Poster Session 1

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THE CRAB PULSAR

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I have performed some work on the determination of the rotation rate, and rate of change thereof, of pulsars including that in the Crab Nebula. I present a poster of my findings.

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COLD CLOUD CORES IN THE CEPHEUS FLARE REGION

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We study the physical parameters of the interstellar medium in the Cepheus Flare region. We investigated the large scale dust temperature and density distribution based on COBE DIRBE, IRAS and ISOSS data. We created optical B band extinction maps of 61 opaque objects in the ~220 square-degree region. We have selected 41 starless, dense cloud cores among these, based on infrared and optical images. As much as 21 cores showed very low (T<15K) FIR colour temperatures. These are considered as candidate pre-protpstellar cores and will be further investigated.

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ADVANCED APPLICATION OF THE QUASI-FREE REACTION MECHANISM TO NUCLEAR ASTROPHYSICS

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Quasi-free reactions (QFR) in heavy ion nuclear collisions at low energy have been widely investigated since 70's and general properties of nuclear structure have been inferred in the framework of the simple plane-wave impulse approximation PWIA and distorted-wave Born approximation DWBA[1]. In most cases it has been possible to deduce the inter-cluster wave function and momentum distribution of several light nuclei such as ^{6}Li, ^{2}H, ^{7}Li. More recently a method has been proposed to study two-body processes by means of a suitable three-body reaction proceeding through the QFR mechanism [2,3,4].

We show that this method can be used to measure two-body cross sections at very low energies (1 keV<E<1 MeV) overcoming the problems tipically encountered in direct measurements due to the presence of the Coulomb barrier. Several experimental results and validity tests are shown and discussed for astrophysically relevant reactions such as ^{7}Li(p,α)^{4}He, ^{6}Li(d,α)^{4}He, ^{6}Li(p,α)^{3}He, ^{12}C(α,α)^{12}C.

In this framework the astrophysical factor S(E) can be determined by-passing the screening effect due to the electron clouds, so providing an important tool in order to measure the screening potential U_e. Perspectives and in-progress experiments will be discussed.

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[3] M. Lattuada et al. Astrophysical Journal, Vol 562(2001) 1076
[4] A. Musumarra et al. Physical Review C Vol 64(2001) 068801

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P1 – 53 – C

ANHARMONICITY EFFECTS IN RAMAN-SPECTRA OF ALKANES

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Vibrational spectra of alkanes are rather complex that is determined not only by the polyatomic structure, but also by other factors. One of the factors is that vibrational frequency of them is close to that of the overtone of CH_3 group vibrations and therefore a manifestation of Fermi-resonance becomes possible.

A theoretical and experimental analysis of registered Raman-contours of alkanes (methane, ethane, propane and butane) in the 2000÷3500 cm^{-1} region has been conducted. A structure of spectra being investigated is rather complex. The structure becomes more complex while changing from methane to butane. An analysis of the obtained data was conducted on the basis of the following assumptions:
According to ab-initio calculations, side by side with vibrations in the 2800÷3000 cm^{-1} region there are low frequency vibrations in the 20÷150 cm^{-1} frequency region, which may be responsible for the spectrum formation with high frequency vibrations.
Vibrations in the 3000 cm^{-1} region take part in the Fermi-resonance with 2ν overtone of more low frequency vibrations in the 1450÷1500 cm^{-1} frequency region.
On the basis of the obtained results it is shown that taking into account anharmonic effects, Fermi resonance and strong interactions of high frequency vibrations with low frequency ones we can give an explanation of qualitative peculiarities of alkanes family spectra transformation in the 3000 cm^{-1} region (CH vibrations).

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MOLECULAR AND QUANTUM MECHANICAL SIMULATION AS A USEFUL METHOD OF THE RECONNAISSANCE FOR ORGANOCHEMICAL PROCESSES

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Extensive development of modern organic chemistry requires from researchers colossal efforts and resources. All means have been spent on the iteration of various agents and reaction conditions. However, only a few of the experiments will have been turned out significant. In most cases, computer simulations of organic processes enable to help to separate the essential one.

Various parameter of selected system such as the equilibrium energy and geometry, conformational energy differences, transition–state geometry and activation energy, electron density, electrostatic potential, molecular orbital energies, vibrational frequencies, nuclear magnetic resonance frequencies, and other values might be calculated using molecular and quantum mechanical methods. The obtained data consent to predict the course of reactions, properties of the substrates and the products.

The interaction reactions of some phosphines with boranes are investigated. Products of such reactions may be used, for example, as carriers of chirality in asymmetric synthesis. Theoretically, reactions of this type can lead to a pair of products. The ratio of the latter mostly depends on the substrates nature. The success in applying of obtained compounds depends on their purity.

The most suitable phosphine and borane were chosen after computer simulation of their interaction reaction. In some case, the difference between isomeric products of reaction turned out to be such large that we expect significant excess one of them. High energies of system stabilization permit expect of stability product that is sufficient for isolation as an individual substance. Our simulation relies on semi-empirical[1] AM1, PM3 models in first approximation as well as on advancing "*ab initio*" by Hartree-Fock[2] model calculation. The relation of obtained date with reality was observed by comparing IR and NMR spectra.

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P1 – 55 – C

AN EXACTLY SOLVABLE MODEL OF QUANTUM RELAXATION: CHECK OF THE MODIFIED DAVIES WEAK COUPLING THEORY

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I study an all-fermion modification of the model recently proposed by Capek (Eur. Phys. Jour. B 25(1),p.101 (2002); cond-mat/0012056). It exhibits the feature of breaking the second law in the modified Davies weak coupling limit similarly as the original Capek 's model. The advantage of the present model is that it is exactly soluble in the full range of parameters known from the mesoscopic electronic transport studies. The exact solution is obtained using nonequilibrium Green functions. A non-trivial transformation/mapping to the reduced density matrix formalism can be developed, and this is employed to clarify the essence and explore the validity of the modified Davies weak coupling theory instrumental in the Capek's work on the violation of the Second law.

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QUANTUM SCATTERING PROBLEM AS A BOUNDARY PROBLEM

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A general case of quantum (wave) scattering problem is only feasible for computation by means of direct methods. But conventional direct methods, developed for solution of boundary problems for partial differential equations, are not straightforwardly applicable for the scattering problem, as the latter is defined in open space, the causality condition (plane wave plus outgoing waves) being set at infinity. Although there was proposed a number of direct methods, allowing one to overcome in some extent the difficulty of establishing correspondence with the causality condition, none of those is as universal and efficient as linear direct methods are for differential equation boundary problems in a finite area.

In the present work on the example of one-particle scattering in a finite-range stationary potential field it is shown, that the causality condition is equivalent to a series of linear integral conditions for the wave function on the scattering area boundary. Combininig that system of conditions with the differential equation in the scattering volume, we obtain a mathematical problem, which may well be solved by conventional projectional and finite-difference methods.

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ARTIFICIAL NEURAL NETWORK STUDY OF AlO_xN_y THIN FILMS ANALYSED WITH RUTHERFORD BACKSCATTERING

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We developed an artificial neural network (ANN) algorithm for analysis of Rutherford backscattering (RBS) data. In RBS, fast ions (typically H^+ or He^+) are scattered off a sample. The energies of the backscattered particles provide information on the compositional depth profile of the sample.

Thin AlO_xN_y films were deposited on Si substrates. These oxinitrides are used as barriers in advanced read and recording devices. The RBS data from these films is difficult to analyse, because the interesting N and O signals are small and superimposed to a large background signal from the Si.

We applied the ANN to this problem, and obtained results that compare well with those from traditional analysis methods. The advantage of ANNs, however, is that they are fully automatic, that is, they do not require the involvement of humans to analyse the data, and they are instantaneous, as opposed to manual (or even computer-aided) analysis, that normally takes longer than to collect the data.

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A NUMERICAL MODEL FOR DYNAMICS OF SPECKLED LIGHT SCATTERED BY CELLULAR SUSPENSIONS

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The coherent light intensity scattered by a collection of microparticles in suspension, has a very complex spatio-temporal pattern known in the literature as laser speckle. The interference pattern has also a relatively complex temporal behavior dictated by the dynamics of the suspended microparticles. The light intensity forward scattered at small angles is usually detected by a photodiode, the signal is amplified and transferred to a PC computer by an A/D converter.

Digitized data obtained in scattering experiments have in general significant temporal fluctuations and represent a dynamic fingerprint of the behavior of suspended microparticles.

Our work is an attempt to compute the dynamic fluctuating response of the system using a numeric model with controlled values of some physical parameters of the suspended microparticles: mean sedimentation rate, microparticle concentration, the amplitude of the random dynamics (hydrodynamic and Brownian) and a set of temporal and geometric parameters related to the experimental set-up (the sampling rate, the sample - detector distance, the detector area, the detecting angle).

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NUMERICAL PHYSICS SPECIFIC PROBLEMS AND APLICATIONS

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In this period the Numerical Physics most provide: some acurate criteria intended to the evaluation of the compatibility of a theoretical model relative to the experimental results, computing algorithms which ensure satisfactiory accuracy, avoiding the instability and non convergence phenomena and a minimal duration of calculations (numerical simulations). It also has the support of Mathematics and Theoretical Physics providing the necessary algorithms for the computing codes used by the Computational Physics.

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NOISE LEVEL ESTIMATION IN A TIME SERIES

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A method of noise level estimation is presented that can deal with most cases of large amount of noise in a data. This method uses the correlation entropy and a corresponding parameter $K_2(\varepsilon)$, that depends on threshold value ε. The latter function relies in a special way on the noise standard deviation σ, which we exploit for noise estimation by a simple function fitting. The developed method works for Gaussian and other noise distribution including dynamical and measurement noise.

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MAGNETIC AND ELECTRONIC PROPERTIES OF $YNi_{5-x}M_x$ COMPOUNDS WITH M=Cu OR Al

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The $YNi_{5-x}M_x$ compounds with M = Al or Cu crystallize in a hexagonal structure of $CaCu_5$ – type. Magnetic measurements were performed in the temperature range 1.5 – 500 K. The magnetic susceptibilities, χ, for YNi_5 increase with temperature up to a maximum located at T ≅ 100 K. For T ≥ 160 K a Curie-Weiss type dependence was shown. The effective nickel moment determined from Curie constant is 1.64 μ_B/atom. In the low temperature range (T ≤ 10K) the susceptibilities follow a T^2 dependence. When alloying with Cu or Al the maxima in χ(T) are shifted to lower temperatures. In $YNi_{5-x}Cu_x$ system ($0.5 \le x \le 1.5$) the χ^{-1} vs T show linear dependencies for T ≥ 100 K. The effective Ni moment is only little dependent on composition, decreasing from 1.64 μ_B/atom (x = 0) to 1.55 μ_B/atom (x = 1.5). For aluminium doped system the susceptibilities may be analysed considering in addition to a Curie-Weiss dependence a Pauli-type paramagnetic contribution. The effective Ni moments decrease very fast when increasing aluminium content. Values of 1.00 μ_B/atom and 0.54 μ_B/atom were evidenced for samples having x = 0.5 and 1.0, respectively. Band structure calculations show that there is a weak hybridization between Ni 3d and Cu 3d states while Ni 3d and Al 3p states are strongly hybridized in agreement with the results of magnetic measurements. The magnetic properties of the $YNi_{5-x}M_x$ (M = Cu or Al) systems are determined by that of nickel. The nickel magnetic behavior as function of temperature change from a Pauli-type paramagnetism to one characteristic for localized moments. The above behavior is analyzed in models, which take into account the electron correlation effects in d-band, as spin fluctuation model and dynamical mean field theory. These models can explain the transition from a T^2 dependence at low temperatures to a Curie-Weiss behaviour in high temperature range.

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BROAD DIELECTRIC RESPONSE IN FERROELECTRICS AND RELATED MATERIALS

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The aim of a broad-band dielectric spectroscopy is to connect different processes which take place in the lattice and which frequently were studied separately. The use of combined techniques (IR spectroscopy, time-domain THz spectroscopy, BWO spectroscopy, high-frequency coaxial technique, audio-frequency dielectric spectroscopy) allows to cover the frequency range 10^2-10^{14} Hz ($\lambda \approx$ km-μm) in order to study the dielectric response of materials and discuss its mechanisms. These techniques provide the complex dielectric function, that is both permittivity ε' and dielectric loss ε''. Excitations connected with phase transitions as soft modes, relaxations and central modes, can be studied as well as the effect of the disorder in the lattice dynamics.

Ferroelectric and related materials have interesting dielectric properties for applications and undergo phase transitions with temperature, therefore they are excellent candidates for these studies. We present here a selection of results obtained in different types of materials: ordered single crystals, structurally disordered systems like relaxor ferroelectrics or dipolar glasses, and ceramics. Different models are discussed depending of the type of material. We show that generally below optical phonons another excitation connected with dynamic disorder exists. For some disordered systems a frequency-independent loss mechanism is found at low temperatures in a broad frequency range.

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SELECTIVE MAGNETOFLUIDIC VALVE

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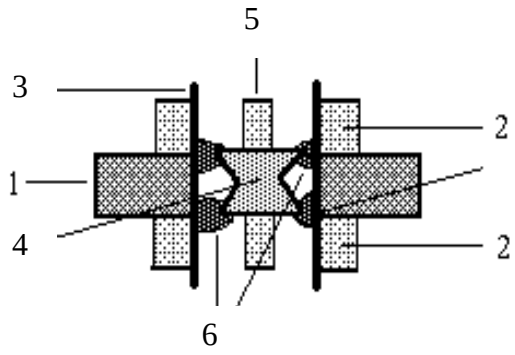
One of the most known applications of magnetic fluids is the magnetofluidic seal. The separation of two different (fluid) zones is realized by a narrow cylindrical shaped gap in which a non-uniform magnetic field is created using a permanent magnet. If a magnetic fluid is placed in the gap, the magnetic forces acting on it determine the formation of a continuous ring of magnetic fluid in the gap, separating the two zones. Usually, the magnetofluidic seals separate two quasi-homogeneous fluid media. Our purpose was to design the seal so that it separates a vertical liquid column containing dispersed small heavy particles (toxic heavy metals, metallic mercury) from a collecting container. Such a seal must support an asked differential pressure, as typical seals, but also must allow to the heavy particles to pass through, not to be floated by the magnetic forces inside the magnetic fluid rings.



The schematic diagram of the simplest magnetofluidic valve is presented in the figure below. A ring shaped permanent magnet (1) is fixed using the ring shaped nonmagnetic pieces (2) on a nonmagnetic tube (3). The ferromagnetic piece (4) is fixed on the ferromagnetic axe (5) and have the role to create a higher magnetic field gradient in the gap where the magnetic fluid rings (6) are formed. The tube (3) ensures both the rigid structure of the valve and its coupling to the water column (on the top end) and particle recovery vessel (on the bottom end).

We have experimentally determined the magnetization curve of the used magnetic fluid and the magnetic field structure in the valve gap. This allowed us to determine by numerical methods both the differential pressure supported by the valve and the minimum density of the particles passing through the valve. The two physical parameters, strongly depending on magnetic fluid characteristics and gap thickness, have values going up to $5 \cdot 10^3$ N/m^2 (for the supported differential pressure) and $5 \cdot 10^3$ kg/m^3 (for particles minimum density). If the technical flux requires a higher differential pressure, a similar valve, containing a higher units presented in figure, must be used.

