetic pulses with superconducting qubit units where the coupling between the two yields properties such as self-induced transparency and super radiance. The appearance of these complex phenomena will be linked to possible technological applications.

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Gas phase of nanoparticle production at large scale

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Nanopowder production is associated with a number of technological challenges. The most common of existing production methods involve chemicals which can be dangerous and environmentally harmful. The gas phase ways provide the most promising perspectives in nanopowder quality and nomenclature. At the heart of our process is a method of obtaining powders by the evaporation of the raw material on industrial electron accelerator with power up to 100 kWt and energy 1.4 MeV followed by cooling the high-temperature vapor and condensation of substance into very small particles (nanoparticles) which then become highly dispersed (nano-size) powders. From fundamental view it can be related with the generation of high-temperature aerosol. The method is universal for a wide range of simple materials, nanopowder is produced in one stage, the technology allows to control the key parameters of finished products and is environmentally friendly. Advantages of the technology result in the advantages of the final products, that suit to the needs of different applications. For some nanopowders the very large volumes had been produced at the semi-industrial installation.

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Recent research progress of photovoltaic materials for high performance polymer solar cells

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Polymer solar cells (PSCs) have attracted great attention in the past decade, because of the advantages of a simple device structure, lightweight and capability to be fabricated into flexible and semi-transparent devices. The key photovoltaic materials of PSCs are conjugated polymer donors and the fullerene or non-fullerene acceptors. Recently, the non-fullerene n-type organic semiconductor (n-OS) (such as the low bandgap n-OS ITIC) acceptors have attracted great attention for their high photovoltaic performance. To match with the low bandgap ITIC acceptor, we developed a series of medium bandgap 2D-conjugated D-A copolymer donors based on bithienyl-benzodithiophene (BDTT) as donor unit and fluorobenzotriazole (FBTA) as acceptor unit. The D-A copolymer donors possess complementary absorption spectra and matching electronic energy levels with ITIC acceptor. By side chain engineering (alkyl-thienyl, alkylthio-thienyl, trialkylsilyl-thieny or alkyl-difluorothienyl substitution) on the thiophene conjugated side chains of the medium bandgap polymers, the power conversion efficiency (PCE) of the PSCs with the polymers as donor and ITIC as acceptor reached 9.26%5~11.63%. By side chain isomerization of ITIC, the PCE of the non-fullerene PSCs was further improved to 11.77%6~12.05%7. The results indicate that the side chain engineering of the conjugated polymer donors and n-OS acceptors are an effective way to improve photovoltaic performance of the PSC. In addition, we also developed high-performance low bandgap n-OS acceptors and low cost conjugated polymer donor materials recently.

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Air-stable high efficiency perovskite solar cells fabricated with graphene and metal oxide based nanocomposites

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The poor air-stability and reproducibility of hybrid solar cells have prevented the practical applications of the devices that can withstand sustained operation under ambient air conditions. To solve this issue, we developed simple methods for the production of silver nanoparticles (AgNPs) and reduced graphene oxide (rGO) in the form of Ag-rGO composites by one-step microwave-assisted reduction (MWAR) for bulk-heterojunction solar cells (BHJ-SCs) and the synthesis of perovskite-metal oxide composite for perovskite solar cells (PSCs). The field-effect transistor fabricated with the Ag-rGO composite showed p-type behavior with a high mobility of 3.3x105 cm2V-1s-1 and conductivity of 9x106 S/m which is one-order of magnitude greater than pristine graphene (1.59x105 S/m). As-synthesized Ag-rGO composite was introduced into the active layer of bulk heterojunction solar cell based on P3HT:PCBM. Compared to the P3HT:PCBM only device, the Ag-rGO implemented device showed 33% increase in photocurrent density and 42% increase of power conversion efficiency (PCE) due to enhancement of the charge carrier generation and fast extraction of holes to the electrode. By introducing the perovskite-metal oxide composite into PSCs with Al2O3/NiO interface engineering, we obtained a high efficiency of 18.14% for a champion device and excellent reproducibility of average 16-18% PCE for 35 devices which were all fabricated under ambient-air conditions, not in a glove box. More importantly, the devices without encapsulation showed a significant enhancement in long-term air-stability; the device photovoltaic parameters stabilized after 20 days and sustained its stability over 210 days with retaining ~100% of its original Voc, ~94% of Jsc, ~91% of FF and ~86% of PCE in an ambient environment.

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Extended adaptive control for electrical discharge machining

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Electrical discharge machining (EDM) has been used widely in industries over 8 decades because of its two remarkable advantages over conventional machining technologies: non-contact machining and machining conductive materials of any hardness. However, its essentially weak stability of machining restricts sustained machining in poor flushing conditions, especially in machining materials of high melting points like molybdenum-titanium-zirconium (TZM) alloy and the materials of low thermal conductivities like titanium and Inconel 718, etc. To solve this issue, some efforts of analyzing and disclosing EDM process dynamical properties had been paid. EDM process is, in fact, a non-stationary and nonlinear process with strong stochastic disturbances and the adaptive control theories seemed most likely fit for it. However, the first developed adaptive control system with minimum-variance control law, though the machining rate has been doubled, still had troubles in stabilizing EDM processes, especially in non-stationary stages. A new approach with minimum-variance and pole-placement coupled control law was studied and testified more feasible in dealing with machining in non-stationary stages. However, significant improvements had been achieved when two-step-ahead prediction control law was studied. Further explorations of EDM processes revealed that both of machining situation and machining state were changing all the time while in machining. If machining situation and machining state were considered simultaneously, more robust control systems for EDM would become possible. Thus, a new control system which was called an extended adaptive control system has been developed. In this system, there were two control variables working harmoniously in parallel to control the machining situation and the machining state respectively. This control system not only sustained fast and stable EDM, but also extended its efficient machining in machining molybdenum-titanium-zirconium (TZM) alloy, titanium alloy, and Inconel alloy, as well. More importantly, this new approach solved an issue once considered bottleneck constraint in 1991 that there existed coupling disturbances from one control variable to another in machining which has restricted the development of multivariable control systems for EDM.

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