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THE HYPERFINE MAGNETIC FIELD AT HF SITES IN $HfFe_2$

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The time-differential perturbed angular correlation (TDPAC) experiments involving the 133-482 keV gamma-gamma cascade in ^{181}Ta ion probe, have been performed in the absence of polarizing external magnetic field to measure the hyperfine magnetic field experienced by ^{181}Ta nuclei at the Hf site in Laves phase compound $HfFe_2$. This phase crystallizes into the cubic $MgCu_2$ (C15) structure, the hexagonal $MgZn_2$ (C14) and the $MgNi_2$ (C36) structure. The subtle results of TDPAC measurements at ^{181}Ta sites in the multi-phase polycrystalline $HfFe_2$ sample have demonstrated the possibility of measurements of the hyperfine magnetic field for every particular structure independently. In our sample the existence of the cubic $MgCu_2$ phase in an amount of 65% and the hexagonal $MgZn_2$ phase in an amount of 35% is established, which changed after annealing the sample in favor of the cubic structure (80%). The presence of the third phase $MgNi_2$ (C36) is not observed in the investigated sample. The hyperfine magnetic fields measured at 293K are H_{hf} = 13.8±0.1T in the cubic (C15) and H_{hf} =7.9±0.2 T in the hexagonal (C14) phase and they haven't changed significantly after annealing the sample (the changes are within experimental errors). Differences of the H_{hf} values in the two structures seems to originate in the crystal structure effects.

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LIFETIME DISTRIBUTION OF ELECTRIC CARRIERS IN CdSe EPITAXIAL LAYERS

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CdSe layers have been deposited on (0001) mica substrates at various substrate temperatures (730°C, 752°C and 770°C) by vapour epitaxial method. Information about growth conditions structure, microstructure and chemical compositions of these samples were obtained from X-ray diffraction and by scanning electron microscopy. Epitaxial layers of photoconducting CdSe reveal superior photosensitivity of the order of 10^9-10^{11}. These layers have the high sensitivity response in the visible range (400-800nm) matching well with the human eye. The study of recombination kinetics and carrier lifetime distribution in the CdSe epitaxial layers is measured using photoconductive frequency-resolved spectroscopy. The carrier lifetime distribution in a semiconductor is important for material characterization and device evaluation. The obtained lifetime data reveal, for all investigated samples, three recombination mechanisms associated to (*i*) band-to-band recombination, (*ii*) surface recombination associated with chemical impurities and (*iii*) surface recombination associated with structural defects.

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PARAMETERISATION OF ENERGY STRUCTURE OF THE RARE-EARTH IONS DOPED IN CRYSTALS AND GLASSES

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Rare-earth (RE) ions are well known activators for laser materials. At the same time the RE ions are widely used for doping various crystals and glasses because they can cause some desirable changes of the physical properties of these compounds (can to compensate effects of uncontrolled impurities as well as change some crystal parameters to better ones) [1].

Transition of the RE ions from a free state to a state in a crystal causes an additional whole or particular splitting of degenerated J-levels on the components characteristic crystal field of the certain symmetry. In order to identify spectral lines we have carried out the simulation of average values of energy matrix for the RE^{3+} ions in various dielectric crystals and glasses using parameterisation procedure for impurity ions in crystals [2]. Obtained F^k (nl, nl) parameters were used for solution of a direct spectroscopy task - calculation of the energies of all actual in the luminescence levels on impurity ion. Computer simulation was also applied for analysis of absorption spectra and study of probabilities of radiation transitions using Judd-Ofelt's theory.

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P1 – 67 – C

POLYELECTROLYTES OBTAINED BY ELECTRON BEAM AND MICROWAVE IRRADIATION

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The results obtained by accelerated electron beam, microwave and simultaneous microwave and electron beam application to the acrylamide-acrylic acid co-polymers curing are presented. The analysis of the experimental results concerning the acrylamide and acrylic acid copolymer parameters demonstrated that MW heating always produces high water solubility (low values for Huggins constant, k_H=0.015-0.5) but median values for molecular weight (M_w =3-5 x 10^6 amu) and conversion coefficient (CC=75%-95%). The ionizing radiation-induced polymerization gives high conversion coefficient (CC=95%-100%) and high molecular weight (M_W = 4 -16x10^6 amu) but poor water solubility (cross-linked structure) of acrylamide-acrylic acid co-polymers. Thus, our interest was focused upon the methods, which lead to the simultaneous optimization of M_w, CC and k_H of the acrylamide-acrylic acid copolymers. The main idea of this paper was to combine the ionization effects of accelerated electron beam and heating effect of microwaves to obtain this desire in the acrylamide-acrylic acid copolymer processing.

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PLASTICITY - STOCHASTIC DISLOCATION DYNAMICS SIMULATIONS FOR THE UNDERSTANDING OF DISLOCATION PATTERNS

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It is well known that during the plastic deformation of crystalline materials the dislocation distribution does not remain homogeneous. In spite of the increasing experimental and theoretical activity in this field we are far from the understanding of this typical self organisatory phenomenon. A crucial open question is whether the elastic part of the dislocation-dislocation pair interaction which is dominant at long distances and does not have an intrinsic range can lead to spatial patterns which may exhibit well-defined characteristic scales.

A possible approach for the modelling of these pattern formation processes is to investigate the collective behavior of systems consisting of individual dislocations by computer simulation. However, because of the long range character of the elastic pair interaction the direct numerical integration of the equations of motion of dislocations is very computation expensive restricting considerably the affordable dislocation number or simulation volume. The aim of the investigations presented is to overcome this restriction by taking into account the statistical properties of the dislocation assembly.

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SIMULATION OF A SI BASED STATIC INDUCTION TRANSISTOR

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Now semiconductor structure simulation is widely used in electronic industry. For example, software environment such as SUPREM, Tide and etc. are very popular in developing technology of intermittent devices or integral scheme elements. Mentioned software tools give the possibility to receive the potential, impurity, electric field, electrons and holes distributions are formed at developed process flow of production. The received results of calculation are recorded to output file. This output file can be used after some transformations for subsequent calculations of current distributions in received n–p–n structure and volt-ampere characteristic of the device.

In this paper we report about the developed by us program which allows to compute the simple one-dimensional static induction transistor model. This model is based on the fundamental system of semiconductor equations and does not require a complex calculations. The mentioned program is developed in programming environment Delphi. It uses data from the text file created after the simulation by one of the program packages for technology modeling (for example, SUPREM or Tide). Results of computation received from the program packages for technology modeling are further used as input data for calculations of current distributions and volt-ampere characteristic of the device by numerical method.

By means of developed by us program we have calculated the volt-ampere characteristics of static induction transistor. Static induction transistors (SITs) are short channel FET structures which are suitable for high power, high temperature and high frequency applications. The one-dimension simulation of Si based output transistor for voltage regulator (it is static induction transistor in this case) was performed by mentioned program developed in Delphi. The breakdown voltage of the transistor which was calculated is 200 V and collector-emitter saturation voltage is 0.4 V. Initial calculations performed by means of program Tide show that developed structure of static induction transistor has emitter-base junction depth 2.3 μm, collector-base junction depth 5.34 μm, the complete length of calculated structure is 30.7 μm.

The potential, electric field, electrons, holes, current distributions and volt-ampere characteristic have been received by means of program developed in programming environment Delphi. Calculations have been performed at range of emitter-base voltage from 0.0 to 0.8 V and collector-emitter one ~ -3 V. Received results of calculations allow to show changes of volt-ampere characteristic in accordance with changes in production technology or electrical mode of operation.

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ULTRASONIC INVESTIGATION OF NANO-SCALED STRUCTURE OF LIQUIDS

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The formation of particles in the liquids from atoms and molecules leads to an inhomogeneous component distribution on height. The information about inhomogeneity of liquids in gravitational field can be extracted from the results of the sound velocity measurements. An ultrasonic pulse phase technique allows the sound velocity Vs to be determined at various distances h from the bottom of the crucible. Using the obtained Vs(h) curve, the composition of phases, average size and concentration of the particles in the liquid can be estimated.

The ultrasonic method of the investigation of nano-scaled structure of liquids has several advantages. 1) The small absorption of sound by the metallic, organic and inorganic liquids enables the wide use of this method. 2) The method allows us to find the particles size down to 10 nm.

The results of the sound velocity measurements of the Ga-Pb melts that demonstrate the described method are reported. The metastable microemulsion structure, which consists of nano-scaled particles enriched with gallium or lead, is found above the miscibility gap. The process of the formation and destruction of the particles are investigated.

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P1 – 71 – C

VORTEX LATTICE IN TILTED MAGNETIC FIELDS. LOCK-IN EFFECT ON MO/SI SUPERCONDUCTING MULTILYERS AND THIN VANADIUM FILM

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The lock-in transition is observed on artificial superconducting multilayers which takes place in the tilted magnetic fields. The measurements have been carried out on Mo/Si layered systems. At the relatively small tilting angles the confinement of the vortices parallel to the layer planes becomes energetically more favorable than creating of the tilted vortices.

The temperature dependence of the critical angle for the trapping of the vortices in the orientation parallel to the layer planes is determined by the known resistive method, as well as by a new method based on the effect of commensurability between intervortex distance and the period of layering. The critical angle dependences on temperature obtained by the both methods practically coincide. The experimental results are consistent with the theoretical predictions of Feinberg and Villard.

In additional, the lock-in transition conditioned by the influence of the surface barrier is observed for the first time on thin films.

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SIZE DISTRIBUTION AND CONDUCTION ESR OF PLATINUM IN NANOPOROUS Al_2O_3 MEMBRANES

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Anodic porous alumina has recently attracted a great attention as a key material for fabrication of devices on a nanometer scale, such as electronic and photoelectronic devices. Also, nanoelectrodes ensembles can be obtained by using porous alumina as template.

Pt-nanoelectrodes ensembles were created by electrodeposition into the porous layers using hexachloroplatinic acid in sulfuric acid. The structure of these Pt-nanowires was investigated by Fourier transform analysis of the X-ray scattering curve. From the crystallite size distribution function, a value of D_m 9.7 nm was evaluated for the mean diameter of Pt-nanowires.

Metal particle sizes could also be obtained by using the Kawabata theory that relates Conduction ESR linewidth to the metal partcle size. The CESR linewidth of Pt-nanoelectrodes were found to be independent of temperature in the temperature range 6-30 K where the resonances were observed. The evaluated Pt-mean particle diameter from CESR linewidth is about 5.6 nm, which is smaller than the value obtained from X-ray analysis. A discussion is given concerning the validity of Kawabata's theory to such systems.

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SCHOTTKY AND OHMIC CONTACTS TO GALLIUM ARSENIDE

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In this work some aspects that determine the properties of Schottky and ohmic contacts to GaAs are discussed. We pay special attention to Ru and show that its thermal and chemical stability makes it ideal for use in devices operating above room temperature and for experiments involving annealing. We discuss the effect of different metallization methods on properties of Schottky barrier diodes and show that methods which use energetic particles, such as electron beam deposition and sputter deposition, often result in inferior Schottky barrier diodes properties-the consequence of electrically active defects introduced by the energetic particles at and close to the semiconductor surface. The advantages of using Ru as contact material to GaAs are that it forms high quality, thermally stable Schottky contacts to n-GaAs and thermally stable ohmic contacts with low specific contact resistance to p-GaAs. The versatile applicability of Ru contacts makes them extremely important for future use in devices such as heterojunction bipolar transistors and solid state lasers.

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THE INFLUENCE OF DEPOSITION PARAMETERS ON THE ELECTRICAL PROPERTIES OF INDIUM OXIDE THIN FILMS PREPARED BY AN ULTRASONIC SPRAY CVD PROCESS

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In the present study we have investigated the electrical properties of indium oxide thin films prepared by an ultrasonic spray CVD process. Using an ultrasonic exciation (824kHz, 40W) and a carrier gas (N2) an aerosol containing the precursors of the films ($InCl_3 \times 4H_2O$) was generated and transported to the reaction zone. Films were deposited on glass substrate heated at temperatures ranged between 623 and 773 K. XRD studies showed that films are polycrystalline in nature and the micrographs, obtained by SEM of some typical films, demonstrate that film deposition was homogenous. A minimum resistivity of 6×10^{-3} Wcm and optical transmission >85% for typical In_2O_3 films 1600 Å thick were achieved. The electrical resistivity behavior during many cycles of heating-cooling was investigated for films deposited at different temperatures. Were established the conditions in which the films electrical conductivity could be improved.

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STUDY OF HETEROGENEOUS SYSTEMS BASED ON MOLECULAR SIEVES OF MeMCM-41 TYPE

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Heterogeneous systems, formed by inclusion of different organic fillers into the inorganic porous matrices, are characterized by non-additive combination of physical and chemical properties of their components. One reason of such behaviour is the interaction between filler molecules and active centers located on the channel surface of these matrices, and investigations of processes in these systems are found to be very interesting.

We have carried out IR spectroscopic and calorimetric studies of heterogeneous systems based on molecular sieves (Si,Al-MCM-41 type, channel diameter4 nm) and the same sieves modified by bivalent metal ions (Mn, Co, Ni, Fe, Cu, Zn) filled with 4-alkyl-4'-cyanobiphenyles (nCB, n=2-9). Changes in IR spectra originate from interaction of adsorbed molecules with active centers of the channel surface, namely Al(Si)-OH groups (of H-bonding type) and cations (of coordination type). Also relatively strong changes have been observed when these samples were heated up to temperatures of about 200 C, which assigned to the dehydration of MCM channel surface. The dependency of this process on the type of cation used has been found.

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RADIATION-STRUCTURAL TRANSFORMATIONS IN VITREOUS LAYERED AND CROSS-LINKED SEMICONDUCTORS

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Chalcogenide vitreous semiconductors (ChVS) are intensively studied in last years owing to their wide application in optoelectronics and dosimetry of ionizing irradiation. However, the microstructural model for radiation-induced effects is developed only for simplest and binary ChVS compositions.

In the present report, an attempt to develop the coordination defects (CD) formation model for γ-induced (^{60}Co source) structural transformations was made at the example of structurally complicated ChVS of As-Ge-S system. These disordered objects possess the mixed layered and cross-linked structural types in dependence on their composition.

It was shown that fundamental optical absorption edge of all investigated ChVS shifted towards lower photon energies after γ-radiation treatment. The topological schemes of the CD formation were proposed, taking into account results obtained by IR Fourier spectroscopy method of additional reflectivity in 400-200 cm^{-1} range.

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COMPARISON OF THE OPTICAL PROPERTIES AND MECHANICAL – ELECTRICAL DEGRADATION OF SOME PE, PP BASED POLYMER COMPOSITES

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There has been increasing interest in preparing polymers that possess high optical stability and good mechanical properties. In this study the optical properties of low-density polyethylene-LDPE/fiber (10-50% PPfiber); polypropylene-PP/fiber (10-50% PPfiber) and LDPE/diamond (0.3-3% diamond) composites which are prepared by hot pressing method, with the thicknesses of 57-70 μm are compared with their mechanical and electrical degradation properties. UV-Visible spectra in the wavelength range 200-2500 nm are examined. Optical absorption spectra and Tauc graphs are presented. Determined values of optical energy gaps (E_d , E_i , ΔE) ultraviolet transmittance (T_{uv}) are listed.The direct E_d and indirect E_i values are in the range of 3 – 3.14 eV and 1.52 - 2.9 eV respectively for organic composites.

The electrical strength (E) and the mechanical stress (σ) have been investigated and the graphs (the dependence of the durability $\log\hat{o}_E$ on E) are given.The experimental results are analysed related to the validity of the thermofluctuation theory.

Intensive absorption bands with double peak are observed in the range of 200-500nm for 20% fiber and 3% diamond additives.Durability (ô) and E ($\hat{o}_ó$=1.2x10^8 - 1.5x10^{12} sec; $\hat{o}_E$=3.5x10^3 - 7.2x10^4 sec ; E=80 - 86x10^6 Vm^{-1}) pass through the maximum and structure-sensitive parameters [÷=0.30-0.65x10^{-6} (kJ)Vm^{-1}/mole; ã=0.88-1.42 (kJ)MPa/mole] through the minimum for the same amount of additives, showing that the composites are more stable and homogenious.

The results indicate that the organic additive, forming polymer-polymer composite play a filler role and also change supramolecular formations (SMF). The inorganic additive (diamond), give rise to significant changes in SMF and affect composites chemically, until it forms a monolayers at the boundaries of SMFs.

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THERMALLY STIMULATED CURRENTS AND THE GLASS TRANSITION

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The consequences of the glass transition for various macroscopic properties of a system can provide a simple means of detecting and characterizing this transition. It was noted by Sauer and his co-workers (Sauer B B and Avakian P, Polymer 33 (1992) 5128) that a sharp increase in the apparent activation energy of thermally stimulated currents, as detected by the thermal slicing technique, occurs at the glass transition temperature. In order to examine this effect and its possible causes, computer simulations were performed on a thermally activated version of the facilitated kinetic Ising model which we proposed recently (Halpern V and Bisquert J, J. Chem. Phys. 114 (2001) 9512), with the dipoles of molecules in the liquid-like A state changing their orientation much faster than those of molecules in the solid-like B state. The results of calculations on this model system show that the increased activation energy is associated with a rapid increase in the current when a small rise in the temperature enables molecules to switch rapidly from states B to A. The significance of these results will be discussed.

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ON MAGNETORESISTANCE OF ORGANIC LAYERED CONDUCTORS

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At low temperature and arbitrary orientation of a quantizing strong magnetic field H the asimpthotic behavior of magnetoresistance in organic layered conductors is analyzed. It is shown that when current flows along the normal to the layers n, the amplitude of Shubnikov - de Haase oscillations have sharp peaks as a function of the angle between the vectors n and H. Value and position of these peaks are sensitive to the form of quasi-two-dimensional electron energy spectrum. We consider also the galvanomagnetic phenomena in layered conductors whose Fermi surface consists of a Q2D cavity and Q1D cavity. The experimental investigation of the magnetoresistance in these conductors open up the possibilities of studying in detail the energy spectrum and relaxation properties of charge carriers.

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P1 – 80 – C

ENERGY TRANSFER AND MIGRATION IN LIGHT-EMITTING POLYMER SYSTEMS

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Polymer blend systems have become increasingly attractive as active layers in organic light emitting diodes, as they exhibit several advantages over single polymer layers. Improved device luminescence may be achieved by balancing electron and hole injection by using polymers with different electrical properties. Efficient Förster transfer from the host polymer to the guest effectively red-shifts the fluorescence emission, reducing self-absorption losses.

We have investigated the effect of guest-host separation and temperature on the rate of Förster transfer and energy migration between two commercially important fluorescent polymers, namely poly(9,9-dioctylfluorene) (F8) and poly(9,9-dioctylfluorene-co-benzothiadiazole) (BT). We find that increasing the average distance between guest (BT) and host (F8) molecules results in a reduced transfer rate, attributed to the decrease in strength of the dipole-dipole interaction. Reducing the temperature has no effect on Förster transfer, but does reduce the energy migration rate.

The Förster radius, defined as the distance between molecules at which excitations are as likely to undergo Förster transfer as decay via any other route, is still a subject of some debate in these systems. Calculations of this distance from spectral overlap data suggests that in a blend of F8 and BT the Förster radius is approximately 5nm. Here we present experimental data from picosecond time-resolved studies on two such systems.

Simple blends of varying concentrations from 50% to 0.01% BT were prepared by spin-coating from solution. The excitation dynamics of the host were observed over a range of temperatures, and were found to exhibit both Förster transfer and, in the case of lower guest concentration blends, energy migration [1].

More complex layered structures were then fabricated by first spin-coating F8 onto a substrate, then depositing an optically inert spacer layer via the Langmuir-Blodgett technique. Finally, BT was spin-coated onto a second substrate and transferred on top of the spacer layer using a water floating technique, to form a sandwich type structure. By varying the number of monolayers in the inert spacer, control over the Förster transfer mechanism was achieved (without affecting energy migration in the F8), and the Förster radius calculated.

[1] A. R. Buckley, M. D. Rahn, J. Hill, J. Cabanillas-Gonzalez, A. M. Fox, D. D. C. Bradley, Chem. Phys. Lett. 339, 331-336 (2001)

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P1 – 81 – C

ELECTRONIC STRUCTURE OF PERFECT AND DEFECTIVE LEAD TUNGSTATE CRYSTALS $PBWO_4$

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Well known scintillator, lead tungstate $PbWO_4$ is assumed to be the working scintillation material for Large Hadron Collider device at CERN. While it's lumenescent features are well studied experimentally, the origin the lumenescence in $PbWO_4$ remains to be the subject of discussion. For successful clarification of lead tungstate luminescence centers the electronic structure calculations are necessary. In order to investigate the interplay between cationic (Pb ions) and anionic (WO_4 molecular anions), that possibly takes place during the photolumenescence processes in a perfect $PbWO_4$ crystal, we specificate the electronic structure of complex lumenescent center $Pb•WO_4$ surrounded by several decades of the nearest formula units of $PbWO_4$. For this purpose we calculate by *ab-initio* RHF method [1] the electronic structure of several $PbWO_4$ molecular clusters with different amount of atoms.

In order to explain the lumenescent properties $PbWO_4$ crystal with oxygen vacancies and molybdenum impurities we carried out the calculations for the same set of clusters, in which V_o and W substitution by Mo were modelled. Comparing density of states (DOS), partial DOS and interband DOS calculated for perfect and defective clusters and analysing the electronic density spatial distributions we determined the influence of these defects on the character of interband optical transitions.

1. M. W. Schmidt, K. K. Baldridge, J. A. Boatz, et. al. *J. Comput. Chem.*, 14 (1993) 1347-1363

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P1 – 82 – C

COMBINED MICROWAVE AND ACCELERATED ELECTRON BEAM IRRADIATION FOR APPLIED PHYSICS

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A new method based on microwave energy addition to accelerated electron beam energy for material processing was developed. In order to investigate this method, several special designed facilities which permit simultaneous microwave and electron beam irradiation were carried out. These facilities and the associated microwave and electron beam injection systems are described. The main idea of this paper was to combine the effects of both electron beam irradiation and microwave heating in order to provide new approaches for applied physics. This idea was suggested by the observation that both, accelerated electron beams and microwaves, in their separate passage through matter, produce by different physical action principles, the same final effects, such as: polymerization of monomer/oligomer systems, crosslinking, grafting and degradation of polymers, degradation of pollutants in air or water, food preservation, sterilization of medical supplies etc. The examination of this aspect suggests that by combining the ionization effects of accelerated electron beam and heating effect of microwaves it could be possible to obtain new and promising results in the material-processing field.

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THE CUMULANT METHOD FOR CALCULATION OF IMPLANTED IONS DISTRIBUTION

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The new efficient theoretical method of finding a spatial distribution function of implanted ions has been developed. This method is based on describing distribution function by using cumulants, instead of moments, which are used in usual theoretical methods . This lets obtain several great advantages of the cumulant method in comparison to usual methods.

The main application of the cumulant method is in calculations of particle distributions for any ion-target combination and for a wide range of initial energy of particles (1 kEV- 1 gEV). Calculations are precise within the whole energy interval, while usual methods loose accuracy at the definite interval, which depends on ion-target combination. Relative to statistical methods, the cumulant method allows for precise calculations two orders of magnitude faster than statistical methods.

The future development of the cumulant method is probable as its advantages lend themselves for use in nano-tubes and nano-electronics technologies. In addition, this more detailed investigation of the distribution function may reveal new mechanisms of atom scattering and interactions within solids.

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EFFECT OF CARBON MONOXIDE ON PTCR CERAMICS

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Semiconducting Y-doped $BaTiO_3$ ceramics were prepared by the conventional ceramics technology. These ceramics have got PTCR effect. The values of the temperatures giving the maximum resistivity are discretly situated between 60 and 95ºC. The effect of the carbon monoxide gas on the resistivity of Y-doped $BaTiO_3$ ceramics is studied. The potential utilisation of these ceramics as CO sensor in concentration less than 1% is discussed.

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P1 – 85 – C

STUDIES ON THE ELECTRONIC TRANSPORT AND OPTICAL PROPRIETIES OF F DOPED SNO_2 THIN FILMS

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Flourine doped tin oxide thin films (d=0.10-1.50 μm) were deposited onto glass substrates by spray pyrolysis. Substrate temperature ranged between 625 K and 775 K. The film structure was analysed X-ray and scanning electron microscopy. The obtained films are polycrystalline and have a tetragonal structure.

The spectral dependences of the absorption coefficient were calculate (in visible and near infrared range) from transmission and reflection spectra. The values of band gap energy determined from absorption spectra ranged between 3.30 and 3.70 eV. The temperature dependence of the electrical conductivity was studied using surface-type cells and static electric films with intensity lower then 102 V/cm.

The influence of the flour concentration on the optical and electrical properties of SnO_2 films is also discussed.

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SIMPLE APPARATUS FOR MEASURING SPECIFIC HEAT BETWEEN 5 K AND 20 K

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The measuring system for adiabatic specific heat measurements of potential thermal regeneration materials between 5 K and 20 K was designed. The sample is mounted on a thin film resistance temperature sensor which is weakly coupled to a copper thermal shield. The temperature sensor measures the temperature of the sample and is also used as a sample holder and a sample heater. Resistance of the sensor is measured in a four-lead configuration using a current reference and analog to digital voltage converter. Thermal shield temperature is monitored by a second temperature sensor, attached to the shield. An electric heater is used to control the temperature of the thermal shield. The apparatus is enclosed in a vacuum chamber which is immersed in a liquid helium bath. Shorter cool-down time is achieved using a thermal switch. The switch thermally couples the copper thermal shield with a cold vacuum chamber wall during the cool-down.

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MODELING OF HEAT SOURCES IN NIS JUNCTIONS

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The most significant heat sources which decrease the cooling capability of the NIS junction based Peltier refrigerator in temperature region of few tenths of K are:
a) heating by the formation of Cooper pairs in the superconductor part of the junction,
b) heating by the back tunneling of quasi-particles,
c) heating by the sub-gap current: this contribution can be described by the dynamic resistance obtained from measurements.

These three contributions quantify heat sources and appear in two equations describing the net heat flows into the electron and the phonon system in the normal metal part of the voltage biased NIS junction. Therefore, the coupled system of two equations can be formulated with two free parameters. By fitting the model to the measured data the heating contribution of back tunneling and of Cooper pair formation can be determined separately.

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THE INVESTIGATION OF NUCLEUS AND ELECTRONIC SPIN SUBSYSTEMS OF PARAMAGNETIC COMPLEXES Cr(V) USING FOR ACHIEVEMENT OF THE HIGH NUCLEAR POLARIZATION

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In this work the investigation of chromium (V) complex solutions in propanediol such as EHBACr(V), HMBACr(V) and its deuterium analog using as the polarized nuclear targets is presented. In this substances dynamic nuclear polarization (DNP) method is used for achievement of the high nuclear polarization.

The following measurements were carried out, namely: electron spin resonance (ESR) and transition processes in the nuclear subsystem under DNP conditions. We have measured the following parameters of these substances: both g-factor components and the nuclear spin-lattice relaxation time. The studies were performed on the spectrometer-relaxometer in the temperature range 1.7-4.2 K, ESR frequencies were 123-135 GHz.

Nuclear relaxation spin-lattice relaxation time in EHBACr(V) complex is higher by 20 % than that in HMBACr(V). This fact explains that EHBACr(V) complex is more effective one as the PNT substance. Such effects as the non-monotone relaxation process and the dependence of the free spin-lattice relaxation time on nuclear polarization taking place until the start of the transition process were revealed. Theoretical models describing these effects are discussed.

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A NEW APPROACH TO THE RADIATION-INDUCED PHENOMENA IN AMORPHOUS CHALCOGENIDE SEMICONDUCTORS

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There are different approaches to the explanation of induced phenomena in amorphous chalcogenide systems (AChS). The approaches, based on the metallization and the redistribution of chemical bonds as well as the free volume concept, have already been used. The last has been successfully applied in interpretation of the photoinduced phenomena in AChS. According to this concept, for explanation of the photoinduced phenomena in AChS, the parameter of free volume that includes atomic compactness of the structure and concentration of heteropolar bonds has been proposed.

The analysis of radiation-induced phenomena, stimulated by gamma-quanta (1.25 MeV energy, 3 MGy dose) in Ge-Sb-S AChS demonstrated that the concept of free volume is the most adequate and applicable one for interpretation of these phenomena. In this work a new approach based upon the concept of free volume, where the parameter of free volume includes atomic compactness and concentration only of such chemical bonds that facilitate the occurrence of radiation-induced changes, has been proposed. In order to identify these bonds a new model of radiation-induced chemical bonds redistribution has been created.

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P1 – 90 – C

ELECTRICAL PROPERTIES OF $Li_{1+x+y}Sc_xY_yTi_{2-x-y}(PO_4)_3$ (WHERE X=0.2, 0.25, 0.3; Y=0.01, 0.02, 0.03) CERAMICS

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The development of lithium-ion batteries and CO_2 gas sensors stimulates the development of solid lithium ion conductors with high ionic conductivity and low activation energy. It has been already reported that the conductivity of $LiTi_2(PO_4)_3$ increases appreciably if Ti^{4+} in the phosphate is partially substituted by a larger cation such as Sc, Y, Al, Fe. In this paper compounds of the $Li_{1+x+y}Sc_xY_yTi_{2-x-y}(PO_4)_3$ system are prepared and their structure parameters, ionic conductivity and electric permittivity at high frequencies and in the temperature range 300-600 K are investigated.

The powders of $Li_{1+x+y}Sc_xY_yTi_{2-x-y}(PO_4)_3$ (where x=0.2, 0.25, 0.3; y=0.01, 0.02, 0.03) compounds were prepared by solid state reaction. The structure parameters were obtained using diffraction of $CuK_{\alpha 1}$ radiation from the powder. The ceramic samples were sintered for the investigation of electrical properties.

Two relaxation dispersions related to the fast Li^+ ion transport in bulk and grain boundaries of the ceramic samples were found. The changes of x and y factors in the $Li_{1+x+y}Sc_xY_yTi_{2-x-y}(PO_4)_3$ system leads to the changes of the values of ionic conductivity, their activation energy, electric permittivity and relaxation frequency of relaxation processes caused by ionic transport in the compounds. The values of the activation energy of the bulk ionic conductivity (σ_b) and relaxation frequency (f_b) in the bulk were found to be very similar in all investigated materials. That can be attributed to the fact, that the temperature dependences of σ_b are caused only by the mobility of the fast Li^+ ions, while a number of charge carriers remains constant with temperature.

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P1 – 91 – C

HIGH-TEMPERATURE STIMULATED EMISSION IN HOMOEPITAXIAL GAN

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III-nitride semiconductor compounds attract considerable attention as potential ultraviolet light emitters. Short-wavelength emission of GaN-based lasers enables fluorescence chemical sensing, ultra-high-density optical storage systems, high-resolution printing, undersea optical communications, and high-efficiency lighting. Further development of III-nitride-based lasers requires deeper understanding of basic phenomena responsible for stimulated emission in GaN. From both fundamental and practical points of view, it is important to reveal contribution of excitonic effects on stimulated emission at elevated temperatures.

We report on mechanisms of stimulated emission in homoepitaxial GaN layers grown by using MOCVD technique. Stimulated emission was studied in a wide range of temperatures (8–600 K) by measuring spectra of luminescence from a photoexcited stripe in a lateral geometry. Application of both quasi-resonant (3.50 eV) and non-resonant (4.66 eV) photoexcitation enabled us to distinguish between the effects caused by carrier temperature and carrier density.

The emission spectra consisted of two bands: a shorter-wavelength band with a lower threshold and a longer-wavelength band with a higher threshold. The width and peak position of the shorter-wavelength band were found to weakly depend on the carrier density, whereas the band broadens and redshifts with increasing temperature. This is consistent with the model of inelastic exciton–exciton interaction and gives clear spectroscopic evidence in favour of excitonic origin of stimulated emission in the entire temperature range. Meanwhile, the longer-wavelength band broadened and redshifted with increasing both the carrier density and temperature. This behaviour is typical of electron–hole plasma (EHP). It is worth noting that the excitonic band persisted up to the highest pump intensities used. We attribute the coexistence of two emission mechanisms to a spatial separation of EHP and excitons. With increasing of photoexcitation intensity, EHP is formed at the very surface of the photoexcited layer, whereas dense exciton system persists deeper in the sample.

In conclusion, we demonstrate that both electron–hole plasma and inelastic exciton collisions are the intrinsic mechanisms of stimulated emission in homoepitaxial GaN even above the room temperature. Our results indicate that the high quality of homoepitaxial GaN layers facilitates longer exciton lifetimes and enables the coexistence of two gain mechanisms.

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INSTABILITY OF OXYGEN VACANCY ORDERING AT METAL-INSULATOR TRANSITION IN IRON DOPED $TbBaCo_2O_{5.5}$ LAYERED PEROVSKITE

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Transition metal oxides are known to exhibit a wide variety of the electrical properties from profound insulator up to metal. Some of the oxide compounds show a temperature induced first order metal - insulator transition (MIT). Among different oxide compounds exhibiting MIT one can distinguish $RBaCo_2O_{5.5}$ (R - rare earth ions) layered - type perovskites which are insulators below $T_{IM} \sim 350$ K and metals above this temperature. These oxygen deficient perovskites have been obtained recently and attracted attention of many investigators in the field of materials research. However, in spite of considerable efforts the nature of the MIT in these compounds is still matter of discussion. In present work the metal-insulator transition has been investigated by Mössbauer spectroscopy method in the $TbBaCo_{1.92}Fe_{0.08}O_{5+\delta}$ perovskite. It was found that the Fe^{3+} ions have two different positions in the low temperature insulator phase (at $T < T_{MI}$) and predominantly one position in the high temperature metallic area above $T_{MI.}$ X-ray diffraction experiment has revealed an orthorhombic - tetragonal crystal structure transformation taking place at T_{MI}. These results have been interpreted in favour of an oxygen vacancies order - disorder transition that occurs simultaneously with metal - insulator one. Thus according to the obtained results the high temperature metallic phase for the $TbBaCo_{1.92}Fe_{0.08}O_{5+\delta}$ is characterized by the tetragonal symmetry with disordered oxygen vacancies in the $[TbO_\delta]$ layer. Therefore one can conclude that the oxygen vacancy ordering does not play key role in the formation of the metallic properties of $RBaCo_2O_{5.5}$ perovskites. Most of works devoted to the investigation of the MIT in the $RBaCo_2O_{5.5}$ agree that given transition is induced by the spin state transition of Co^{3+} ions. The sharp increase of the effective paramagnetic moment at T_{MI} is the satisfactory argument in favour of this assumption. However, two nonequivalent positions of cobalt ions (octahedral and square pyramidal) in the $RBaCo_2O_{5.5}$ lattice (above/below T_{MI}) and three possible spin states of Co^3 ions (LS-low, IS-intermediate and HS-high spin states) give a wide field for speculation. Thus, according to one authors all cobalt ions adopt IS state below T_{MI} and corresponding HS and IS ones in the octahedral and pyramidal coordination above T_{MI}. Another electronic transformation: LS→IS for cobalt in the octahedral position has been also proposed in several works. Recently the $RBaCo_2O_5$ compounds containing all cobalt ions within square pyramids have been investigated by neutron diffraction method, and it was found that Co^{3+} adopts the HS configuration. We suggest the scenario of the MIT involving the IS→HS state transition for cobalt ions with octahedral environment and invariance of HS state for cobalt in the pyramids. In this model the high temperature metallic phase contains all cobalt ions in the uniform spin state which is more probable since there is only one position for cobalt ions above T_{MI} in the $TbBaCo_{1.92}Fe_{0.08}O_{5+\delta}$.

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QUANTUM OSCILLATIONS OF THE IMPEDANCE OF LAYERED CONDUCTORS IN A STRONG MAGNETIC FIELD

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Oscillatory dependence of the impedance of organic conductor with the Q2D electron energy spectrum on an external strong magnetic field, is studied. In the presence of an elastic impurity the high temperature oscillations (HTO), arising from the interference of the oscillations, whose period is related to the extremal cross sections of the Fermi surface, are predicted. The temperature of damping for these oscillations is expected to be much higher than that for the de Haas - van Alphen oscillations. The HTO are conditioned by the elastic character of scattering of charge carriers and connected with a small difference between cyclotron masses at external cross sections of the Fermi surface.

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MODEL STUDIES IN ION-INDUCED NUCLEATION

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A new model for ion-induced nucleation and charged aerosol dynamics is presented. The model includes ion-induced nucleation, coagulation, ion attachment and condensation with Coulomb interactions. According to the first results, ion-induced nucleation is found to be able to produce considerable amount of new particles if the pre-existing particle concentration is sufficiently low.

In some simulated conditions the agreement with observed particle formation events in boreal forest environment was achieved. According to results, in certain situations ion-induced nucleation is able to change the charge distribution of the particles which may allow the observation of ion--induced nucleation in the atmospheric conditions.

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THE INFLUENCE OF THE SELF-ORGANIZATION NANO-SIZE STRUCTURES ON THE ELECTRON FIELD-EMISSION

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One of the most promision application of field emission phenomena is ultra high frequency oscillations generation. Enhancement and anomalous properties of the field emission (so named cold electron emission) for quantum-size structures (layered structures, quantum dots and Gunn effect structures.) have been predicted in our publications early. The current-voltage characteristics with oscillations of emission current were observed also at emission from $Si_{1-x}Ge_x$ quantum dots and from GaN microrafless layer on sapphire. These different types of emitters have quite similar emission characteristics. Possible reason of such oscillations can be connected with ultra small size of tips at the surface: the radius curvature of tip's top is about 2 nm and tip height is ≈10 nm. In this case the electron emission of separate electron from tip can influence on local electric field due to small number of electron in tip volume. Another possible explanation is based on quantum-size effect phenomena in ultrathin tips, which have high resistance. Separate electron levels allow to realize resonance tunneling mechanism.

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MAGNETOSTRICTION OF $Eu_{1+x}(Ba_{1-y}R_y)_{2-x}Cu_3O_{7-d}$ AT SUPERCONDUCTING TRANSITION

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The cryogenic X-ray studies of structure deformations in the vicinity of superconducting transitions in structural series of $Eu_{1+x}(Ba_{1-y}R_y)_{2-x}Cu_3O_{7-d}$ was performed. As superconducting transition is the second order phase transition, the accompanying strains may be considered as spontaneous striction and attributed to the pressure dependence of the superconducting transition temperature TSN. Though the pressure effect on TSN in $RBa_2Cu_3O_{7-d}$ series proved to be important insight into major properties of the high temperature superconductors, it is not understood by now. The performed investigation of temperature effect on position and shape of diffraction maxima at cooling below TSN of the samples with the different radii of the Rare Earth ions allowed us to find spontaneous magnetostriction in these compounds, estimate pressure derivative of TSN and make comparison with existing models. The proposed experimental procedure enabled us recently to find out the magnetostrictive deformations in the CMR (colossal magnetoresistance) compounds with perovskitelike structure similar to that of the materials under current study.

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CONCENTRATION FLUCTUATIONS IN BINARY LIQUID METAL ALLOYS

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The study of the Bhatia-Thornton [1] structure factor "concentration – concentration"; for binary alloys in the long-wavelength limit, is topical, since the structure factor dependency on alloy composition is connected with tendencies for phase separation or strong association in system.

We theoretically investigate for Na-K, Na-Cs, Na-Rb, K-Rb, K-Cs and Rb-Cs systems at T=373K. For this aim, the local Animalu-Heine [2] model pseudopotential and variational method of the thermodynamic perturbation theory are used. The exchange - correlation function is considered in the Vashishta - Singwi approximation. Earlier, this method was successfully used for thermodynamic studies of the systems under consideration [3]. In the most cases, good agreement of our results with experimental data and other theoretical results is achieved.

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MAGNETIC BEHAVIOR OF $HoNi_{5-x}Al_x$ SYSTEM WITH x £1.5

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The $HoNi_{5-x}Al_x$ compounds crystallize in a $CaCu_5$-type structure for x 1.5. Magnetic measurements were made in temperature range 4.2 – 300 K and fields up to 9 T. The Curie temperatures decrease from T_C = 12 K (x = 0) up to 5 K (x = 1.5). The saturation moments per formula units extrapolated at 0 K are ~ 9.2 μ_B which show negligible crystal field effects. In the paramagnetic range, at T 80 K, linear variations of reciprocal susceptibilities as function of temperature are evidenced. The Curie constants are greater than those expected for Ho^{3+} free ion suggesting the presence of additional contribution from nickel atoms. According to addition law of susceptibilities we determined the contributions of nickel atoms to Curie constants, the effective nickel moments, M_{eff}(Ni) respectively. The M_{eff}(Ni) values decrease from 2.25 μ_B (x = 0) up to 1.05 μ_B (x = 1.5) suggesting a strong hybridization of Ni3d and Al3p states.

Band structure calculation on $HoNi_{5-x}Al_x$ show that the nickel moments at 0 K are 0.160 μ_B for 2c and 0.242 μ_B for 3g sites antiparallely oriented to holmium moment. The Ho5d band polarization is $M_{5d} \cong 0.150$ μ_B/atom parallel to holmium moment. The total contribution of Ni atoms to the magnetization, at 0 K, is smaller than 9 % from that of holmium; the magnetic behavior of $HoNi_5$ is mainly determined by the rare-earth. When replacing Ni by Al the nickel magnetic contributions decrease and are near nil for a composition x = 1.5. Thus, as function of aluminium content, there is a transition from a ferrimagnetic to ferromagnetic type ordering.

The magnetic behavior of nickel which show a very weak or nil magnetic moment at 0 K and well defined values in the high temperature range is analyzed in spin fluctuation model. This model uses the concept of temperature induced moments. The average amplitude of spin fluctuations increases with temperature and reaches an upper limit determined by charge neutrality condition at a temperature T* ≅ 80 K. For T > T* a Curie-Weiss behavior is shown, similar as in a system having local moments. The moments in this case are localized in q-space.

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APPLICATION OF ION BEAM TECHNIQUES TO STUDY THE OXYGENATION OF YBaCuO THIN FILMS

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The physical properties of YBCO compound are very sensitive to the amount and the order of the oxygen atoms in the crystal lattice. In this way, $Y_1Ba_2Cu_3O_6$ is an antiferromagnetic insulating, whereas $Y_1Ba_2Cu_3O_7$ is a high temperature superconductor. $Y_1Ba_2Cu_3O_{7-x}$ thin films were grown “in situ”by cathodic sputtering on $LaAlO_3$ single crystal substrates. The $^{16}O(á,á)^{16}O$ resonance at 3.045 MeV was applied to determine the oxygen content and its depth distribution. High energy RBS was used to measure the cationic composition of the samples. Oxidation potential of the oxygen plasma at low temperatures was studied by using these ion beam analytical techniques and the results will be presented.

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PHOTOINDUCED CAPACITANCE EFFECTS IN POLYCYCLIC 4-NITRO-4'AMINODYPHENILE

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The investigation of the light exposure influence on the charge generation processes is the actual problem in the physics of organic materials.

Photocapacitance properties of organic semiconductor 4-nitro-4'-aminodyphenile thin films were studied under photoexitation in 340-1000 nm wavelength range.

It was established that photocapacitance value depends on the light intensity, its wavelength, duration of photoexposure t and temperature. The regularities of photocapacitance kinetics under illumination and without it were determined at different t values. The photocapacitance memory effect after switching off the illumination is observed at the high t values due to photopolarization effect occurance.

It was shown that photocapacitance maxima coincided with the position of photoconductance and photopolarization peaks on the proper spectral dependencies. It must be mentioned that the photopolarization phenomenon complicated the determination of photocapacitance parameters.

The mechanism of photocopacitance formation taking into account the photopolarization effect was proposed.

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RUTHERFORD BACKSCATTERING ANALYSIS OF ROUGHNESS IN TiAlN/Mo MULTILAYERS WITH ARTIFICIAL NEURAL NETWORKS

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Multilayered $Ti_{0.4}Al_{0.6}N$/Mo coatings deposited on Si. The thickness of individual layers is between 1 and 5 nm. A strengthening effect can be obtained by using alternate layers of materials with high and low elastic constantsThis behaviour requires a multilayer periodicity below a certain value in order to reduce dislocation motion across layer interface. Below this critical period, in most cases the hardness decreases as the period decreases. The multiple interfaces have an important role on this behaviour, working as stress relaxation areas and preventing crack propagation, influencing the mechanical properties of the system.

Understanding the origin of these effects requires knowledge of the interface structure, where the interfacial roughness is of prime importance. TEM and AFM results shown roughness in the nm scale. We used Rutherford backscattering (RBS) to study roughness in a quantitative way, and developed an artificial neural network (ANN) algorithm dedicated to the analysis of the RBS data. The results compare very well with the microscopy data.

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ELECTRICAL, OPTICAL AND ELECTROCHEMICAL PROPERTIES OF NAPHTHALENE SULPHONIC DOPED POLYPYRROLE

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Polypyrrole (Ppy) is one of the most attractive conducting polymers because of its high conductivity, good environmental stability and a large variety of potential technological application.

Recently soluble Ppy has been prepared by chemical polymerization of pyrrole (Py) monomer in the presence of β-naphthalene sulphonic acid (NSA) as a dopant.

The purpose of this article is to study the correlation between the synthesis conditions and the electrical, optical and structural properties of the soluble naphthalene sulphonic (NS) doped Ppy.

It is very interesting to find that the morphology of Ppy(NS) synthesized by the in situ doping polymerization of Py exhibits a fibrilar morphology. SEM images proved that tubular Ppy(NS) could be synthesized by this method.

The structure of Ppy(NS) is strongly influenced by the concentration of NS doping ions, the oxidant ands solvent nature.

The behavior of the electrical conductivity for Ppy(NS) in the temperature range 5-300 K was investigated. The main conducting mechanism is very able range hopping. The typical value of the electrical conductivity is 5 S/cm.

The particularities of the molecular and electronic structure of Ppy(NS) were investigated by FTIR and UV-VIS spectroscopy.

Moreover, we were focus on the investigation of metal-Ppy(NS) interaction. Metal ions like Au(I), Ag(I), Cu(II) and Pb(II) were chosen for study because of their possible affinity to Ppy(NS).

The scanning electron microscopy (SEM) and cyclic voltametry (CV) studies demonstrated that the metal-Ppy(NS) interaction may involve complex formation rather than ion absorption. This fact is also supported by the UV-VIS spectra of Ppy(NS) after the interaction with the metal ions.

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LATERAL INTERACTION AND Co ADLAYER STRUCTURES ON THE Pt(111) SURFACE

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We have revisited the structures for CO films adsorbed on the Pt(111) surface and simulate the diffraction patterns. In particular, we suggest alternative placement of the CO molecules in the unit cell of the c(4×2) structure for CO on Pt(111) at coverage 0.5. To correctly explain the LEED pattern, found from experiment at coverage 0.5, the cell ultimately should be asymmetric. This agrees with recent STM results for similar CO structures on Ni(111). Parameters of the lateral interaction, evaluated from the Monte Carlo simulations, are in excellent agreement with recent first-principle calculations. Formation of the stable CO adlayer structures on Pt(111) appears to be dominated by a superposition of the dipole-dipole and indirect interactions, which provide the attraction between the molecules at characteristic spacing. Trio interactions are also found to be important and may originate from characteristic pairs of molecules in adsorbtion sites of different types.

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DEPOSITION OF DOPED SNO_2 THIN FILMS FOR GAS SENSING APPLICATIONS

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With the increase of pollution that has been seen in our atmosphere, there is a need to develop gas sensors which are able to detect small traces of toxic gases, in a short period of time, this way reducing the danger of exposal. Therefore, there is in the Physic Department, at University of Minho, an research project in materials area whose goal is to develop thin films of tin oxide for gas resistive sensors devices. One of the Tin dioxide deposition techniques is reactive magnetron sputtering, which allows us to change some deposition parameters, as the oxygen flow, the magnetron power and the temperature, obtaining this way films with different structures and with different physical and sensitive properties. In some films, we have studied the doping influence, with iron or molybdenum in its sensitivity.

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ON THE ELECTRICAL AND OPTICAL PROPERTIES OF POLYCRYSTALLINE ZNSE THIN FILMS

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Zinc selenide (ZnSe) thin films (with thickness ranged between 0.15 μm and 1.20 μm) were deposited onto glass substrates by the quasi-closed volume technique under vacuum.

The film structure was studied by X-ray diffraction technique, scanning electron microscopy and atomic force microscopy. The investigations shown that films are polycrystalline and have a cubic (zinc blende) structure.

Some correlations between film structure and deposition conditions were established. The films with stable structure can be obtained if they, were submitted to a heat treatment, this consists of several succesive heating / cooling cycles within temperature range ÄT = 300-450K. The values of thermal activation energy of electrical conduction, calculated from temperature dependence of the electrical conductivity, ranged between 2.20 and 2.50 eV.

The spectral dependences of the absorption coefficient were calculated in the range 330 nm – 1260 nm from transmission spectra. The influence of heat treatment on the shape of the absorption spectra is studied for samples with different thinckness. After heat treatment absorption coefficient decreases for films with smaller thickness. This fact indicates an increase in crystallite size and a decrease of the concentrations of impurities and structure defects. The values of bandgap energy determined from absorbtion spectra ranged between 2.50 and 2.70 eV.

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IR SPECTRA OF SOME POLYMER BLENDS CONTAINING LIQUID CRYSTALLINE COMPONENT

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The IR characterization of some binary blends of cholesteryl palmitate (CP), which is a low molecular-weight liquid crystal with two isotropic *semi*crystalline polymers such as: poly(ethylene adipate) (PEA) (M_n=2000g/mol) and polytetrahydrofuran (PTHF) (M_n=2000g/mol) has been made. These blends have been prepared by solution casting. Two kinds of FT-IR experiments were performed: at room temperature and by heating up to 120^{o}C followed by cooling. The heating and cooling rate were of ~1^{o}C/min.

The experimental spectra of the blend recorded at room temperature have been compared with the calculated ones by aditivity rule supposing no interactions between the components of the blends. Some differences have been evidenced in 2700-3200 cm^{-1} and 1200-1600 cm^{-1} assigned to hydroxyl, ether and ester bonds. These could be due to either some interactions between components, to conformational changes or to the phase transitions. To clarify these aspects, supplementary information has been obtained by recording spectra during heating and plotting the dependence of integral absorbance of several characteristic bands on temperature.

Some blends exhibit a sudden increase of the absorbance at two temperatures of ~50^{o}C and ~72^{o}C, which correspond to the transitions found for the components of the blends, while other blends (mainly those at the extreme composition range) a continuous change of absorbance with temperature was observed.

Therefore, it was concluded that the components exhibit a poor miscibility at certain mixing ratios (middle composition range); this conclusion being in good accordance with DSC and optical microscopy results, previously presented [1]; the IR spectroscopy being a reliable method to determine transitions in systems containing liquid crystalline components.

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SINGULARITIES OF PHASE TRANSITION IN THE SILICON NANOCLUSTERS

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Using Stillinger-Weber potential we analyzed the peculiarities of silicon nanoclusters with atomic number Si_n (n=6,13,55).

The transition between configurations (the process of isomerization) is accompanied by the displacement of atoms in the new sites. The isomers of Si_8 represent the bipyramid with the covered face and dodecahedron; Si_{14}–is an icosahedron with capping atom over the face. One of peculiarities of cluster phase transition lies in the different bond energy for inner and outer cluster atoms. So the phase transition in the cluster occupies some area of temperatures. Atoms can exchange by their positions like the liquid. At the same time the inner atoms attached in the definite sites answer the crystal state. So, the phase transition doesn't connect with transition of definite atoms, but with peculiarities of atomic movement as a collective. For clusters with two coordinating shells the "quasi-melting"effect was noted. In that way the phase transition in the system of connected atoms one can explain as a result of non-linear oscillations on the modes changing the configurations for clusters, arranged from lattice atoms.

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EPR INVESTIGATIONS OF COLOSSAL MAGNETORESISTIVE PEROVSKITE $La_{2/3}Ca_{1/3}MnO_3$ DOPED WITH DIAMAGNETIC IONS

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The manganese perovskites have been widely studied since the discovery of colossal magnetoresistence (CMR) effects. EPR spectroscopy is a powerful tool to study the complex magnetic state in these materials [1].The linewidth in CMR manganites was considered to be caused by spin – lattice relaxation of the exchange coupled Mn^{4+} ions via Mn^{3+} JT – ions to the lattice under the condition of a strong relaxation bottleneck [2].

In this contribution, we have analyzed the effects of Mn- site substitution by diamagnetic ions on the spin dynamics in $La_{2/3}\ Ca_{1/3}\ Mn_{1-X}\ M_X\ O_3$ (M = Al, In, x 0.05) perovskite manganites. The temperature and x dependence of the resonance linewidth and EPR integral intensity have been investigated and discussed in terms of the bottlenecked spin relaxation and small polaron hopping model. In the paramagnetic regime, the exchange coupling integral, J , between Mn^{3+} and Mn^{4+} ions shows a decrease with increasing x. It could arises from weakening of the double - exchange interaction by M - doping which reduces the exchange field at the Mn–sites.The changes in J produced by the substitution of Mn with In are larger than those produced by the substitution with Al due to the larger ionic size of In^{3+}.

The activation energy, E_a , for the hopping motion of small polarons as function of x and M was also evaluated and compared with the results of other experiments.

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OXYGEN INFLUENCE ON THE ION BEAM SYNTHESIS OF HAFNIUM SILICIDES: HIERD AND RESONANT SCATTERING ANALYSIS

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Hafnium disilicide ($HfSi_2$) has one of the lowest resistivities and highest melting points among refractory silicides. Ion Beam Synthesis (IBS) techniques have been shown to promote $HfSi_2$ formation at lower temperatures and continuous stoichiometric layers have been prepared by channeled implantation [A.R.Ramos et al, Nucl. Instr. and Meth. B161-163 (2000) 909]. Hafnium is, however, a known oxygen getterer: hafnium oxide precipitates may prevent complete epitaxial regrowth [C.S. Chang et al, J. Appl. Phys. 61 (1987) 2393] and hinder the $HfSi_2$ layer's electrical properties.

We have studied the oxygen distribution behavior during the IBS of $HfSi_2$ by HIERD and oxygen Resonant Scattering. Czochralski and Float Zone silicon substrates were analysed. The low oxygen concentration results in low statistics, shadowing results. Therefore, $HfSi_2$ layers were prepared on oxygen pre-implanted samples and the oxygen redistribution resulting from Hf implantation studied. Results show no oxygen incorporation in the Hf implanted layer.

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MODEL CONCEPTS FOR THE GETTERING METAL IMPURITIES IN STRUCTURES BASED ON Si WITH DEVELOPED SURFACE

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Metal impurities in Si wafers are known to create deep levels in Si band gap. To remove them and to stimulate the decomposition of defect-impurity internal complexes a gettering was applied with a getter consisting of a chemically etched Si layer with developed surface. Al film was deposited on this layer by vacuum sputtering. The gettering anneals were carried out at the temperatures of 600-1100ºC.

To describe the mechanisms responsible for metal impurities removal the ability of described getter to extract copper, iron and gold atoms was studied for rapid thermal and furnace anneals. The recombination-active metal atoms were introduced by ion implantation or diffusion from the infinite source. The impurity distribution in wafers was measured by the mass-spectrometry of neutral atoms.

On annealed samples with getter essential increase of minority carriers lifetime was observed. Obtained results allow proposing the mechanisms for performance of described getter. One of the possible mechanisms may be the emission of vacancies from the gettering region, which stimulate Si interstitials flow to the getter and promote to the change of impurity precipitation kinetics in wafer bulk.

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SPIN PRECESSION OBSERVATION IN QUANTUM CORRECTIONS TO RESISTANCE OF $Si_{0.7}Ge_{0.3}$/ $Si_{0.2}Ge_{0.8}$ HETEROJUNCTION WITH TWO DIMENSIONAL HOLE GAS

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The two dimensional hole gas (2DHG) magnetoresistance of $Si_{0.7}Ge_{0.3}/Si_{0.2}Ge_{0.8}$ heterojunction in a wide range of temperatures T = 0.335K-20K, magnetic fields

–110 kOe < B < 110 kOe, and transport currents I = 100 nA - 50 ìA is measured. In the vicinity B = 0, the sharp and positive in sign feature on smooth negative magnetoresistance is observed at lowest temperatures. The amplitude of this feature quickly fades with temperature and transport current. For experimental data analysis the theory of weak localization for 2DHG is applied.

We use this analysis for extraction of following carrier relaxation times: *(i)* transport $t_{tr} = 1.45\times10^{-13}$ sec, *(ii)* inelastic $t_j = 4.5T^{-1}\times10^{-12}$ sec, and *(iii)* spin-orbit

$t_{SO} = 4.41\times10^{-12}$ sec. Nearly-zero-magnetic field position, positive sign and amplitude of observed magnetoresistance feature (MRF) allow one to connect its origin with spin splitting caused by spin-orbit interaction in a zero magnetic field. The values obtained t_{SO} and t_{tr} are used for the first time to define zero magnetic field splitting in the hole energy spectrum for a $Si_{0.7}Ge_{0.3}/Si_{0.2}Ge_{0.8}$ heterojunction: Δ=1.65 meV. The experimentally observed temperature and transport current MRF amplitude damping is in good agreement with quantitative estimations.

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ELASTIC STRAIN FORMATION AT Ge QUANTUM DOT HETEROSTRUCTURES IN Si(SiGe) MATRIX BY MBE

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MBE technological development essentially enlarge application prospect of new class materials based on solid solutions $Si_{1-x}Ge_x$ of different types and especially Ge quantum dot system in Si matrix or $Si_{1-x}Ge_x$. Elastic strain initiation in SiGe system determine zone structure of obtained sample and correspondingly its optical and electronic properties. Strain distribution homogeneity in layers predecessor to the active layer, i.e. the layer forming Ge quantum dot system, and also possibility of residual strain fixing within required bounds take on special significance in this case.

The main idea of the experiment lies in Si-substrate initial surface serial transformation to achieve a uniform and possibly regular distribution of deformation forces at the N-layer surface and therefore to create such conditions that island nucleation and formation happen actually simultaneously overall the substrate surface according to its relaxation mechanism.

Investigation data of island density and dimensional characteristics dependences on the number (N), thickness (d), Ge mole fraction (x) and growth rates (V_{Ge} and V_{Si}) of intermediate layers $Si_{1-x}Ge_x$ are given at the work proposed.

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THE STUDY OF MAGNETIC ANISOTROPY DISPERSION IN PARTICULATE MEDIA BY MAGNETIC GYROREMANENCE MEASUREMENTS

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The study of angular dependence of Gyroremanent Magnetization (GRM) on samples containing dispersed ãFe_2O_3 particle is made in a cartesian coordinates system associate of the sample.

Was used two types of samples: one consisting by rocks containing particles very dispersed in volume with a weak anisotropy and interaction field and another category of samples consisting by multiple layers of magnetic recording media that presents a higher interaction field and anisotropy.

The Fourier analysis of this angular dependence was compared with case of sin 2è function and was observed a closer dependence to sin 2è function for samples with weak interaction and anisotropy field.

Fourier analysis of experimental dates obtained give the possibility of determination of particle anisotropy dispersion and global anisotropy of the sample.

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INFLUENCE OF DIMENSIONALITY ON EXCITON CHARACTERISTICS IN LUMUNESCENT SEMICONDUCTOR STRUCTURES

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In this presentation the parameters of phonon-assisted transitions have been investigated in dependence on the dimensionality of semiconductor structures. Experimentally measured low-temperature photoluminescence spectra of GeS_xSe_{1-x} for different alloy compositions as well as resonantly exited spectra of oxidised porous silicon have been analysed. The effective medium theory has been used to calculate the dielectric constants of the structures. To calculate binding energy of the localised centre or exciton the Froelich-Hopfield relation has been used. Such parameters of phonon-assisted transitions as binding energy and Bohr radius of the localised centre or exciton as well as the electron-phonon coupling factor and phonon energy have been determined in adiabatic approach for different contents of sulphur/selenium in GeS_xSe_{1-x} alloy (different degree of two-dimensionality) as well as for oxidised porous silicon. Obtained results have been compared with results of calculations of these parameters by other methods. A new method for the estimation of geometrical characteristics of Si nanocrystals has been proposed basing on the determination of nanocrystals optical band gap.

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INVESTIGATION OF MAGNETIC FLUX GRADIENTS IN HARD SUPERCONDUCTORS

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Analytical calculations of the transverse magnetostriction in a thin hard superconductor are presented in relation to the distributions of currents and fields within a superconducting specimen in a varied magnetic field. The approach is successfully tested on high-temperature superconductors. The flux distribution derived from magnetostriction measurements is in satisfactory agreement with that obtained from computer processing of magnetooptical images. The magnetic flux distribution below the irreversibility line of hard superconductors is derived from both original magnetization and magnetostriction measurements and image processing. Perfect consistency of the results is obtained for a family of high-temperature superconductors ($La_{2-x}Sr_xCuO_4$, $Bi_2Sr_2CaCu_2O_x$, $YBa_2Cu_3O_{7-x}$).

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EFFECT OF BERRY'S PHASE ON THE CONDUCTION ELECTRONS g FACTOR IN Zn

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In metals, Berry's phase is nonzero when the electron orbit links to band-contacts lines of the metal. This result is closely analogous to the Aharonov-Bohm's effect provided the band-contact line plays the role of the infinitely thin “solenoid”with the fixed “magnetic flux. “When Berry's phase is nonzero, even a small spin-orbit interaction leads to an essential difference of the conduction electron g factor from its free electron value, g = 2. In other words, the electron g factor is determined not only by the strength of the spin-orbit coupling but also by the linkage of the semiclassical orbit with band-contacts lines. To clarify this point, we calculate and analyze the g factor in the framework of the three-band model of the electron spectrum which can describe the so-called needles around K in Zn. In hcp metals (Be, Mg, Zn, Cd) several band-contact lines are in the vicinity of the symmetry point K of the Brillouin zone. We show that in zinc Berry's phase effect on the electron g factor is comparable with the spin-orbit contribution to it. This provides possibility to detect the Berry's phase effect in Zn.

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INVESTIGATION OF PHASE TRANSFORMATIONS AND CHANGES OF ELECTROPHYSICAL PROPERTIES Ti/Si SYSTEMS BY TREATMENT WITH PLASMA OF ARC DISCHARGE

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In this work by using electron diffractography and Auger spectroscopy methods (an E ÌR-102 electron diffractograph and a PHI-660 scanning Auger spectrometer) we have studied phase transformations in a Ti-Si system irradiated with hydronitrogen and hydrocarbon plasma of arc discharge. Electrical and physical parameters of the Ti-Si contact depending on plasma treatment conditions have been determined by measuring current-voltage characteristics.

The results of studies show that the titanium films obtained are polycrystalline and fine-grained, with the average grain size of ~5-10 nm. When the Ti-Si system is exposed to hydronitrogen plasma at 500 °C, TiN and Ti_2N are formed on its surface. As treatment temperature is increased to 600 °C, the nitride phase having a small amount of nitrogen disappears, and a film of golden colour, consisting entirely of TiN, is formed on silicon. Further increasing of temperature to 700°C does not change phase composition at the surface of the Ti-Si system. At the metal-semiconductor interface $TiSi_2$ in modification C-54 is formed. Temperature-dependent changes in the phase composition of the titanium-silicon system under irradiation with hydronitrogen plasma proceed along the following scheme:

$$\text{Ti /Si} \xrightarrow{500\ ^\circ\text{C}} \text{TiN} + \text{Ti}_2\text{N/TiSi}_2\text{/Si} \xrightarrow{600\text{-}700\ ^\circ\text{C}} \text{TiN/TiSi}_2\text{/Si}$$

After processing of Ti-Si system in hydrocarbon plasma at 500 °C titanium carbide TiC is formed on its surface. Increasing of temperature to 600-700°C does not change phase composition at the surface of the Ti-Si system:

$$\text{Ti /Si} \xrightarrow{500\text{ -}700^\circ\text{C}} \text{TiC/TiSi}_2\text{/Si}$$

Phase transformations that occur in the Ti-Si system result in changes in the electrical and physical parameters of the contact as evidenced by forward-bias regions of the current-voltage characteristics measured on the starting and plasma-irradiated specimens. In our opinion, this is probably caused by formation of TiN or TiC on silicon and $TiSi_2$ at the metal-semiconductor interface.

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ELECTRO-OPTICAL EFFECTS IN THE IN-PLANE SWITCHING OF NEMATIC LIQUID CRYSTALS WITH THE STRONG DIRECTOR ANCHORING

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In the IPS mode an electric field is applied to the liquid crystals along the direction, which is parallel to the plane of the substrates with interdigital electrodes. The threshold behavior and response characteristics of the liquid crystals in the IPS mode were studied in assuming uniform electric field and strong director anchoring at the cell boundaries.

In this paper we calculated an electric field produced by interdigital electrodes in IPS-mode analytically and compare them with our numerical calculations. The results for the threshold voltage in our model and it dependence on the cell sickness and electrode gap are in the good agreement with the experimental data of Matsumoto (et. al). Also we proposed optimized cell geometry for the IPS mode that corresponds to the smallest threshold voltage.

Using the results for the electric field we found the director profile in our model for the nematic cell with the strong director anchoring.

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STUDY OF NUCLEIC ACIDS INTERECTION WITH CARBONACEOUS MATERIALS: SIERA DATA

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The interaction of DNA with carbon-based materials is of great scientific and applied interest. We studied the different structural forms of carbon - graphite and carbon nanotubes (CNT) - and its interactions with nucleic acids. It is important for application and fundamental knowledge, however until now it isn't very clear. We studied the interaction between denatured DNA and CNT by SEIRA spectroscopy. Due to using of gold substrate we observed the effect of SEIRA (Surface Enhanced Infra-Red Absorption) for nucleic acids.

We obtained changes in vibration modes of the marker bands of DNA that can be an evidence of interaction the DNA with CNT. Some transformation of H-bonds in the region of OH-, NH- and CH-vibrations was observed. Relative intensity of base vibrations is increased twice in a spectrum of DNA/CNT in comparison with reference DNA. The stretching asymmetrical phosphate bond shift from 1235 (A-form) to 1225 cm^{-1} (B-form), its intensity was increased by 20% and the halfwidth increased about 5 cm^{-1}. So, we could suppose that CNT causes A-B transition in some fragments of DNA sugar-phosphate backbone that can be in agreement with model of DNA wrapped around CNT.

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X-RAY STUDY OF $Nd_{1-x}A_xMnO_3$ (A=Sr, Ca) MANGANITE STRUCTURE ABOVE AND BELOW THE FERROMAGNETIC METAL – ANIFERROMAGNETIC INSULATOR SPONTENEOUS PHASE TRANSITION

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The crystal structure of the manganite $Nd_{1-x}A_xMnO_3$ (A=Sr, Ca) is studied at temperatures T=300 and 77,3 K by means of an X-ray diffractometer. It is shown that the transition from the ferromagnetic metallic state to the antiferromagnetic insulating charge-ordered state is accompanied by structure deformations. Lowering of the structure symmetry from orthorombic to monoclinic occurs in $Nd_{0.5}Sr_{0.5}MnO_3$. The space-group symmetry of the orthorombic and monoclinic phases is identified as Imma and P21/m, respectively. Twinning of the crystal and the formation of a twin domain structure with coherent boundaries in the (00l) crystallographic planes are found.

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NONDESTRUCTIVE TESTING OF FERROMAGNETIC CONSTRUCTION MATERIALS BY PERMEABILITY MEASUREMENT METHOD

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Despite the long history of investigation of the influence of composition and structure variations of ferromagnetic materials on their magnetic behavior, the question of application of magnetic hysteresis methods for purposes of nondestructive examination of ferromagnetic construction materials is still attracting broad attention of both researchers and industry. Appearance of modern computer-aided magnetic precision instruments gives a powerful incentive to development of this field. The possibility of an easy collection of large volumes of experimental data permits to obtain all the traditional magnetic hysteresis parameters (coercive field, remanent and saturation magnetizations, initial and maximum susceptibilities) as well as novel complex parameters (minor loop susceptibility matrix, Preisach-like matrix, etc.). Fast evaluation of the measured data allows optimization of the information they contain.

For these purposes a special device, able to magnetize samples by a triangular signal and to measure and record a picked-up signal proportional to differential permeability of the sample, was constructed and connected to a steering computer. The experimental data obtained contain detailed information on the magnetization process of the sample and all the magnetic parameters mentioned above.

At the moment investigation of dependence of characteristic parameters of magnetically closed construction steel samples on applied mechanical stress is carried on. The samples are measured in situ in an electromechanical loading machine within the range of both elastic and plastic deformation. Analysis of the magnetic variables of the deformed samples aims at finding the most sensitive and optimized parameters, which could be used for nondestructive magnetic testing of critically distorted materials. The investigation is supported by the Grant Agency of the Czech Republic (project No.101/02/0236) and the first results will be presented.

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MULTIELECTRON BUBBLES IN LIQUID HELIUM: VIBRATIONAL AND ELECTRONIC PROPERTIES

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When the surface density of a film of electrons on top of a liquid helium surface exceeds a critical value, the helium surface becomes unstable with respect to the formation of multielectron bubbles. These fascinating systems are cavities in the helium liquid, containing from a few up to 10^8 electrons. The typical radius of the bubble is 1 micron for an N=10000 electron bubble, and this radius scales as $N^{2/3}$. The electrons in the bubble are not smeared out homogeneously throughout the volume of the bubble, but form a nanometer-thin layer anchored to the spherical helium surface of the bubble.

We have investigated the vibrational modes of the multielectron bubbles. The deformations of the helium surface can be described by ripplon modes, with frequencies in the MHz-GHz region. A remarkable result is that increasing positive pressure on the helium will drive all ripplon modes one by one to zero frequency, whereas a small negative pressure stabilizes the multielectron bubble.

The spherical two-dimensional electron system in the bubble can form an electron gas (weakly correlated phase), or an electron liquid (strongly correlated phase), or an electron solid (Wigner crystallized phase). We have mapped out the phase diagram for this electronic system as a function of the experimentally tunable parameters, namely the pressure, the number of electrons and the temperature. The high compressibility of the multielectron bubbles allows to tune the surface density of electrons over four orders of magnitude. We derive the melting surface of the Wigner crystallized phase and show that it can be determined experimentally by varying the pressure.

Finally, a new experimental scheme to create, stabilize and study multielectron bubbles is proposed. This scheme is being implemented and we will report on the recent progress of the experiments that allow to verify our theoretical results for the vibrational and electronic properties of the multielectron bubbles.

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CHANGES IN INFRARED SPECTRA OF PHTHALOCYANINES DURING OXIDATION: QUANTUM CHEMICAL CALCULATIONS

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Metal–phthalocyanine molecules ($Me^{2+}Pc^{2-}$) are stacked one-dimensionally in a metal-over-metal mode. Because of this arrangement, these compounds create two channels – the metal and ligand ones – in the same molecular column. The iodine doping makes NiPc, CuPc and metal-free (H_2Pc) phthalocyanines metallic at room temperature [1], whereas CoPc was found to be semiconductive [2]. Martinsen *et al.* ascribed these different properties to the difference in the doped channels: CoPcI has a metal-oxidized channel, whereas the NiPcI has a ligand-oxidized channel [2]. If this is the case, the infrared spectra of metal-oxidized and ligand-oxidized compounds should be substantially different, since the former compound has the unoxidized ligand (Pc^{2-}), whereas the latter has the oxidized ligand (Pc^{1-}). Yakushi *et al.* prepared a similar compound $CoPc(AsF_6)_{0.5}$ and found that the infrared spectrum of this compound was essentially the same as that of the ligand-oxidized salt $NiPc(AsF_6)_{0.5}$ [3]. Because the infrared spectra of both compounds were substantially different from those of ligand-unoxidized compounds, CoPc and NiPc, they concluded that the ligand was oxidized in $CoPc(AsF_6)_{0.5}$ in contrast to CoPcI.

In this paper we present the intensity changes of the charge-sensitive vibrational bands (in the oxidized MePc increase the intensities of the bands around 1356 and 1471 cm^{-1}, whereas the intensities of the 1291 and 1533 cm^{-1} bands decrease) as obtained by means of quantum chemical calculation. The calculations were performed by B3LYP method. To provide a theoretical support for the idea of using the charge-sensitive vibrational bands for the characterization of the oxidation process the electronic density and orbital analysis was applied. The obtained results show that NiPc and CoPc lost their electrons during the oxidation from a_{1u} orbitals, which are located in the ligand. According to the charge distribution in NiPc and CoPc neutral molecules and their positive ions we concluded that the metal oxidation is low in both NiPc and CoPc, say on the level of a few percent. The problem of the CoPc cation spin state is also discussed.

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CBE GROWTH AND INVESTIGATIONS OF BE IN III-V ALLOYS/INP

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InP and phosphorus based alloys are important materials system for modern electronic, photonic and advanced device applications. In this work, we present the growth of InGaAs(P) on InP by CBE technique for optical communication applications and also the quality of the grown layers, evaluated by different techniques such as HALL, HRXRD, ECV, absorption and PL measurements. The epitaxial growth was carried out in VG80H CBE system equipped with a homemade gas-handling system. Good quality epilayers were grown on an epiready, exact (001) InP substrates and the growth rate of InP epilayer was 1 μm/h at temperature of 783 K. In the case of lattice matched InGaAs and InGaAsP, the growth rate was 0.65 μm/h and 0.67 μm/h respectively at the growth temperature of 798 K. The MQWs were also grown at 798 K for the realisation of semiconductor optical amplifier. The electrical properties of the layers were characterised by HALL effect measurements. The grown InP samples have mobility values of 70,000 and 2800 $cm^2/V.s$ with background impurities as low as 1×10^{14} cm^{-3} and 2×10^{15} cm^{-3} at 77 K and 300 K respectively. The FWHM of the (004) Bragg reflection peak as narrow as 17 arcsec was obtained for these samples by HRXRD measurements. The RT PL measurements also show typical spectra with a peak FWHM of about 19 nm. Lattice matched $In_{0.53}Ga_{0.47}As$ thick layer were grown on InP and the strain value of the layers was about 6.7×10^{-4}. The HALL mobilities of the thick undoped ternary layer were 5970 (300 K) and 37,550 $cm^2/V.s$ (77 K) with carrier concentration in the range of $1.2 \times 10^{15} – 4.2 \times 10^{14}$ cm^{-3}. Be-doped $In_{0.53}Ga_{0.47}As$ layers with $p_{300K} = 9 \times 10^{18}$ cm^{-3} and $\mu_{300K} = 58$ $cm^2/V.s$ were also grown which exhibits a line width of nearly 25-30 arcsec. $In_{1-x}Ga_xAs_yP_{1-y}$ quaternary epilayers ($x = 0.24$, $y = 0.52$) closely lattice matched to InP have been grown. The HRXRD pattern of the quaternary layers shows a lattice mismatch of 2.4×10^{-3} and a FWHM of 8 meV was obtained by the PL measurements. Further the homogeneity of these layers was checked using FTPL study at different positions of the full wafer and it was extremely good. For InGaAs/InP MQWs (7.0 nm / 7.0 nm, 60 periods), very intense luminescence peak with line width as low as 4.5 meV was obtained by 4 K PL measurements. The RT absorption spectra of the MQWs also show a very sharp peak. Furthermore during ECV measurements, a sudden transition with high carrier concentration variation was observed as soon as the MQW layers were approached. These studies show that the quality of the QWs were good with smooth and abrupt (“Squareness”of the QW) interfaces, few background impurities and a high PL efficiency. A new electrolyte system, which posses better electro-chemical properties has been realised and proposed for ECV profiling of InP based materials. The electrically active concentration of Be has been investigated. The carrier concentration and etch depth values measured by ECV profiler were compared with that of HALL effect measurement and stylus profiler. We observed a discrepancy between ECV and HALL measurements only, at higher concentrations, for InP, but for InGaAs it is less predominant. This discrepancy will be discussed and explained in detail.

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INVESTIGATION OF PROPERTIES OF SOLIDS INTERFACE STRUCTURE BY PHOTOACOUSTIC MICROSCOPY

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Photoacoustic microscopy (PAM) is a new perspective method of non-destructive control of properties of interface structure of solids. The application of PAM for non-destructive control of initial materials and finished products of an electronic engineering during their manufacturing, in particular, diagnostic the quality of microwelded connections of integrated circuits up to a stage of assembling, is presented.

The principle of the PAM is based on the phenomenon of the generation and distribution of both thermal and acoustic waves excited by modulated in intensity laser radiation. The acoustic fluctuations spreading in the object are detected by the piezosensor and converted by it into electrical signal. The computer processing of this signal allows receiving the photoacoustic image of internal structure of researched object under the scanning by a laser beam along the sample surface.

For computer analysis of the photoacoustic images author developed the one-dimensional mathematical model of photoacoustic effect with piezoelectric registration. This model allows to restore the information about physical properties of researched object under the experimentally received amplitude and phase characteristics, estimate a minimal size and a maximal depth of defect and choose optimum modulation frequency for deep profiling of researched object.

The results of investigation of the microwelded connection of IC (“metal – semiconductor”structure) by a photoacoustic microscopy are presented. The possibility of photoacoustic registration and visualization of upper layer's delamination of semiconductor devices at the frequencies up to 10 kHz, for which the upper layer is thermally thin, is shown. The photoacoustic images of “Al-foil – Si-monocrystal' connections are presented. The “metal – semiconductor”connections quality control technique on the photoacoustic contrast is proposed. The PAM allows receive the most complete information about quality of microwelded connections of IC and carry out the computer analysis of connections quality and selection by a principle “valid”- “not valid”.

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GROWTH, STRUCTURE AND INTERDIFFUSION IN SEMICONDUCTOR EUS/PBS SUPERLATTICES

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The ferromagnetic/nonmagnetic, wide-gap/narrow-gap semiconductor EuS/PbS superlattices (SL) were prepared by thermal evaporation of lead sulfide from tungsten boat, electron-beam evaporation of europium sulfide in oil-free vacuum (10^{-5}- 10^{-6} Pa), and alternative deposition of two constituents on (001) KCl and (111) BaF2 at 523 K. The layer thickness and condensation rates were monitored by calibrated quartz resonator. The epitaxial growth and structure of multilayers were studied by transmission electron microscopy (TEM) and X-ray diffraction (XRD). The TEM study showed that EuS and PbS had grown on the top of each other in the layer-by-layer fashion (Frank-van der Merwe mechanism), no presence of misfit dislocation was found. The XRD study showed that it is possible to fabricate quality SL with thickness of layers down to 1 monolayer. Layer diffusion intermixing in epitaxial EuS/PbS SL was studied by means of XRD. The interdiffusion coefficients were determined via near-Bragg peak satellites intensity changes on XRD pattern during annealing for different annealing temperatures: $D=1{,}1.10^{-20}$ cm^2/s (Ò=543 Ê); $D=6{,}4.10^{-20}$ cm^2/s (Ò=593 Ê); $D=1{,}7.10^{-18}$ cm^2/s (Ò=623 Ê). Using Arrenius law values of preexponential factor and activation energy were calculated: $D_0 = 2{,}2\times10^{-9}$ cm^2/s; Å = 1.22 eV. It allowed to estimate value of intermixing zone, which formed at temperature of superlattice preparation: x=0.1 nm (less than thickness of one monolayer). Presence of sharp interfaces in EuS/PbS system was confirmed by measuring several physical properties for which condition of interfaces very important [1-3].

Peaks, that correspond to size quantization levels were observed on photoluminescence spectra of EuS/PbS SL grown on (111) BaF_2 [1].

Enhancement of thermoelectric power factor with decrease of PbS quantum well width was found in EuS/PbS SL on (001) KCl [2].

By means of neutron diffraction antiferromagnetic interlayer exchange coupling was observed in purely semiconductor, ferromagnetic/nonmagnetic EuS/PbS SL on (001) KCl [3].

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THE INFLUENCE OF STRONG SHORT-RANGE INTERACTIONS ON THE BEHAVIOUR OF ONE-DIMENSIONAL PROTONIC CONDUCTOR

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In the recent years the wide experimental and theoretical investigations of superionic crystals with hydrogen bonds and other systems with protonic conductivity have raised the interest to the problems of proton transport considerably.

We consider the one-dimensional hydrogen-bonded chain described in the framework of the orientational-tunnelling model which takes into account proton transfer according to Grotthuss mechanism as well as the strong short-range proton interactions. We use the method of expansion in terms of the irreducible Green functions to obtain the single-particle Green function of the proton subsystem. Thus we calculate the energy spectrum of the system taking into account the first order contributions to the proton self-energy part. The spectrum has a complicated structure and consists of the several groups of bands. Depending on the proton concentration the conductivity of the system can be either of dielectric or metallic type. It is also shown that at some values of concentration the uniform distribution of protons along the chain becomes unstable.

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WANNIER-MOTT EXCITONS IN SEMICONDUCTOR $Zn(P_{1-x}As_x)_2$ AND $Cd_xZn_{1-x}P_2$ CRYSTALS

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Low-temperature (1.8K) absorption, reflection and photoluminescence spectra of excitons in semiconductor mixed $Zn(P_{1-x}As_x)_2$ and $Cd_xZn_{1-x}P_2$ crystals have been studied at small $x < 0.05$. We have found that, likely to "pure"ZnP_2 crystal, in mixed crystals the same excitonic series (C, B, and A) are observed. At the increase of x from 0 to 0.05 the decrease of the energy gap takes place in crystals of both types: 1.6026-1.5801 eV in $Zn(P_{1-x}As_x)_2$ and 1.6026-1.5981 eV in $Cd_xZn_{1-x}P_2$. At the increase of x from 0 to 0.05 the rydbergs of series decrease in crystals of both types as well: 44.0-37.4 meV (B-series), 39.6-33.2 meV (C-series), and 26.5-22.8 meV (A-series) in $Zn(P_{1-x}As_x)_2$ crystals; 44.0-43.6 meV (B-series), 39.6-37.6 meV (C-series), and 26.5-26.1 meV (A-series) in $Cd_xZn_{1-x}P_2$ crystals. It is seen, that the dependences of E_g and Ry on x are considerably stronger in $Zn(P_{1-x}As_x)_2$, where the changes of the energy bands occur, probably, faster than in $Cd_xZn_{1-x}P_2$ crystals.

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VORTEX LATTICE COMMENSURABILITY EFFECTS IN SUPERCONDUCTING LAYERED SYSTEMS

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Novel reentrance phenomenon is discovered in Mo/Si multilayers. It occurs in the magnetic fields H parallel to the layer planes. At some temperature corresponding to the fitting of the vortex cores within semiconducting interlayers a minimum appears on resistivity R vs H dependence. At lower temperatures the minimum becomes more pronounced and at transforms into a large zero resistance region (ZRR). This effect may be explained in terms of the intrinsic pinning and vortex lattice (VL) commensurability with period of layering s. The positions of minima and ZRR correspond to the stable configurations of commensurate VL's.

The oscillations of critical currents Ic is observed in thin vanadium films. This oscillations are explained in terms of commensurability effect between VL parameter a and total thickness of sample D. Two different commensurability effects are observed simultaneously in V/Si multilayers with small numbers of bilayer. One of them is the commensurability effect between a and s and the other between a and D.

It is suggested that resistive method may be used as a new tool of the VL structure study in layered superconductors.

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BISMUTH-INDUCED INCREASE OF IRON GARNETS MAGNETOOPTICS: THEORY AND COMPUTER SIMULATION

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In the framework of the charge-transfer transitions concept, we suggest a quantitative model which explains the strong increase of the circular magnetooptics of iron garnets when doped with bismuth or lead ions. The covalent admixture of their 6p-orbitals (with giant one-electron spin-orbit coupling constant) to oxygen 2p-states causes the growth of the oxygen contribution to the spin-orbit coupling constant of octahedral and tetrahedral Fe-O complexes (main magnetooptically active centers of iron garnets). The enhanced spin-orbit interaction on the oxygen is not the only effect of substitution; it also gives rise to the effective anisotropic tensor addend to the spin-orbit interaction and the circular magnetooptics of iron garnets as well. The computer simulation of bismuth-substituted garnets magnetooptics under the inhomogeneous Bi distribution is made. Estimates of various contributions to the Faraday rotation of garnets are given. Analysis of experimental data supports our theoretical model.

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AN ANALYSIS OF THE LOCAL ATOMIC STRUCTURE OF MATTER BY THE ELECTRON EXTENDED ENERGY LOSS FINE STRUCTURE METHOD

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The oscillating fine structure located on the low energy side of edges of characteristic losses of electrons connected with the ionization of the substance atom inner level is said to be extended energy loss fine structures (EELFS). EELFS spectra by their nature belong to the class of XAFS-like phenomena and are determined by processes of coherent scattering of a secondary electron on the nearest atomic environment of the ionized atom. So, the EELFS spectroscopy, as well as XAFS, allows to perform the experimental analysis of parameters of atomic correlations. In this case the initial atomic locality of the method allows to analyze both crystal and amorphous substances. EELFS, more than XAFS, is capable of analyzing the local atomic structure of light elements of the extremely low (to 1 nm) square resolution and the surface (of tens of atomic layers) sensitivity.

The theory of the EELFS process in the approximation of orthogonalized plane waves and experimental EELS spectra of Al, Si above K-edges of ionization and Fe, Cu above L-edges of ionization are presented in the present paper.

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INVESTIGATIONS OF THE D BAND IN THE RAMAN SPECTRA OF SINGLE WALL CARBON NANOTUBES

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The disorder-induced D band in the Raman spectrum of single wall carbon nanotubes (SWNTs) was investigated theoretically and experimentally. The measured maximum position of the D band for SWNT bundles exhibits an oscillation superimposed on a linear shift, when the laser excitation energy E_{laser} varies in the range of 1.6 - 2.8 eV. Our theoretical calculations show that the D-band intensity of an isolated SWNT has a sharp maximum when E_{laser} of either the incoming or the scattered photon matches a van Hove singularity in the joint density of states. This 'resonance' must be considered in addition to the double resonance from a scattering by an impurity. Calculating the D band of a superposition of all the 114 SWCNTs within a given diameter range both the shift and the oscillation in the experimentally observed spectra were reproduced. The structure of the D band was also examined theoretically and compared to experiments.

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PHOTOLUMINESCENCE OF FULLERITE C_{60} LOW TEMPERATURE PHASE

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The results of studies of photoluminescence spectra of fullerite $\tilde{N}_{60}$ low temperature phase are presented. C_{60} thin films were fabricated by the deposition in vacuum on the heated up substrates (NaCl crystalline plate, mica). The films structures were analyzed by THEED technique. Earlier [1-4] the definite proofs were given that structural defects play the important part in $\tilde{N}_{60}$ photoluminescence spectrum shaping. For clearing up of a nature of defects, researches of an effect of temperature and strains on photoluminescence spectra were conducted. Mainly the structural defects have originated both over difference of $\tilde{N}_{60}$ thin film and substrates thermal expansion coefficients and over a forced bending of $\tilde{N}_{60}$ thin film deposited on mica. Influence of strains was observed on the 1.76 and 1.71 eV defect-related photoluminescence bands at 5 K (see Fig. 1). The features of a temperature behavior of these photoluminescence bands are also investigated. Defects formation, electronic excitations trapping and effects of orientational disorder are discussed.

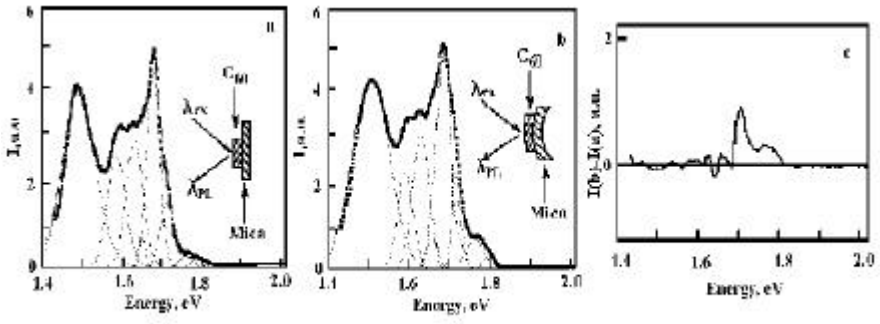

Fig. 1: Photoluminescence spectra of C_{60} thin film of 90 nm thickness deposited on mica: a - plane specimen, b - bent specimen. I is a photoluminescence intensity in arbitrary units. Photoluminescence (λ_{PL}) was excited by the 2.84 eV (λ_{Ex}) radiation at 5K, the curves were best fitted by Gaussians. c – difference of the a and b spectra which have been normalized to their integral intensity.

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A METHOD FOR SULFUR ISOTOPES DETERMINATION FROM MINERAL SULPHUROUS WATERS

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Sulfur isotopic ratio in terrestrial samples varies because of the isotopic fractionation by geological and biological process. Sulfur fractionation of mineral sulphurous water offers information about theirs sources and relationship between neighboring hydrocarbon deposits and mineral sulphurous waters. First step for sulfur isotopic analysis from dissolved sulfates and H2S is the samples preparation. For sulfur isotopic analysis, S must be extracted from sample for SO_2. The techniques of preparation must be accomplished three conditions:
- supply an enough quantity of SO_2
- SO_2 hasn't impurities
- don't produce isotopic fractionation long preparation process.

We have reported measurements for 22 samples to verify the method. The results were obtained with a precision of +0.1 per mil.

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SO_2 AND NO_x REMOVAL BY ELECTRON BEAM AND ELECTRICAL DISCHARGE INDUCED NON-THERMAL PLASMAS

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Non-thermal plasmas in which the mean energy of electrons is substantially higher than that of the gas offer considerable advantage in reducing the energy required to remove the pollutants. An installation containing a DC negative corona discharge reactor, a pulse corona discharge reactor and a combined electron beam (EB) and microwave (MW) induced plasma reactor is presented. DC negative corona discharge reactor contains a ceramic tube injector (o.d. 3 cm and 10 cm long) with a hollow electrode (o.d. 0.5 cm and 5 cm long). The pulse plasma discharge reactor is a coaxial one and consists of a centered single discharge wire of 1mm in diameter and a stainless steel tube with 20 cm inner diameter and 250 cm length. The discharge wire is energized by short duration and fast rising positive high voltage pulses from a nanoseconds pulse generator. Combined EB and MW reactor is a multimode rectangular cavity RC. The scanned EB of 5.5 MeV is introduced perpendicular to the RC upper-end plate through a 100 m thick titanium foil while the MW power of 2.45 GHz is coupled to the RC walls via the slotted waveguides used as radiating antennas.

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PRELIMINARY INVESTIGATIONS INTO TOXIC GAS AND VAPOUR SENSING USING LANGMUIR-BLODGETT AND LANGMUIR-SCHAEFFER FILMS OF 4-METHYLBENZENETHIOL-ENCAPSULATED GOLD NANOPARTICLES

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Films of gold nanoparticles encapsulated with 4-methylybenzenethiol ($CH_3C_6H_4SH$) molecules (diameter ~ 5nm) have been deposited via both the Langmuir-Blodgett (LB) technique and the Langmuir-Schaeffer (LS) technique onto glass and silicon substrates (50 layers). Ellipsometry, atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS) and optical absorption measurements show these films to be highly ordered, forming discrete layers. Films of this material have been deposited onto interdigitated gold electrodes across which voltages have been applied. Typically, 5V applied across a 5-layer film produces a current in the order of ~10ìA. On exposure to certain gases (e.g. NO_2) and vapours (e.g. chloroform, toluene, water) of known concentration, a change in electrical current (up to 50%) is observed. Preliminary investigations suggest that some vapours exhibit a unique initial response. This fingerprint may be utilised in order to help identify a specific gas or vapour. The films experience partial recovery in a nitrogen atmosphere, after which they can be re-exposed.

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NON-DESTRUCTIVE PIXE AND XRF ANALYSIS OF ART AND ARCHAEOLOGICAL OBJECTS

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The preservation and conservation of our cultural heritage has become one of the main concerns today all over the world. In particular there is an increasing need for non-destructive investigations, as sampling from the unique and precious objects of art and archaeometry. In addition to the conventional analytical procedures, techniques utilising nuclear instruments and methods play increasing role in this field. The small, portable X-ray fluorescene (XRF) spectrometers using radioisotope excitation allow *in situ* analysis in museum, galleries, on even on field. The special version of the particle induced X-ray emission spectroscopy (PIXE), where the few MeV energy proton beam is extracted to the atmosphere offers unique possibilities for detailed elemental mappings in the laboratory (external beam PIXE).

This paper presents illustrative applications of our external beam PIXE set-up and the XRF device with radioisotope excitation. The PIXE analysis of a medieval small bronze sculpture from Cambodia has furthered to find out the structure of the sculpture, while the detection of the presence of titanium in white spots of a painting provided scientific basis to decide that the painting in question was a fake.

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RADIOACTIVE ISOTOPES ACCUMULATION IN INVASIVE AQUATIC PLANTS

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One of the most important factor of the phytoremediation of the water contaminated with radioactive isotopes is the capacity of the plants to accumulate this isotopes.

In our study invasive aquatic plants was used, from Transylvania region. The gamma spectrometry method was used to determine the concentration capacity of different plants for natural (U, Th^{232} and K^{40}) and artificial (Cs^{137}) radioactive isotopes.

We used two methods: measuring the activity of water before and after the biological decontamination process (experiment made in laboratory conditions) and measuring the specific activity of water and compare to the specific activity of the aquatic plants.

Significant effects was obtained for natural Th^{232} contamination for the acclimatized "Elodea"species in natural condition - up to 10x concentration. Autohtone species "preference"is K^{40} at 20x concentration, and for U both, elodea and autohtone species present a 10x concentration. For Cs^{137} the accumulation in elodea is 25x.

The efficiency of decontamination is 50% for natural isotopes (autohton plants) and 60% for Cs^{137} , but there is results for some species in special conditions up to 80%.

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DEPLETED URANIUM DETERMINATION IN SOIL

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A simple method to determine low activity concentrations of depleted uranium (DU) in soil by means of spectrometry is discribed. The metod is based on the completely violated ^{238}U - ^{226}Ra equilibrium in DU. The detection limit of DU with this method under usual measurement conditions has the order of magnitude of 10 Bq/kg. A number of measurements were made on soil samples and the DU content in soil samples from southern Serbia was determined.

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DYNAMICS OF EVAPORATION OF WATER MICRODROPLET IN PAUL TRAP

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Meteorological models and climate simulations require incorporating microphysics of clouds and aerosols for their proper operation. Complex refractive index of light and size of microdroplets to build clouds and aerosols are very important parameters. Sound knowledge of the parameters at microscopic level would also yield a better interpretation of remote sensing of atmosphere. Fortunately microphysics may be explored experimentally. There is quite a number of well established experimental techniques of investigation of individual microparticles. Techniques of levitation are the most often applied at present e.g. ultrasonic, optical and electrodynamic levitators. We concentrate on electrodynamic levitation of water droplets as suitable for objects of sizes between 0.1 and 250μm. Our investigations are made for range of temperatures, pressures and relative humidity, that are observed in troposphere. We also charge of droplet take into consideration. It changes the properties and a behavior of droplet e.g. evaporation process.

During experiment we record an interference image of microdroplet created by scattered light in space around it, on two perpendicular polarizations. Next this image is analyzed. A base for analysis is Mie-theory that describes a scattering of light on dielectric sphere. The theory include a solution of Maxwell's equation for two perpendicular polarizations (vertical and horizontal) of scattered wave for specific boundary conditions. The solution has a form of infinite series of complex functions with coefficients, that determines radius and complex refractive index of light of scattering microdroplet. This property of coefficients allows us to find size and complex refractive index of scattering microdroplet by comparison experimental image with theoretical image. Because we record a movie, we can analyze an evaluation of microdroplet in time e.g. evaporation of it.

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REINTERPRETATION OF LORENTZ TRANSFORMATION AND RESOLUTION OF SPECIAL RELATIVITY'S PARADOXES

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Lorentz Transformation is reinterpreted. It is shown that by admitting the existence of a frame of reference with synchronized clocks, we conclude that any other frame of reference that moves related to the first has desynchronized clocks. From this conclusion we will arrive at a new expression to relate the time of different frames of reference. We will show that if the maximum speed on a frame with synchronized clocks is the speed of light, then the speed of light varies accordingly to the velocity of the frame of reference. The new interpretation of Lorentz Transformation explains and solves Relativity's paradoxes.

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CROWD BEHAVES AS EXCITABLE MEDIA DURING MEXICAN WAVE

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The Mexican wave (also called La Ola) became widely known during the 1986 World Cup held in Mexico. Since then it has become a paradigm for a variety of phenomena involving an initial perturbation propagating in the form of a "single" planar wave. In addition, La Ola raises the exciting question of the ways by which a crowd can be stimulated to execute a particular pattern of behaviour.

(http://angel.elte.hu/wave)

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CYCLIC MANIPULATION OF CASIMIR CAVITY DIMENSIONS AND ITS IMPLICATIONS

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It has been calculated that rectangular microcavities in metals should produce complex and counteracting atractive forces on the cavity's sides. General properties of the Casimir force are reviewed, with a focus on the geometry of these microcavities. The forces in several simple idealized structures are derived as a starting point to discuss the implications of cyclical manipulation in detecting repulsive forces within the cavity.

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WHAT WILL WE LEARN ABOUT ELASTIC SCATTERING FROM FUTURE COLLIDERS AT RHIC AND LHC?

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We hope and expect that many new discoveries are in store for future machines at RHIC and LHC. Consequently, We hope to have some information about supersymmetry, Higgs, Quark substructure and much more. At the same time, lot of new information is planned through experimental study of elastic scattering. We give a brief survey of what we expect at RHIC and LHC with respect to elastic scattering.

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HIGH-p_T PION PRODUCTION IN HEAVY-ION COLLISIONS

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This presentation summarize pQCD results on p_T production in proton-proton (*pp*), proton-nucleus (*pA*) and nucleus-nucleus (*AA*) collisions. These next-to-leading order (NLO) evaluations applying a *K* factor from jet productions. Using the intrinsic transverese momentum (k_T) we calculate p_T productions fitted to several experimental data, at two differen fragmentation scales ($Q=p_{T,jet}/2$ *and* $Q=p_{T,jet}$). Here we have tested these results on Cronin effect from CERN SPS up to RHIC energies.

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RECONSTRUCTION ISSUES IN COLLIDER PHYSICS

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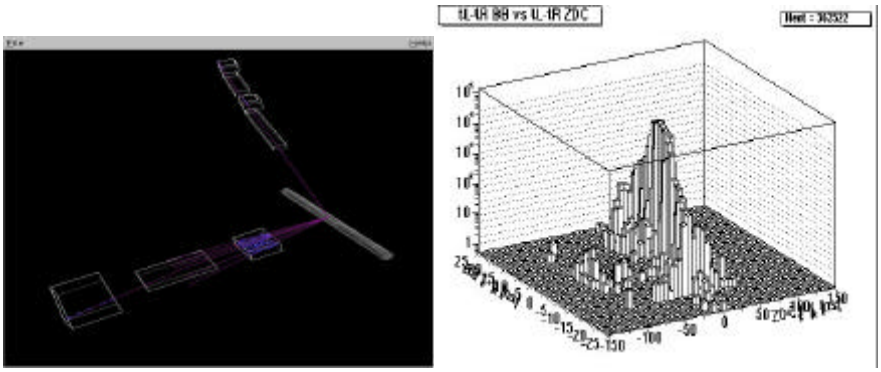
Taking into account the experimental results obtained in one of the major experiments at the Relativistic Heavy Ion Collider from Brookhaven National Laboratory - Upton, New York, USA - namely BRAHMS (Broad Range Hadron Magnetic Spectrometres) Experiment - which studies Au-Au collisions at $\sqrt{s_{NN}} = 200GeV$ energy, we study the collision geometry implications on the experimental yields. Making use of the two spectrometers from BRAHMS - providing very accurate angular distributions - we find out the importance of vertex determination on the physical event reconstruction and on the centrality cuts. The vertex problem is of major importance in collider physics, showing wide distributions. In this analysis of the experimental data are used three groups of detectors, namely: the Beam-Beam Counters and Zero Degree Calorimeters, providing vertex measurements by time of flight right-left methods, and the time projection chambers that reconstruct the vertex by back-projection of the produced clusters. The methods used are presented and a qualitative comparison between the experimental data from Au-Au collisions at $\sqrt{s_{NN}} = 130GeV$ and $\sqrt{s_{NN}} = 200GeV$ energies is made. Finally, we present the main problems regarding the track reconstruction and also some visualization algorithms from peculiar tracking detectors from BRAHMS.



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ASYMMETRIC NUCLEAR MATTER IN THE RELATIVISTIC MEAN FIELD THEORY

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Asymmetric nuclear matter is studied in the frame of relativistic mean field theory, using scalar-isoscalar sigma, vector-isoscalar omega mesons together with their selfinteractions and also vector-isovector rho and scalar-isovector delta mesons as degrees of freedom. The model is used to parametrize the nuclear matter properties results calculated by more fundamental Dirac-Brueckner-Hartree-Fock (DBHF) theory, thus allowing to apply these results also to finite nuclei in contrast to DBHF model. Binding energy per nucleon, meson potentials, uncompressibility, symmetry energy, nuclear pressure as well as proton fraction of matter are further calculated. The behaviour of rho meson coupling constant is discussed. The delta meson is proved to be an usefull degree of freedom for describing of the asymmetric nuclear matter.

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STUDY OF DYNAMICAL AND ENTRANCE CHANNEL EFFECTS IN HEAVY-ION FUSION REACTIONS VIA NEUTRON EVAPORATION

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We had performed two reactions leading to the same compound nucleus ^{80}Sr . In the first reaction ^{80}Sr was formed through symmetric reaction ^{32}S + ^{48}Ti at 120MeV, with angular momentum 41h. In another reaction the same compound nucleus was formed through asymmetric reaction ^{16}O+^{64}Zn at 91MeV, with angular momentum 41h. Neutrons from these two fusion reactions have been measured, in two series of complementary experiments using neutron liquid scintillators.. Both the neutron energy spectra reveal significant quantitative differences in the decay patterns of the two reactions studied. It is shown that these differences can not be understood in terms of decay cascades proceedings through states of enhanced collective energy, such as the superdeformed state, suggested in earlier studies. Instead, they can be explained consistently within the frame work of a statistical decay model, if different effective level density parameter are allowed for the evaporation chains of the two composite systems.

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HEAVY-ION COLLISIONS: THE STUDY OF ELLIPTIC FLOW OF NEUTRAL MESONS IN Au+Au REACTION AT 800 A MEV

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The heavy-ion collisions at incident energies of 1-2 AGeV are a unique tool to investigate the properties of nuclear matter at high temperature and density – one of the major goal of contemporary nuclear physics. According to various theoretical model calculations nuclear matter can be compressed to 2-3 times the normal nuclear density and heated to temperatures in the order of 100MeV in this energy regime. In addition, during the compression phase of the heavy-ion collision a significant fraction of the participating nucleons is excited to short-lived resonance states, which subsequently decay via meson emission.

Experimentally, this can be studied by measurements of meson yields as a function of the system mass, the beam energy and reaction centrality, momentum distribution and emission patterns relative to the reaction plane.

An experimental program to study neutral meson production (π^0,η) was realized at SIS facility at GSI Darmstadt, Germany by the TAPS collaboration. The combination of the photon spectrometer TAPS – an electromagnetic calorimeter with good energy, time and spatial resolution – and the charged particle-detecting KAOS Forward Wall (FW) offers the possibility to study azimuthal distribution of neutral mesons relative to the reaction plane. The experimental data from the Au+Au reaction at 800 MeV were analyzed. The reaction plane was determined on an event by event basis and angular distribution of π^0 and η mesons was reconstructed.

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SOME PREDICTIONS AND EXPERIMENTAL RESULTS ON THE POSSIBILTY OF QUARK–GLUON PLASMA FORMATION IN ULTRARELATIVISTIC NUCLEAR COLLISIONS

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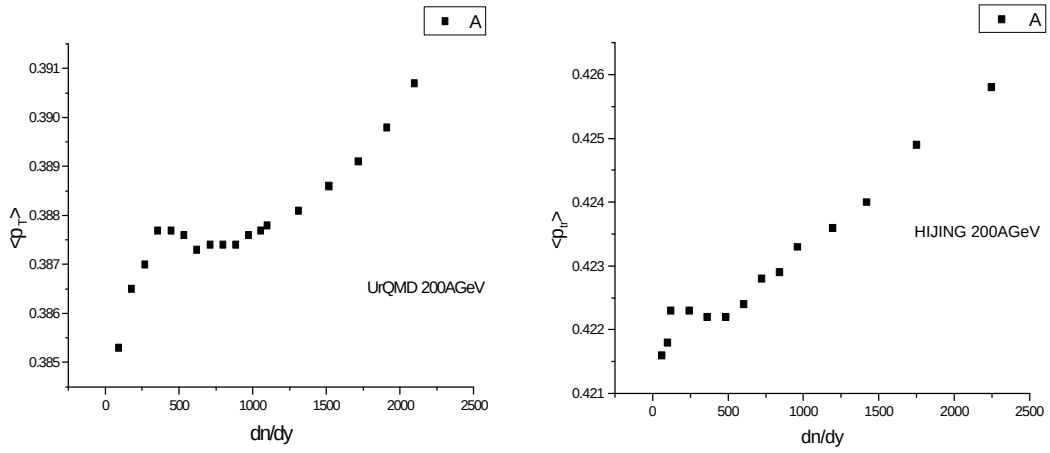
Ultrarelativistic heavy ion collisions are useful to investigate highly excited dense nuclear matter. At sufficiently high temperature, nuclear matter is expected to undergo a phase transition to quark-gluon plasma. Some predictions on the particle production yields, rapidity and pseudorapidity distributions, and hadron spectra using UrQMD and HIJING codes are presented in this paper. The rapidity density, respectively, pseudorapidity density could be used to estimate energy density in the collision.

Transverse mass spectra and transverse momentum spectra for pions, kaons, protons and antiprotons from the symmetric heavy ion collisions Au+Au at $\sqrt{s_{NN}} = 200\ GeV$ are presented. Comparisons with experimental results obtained at BRAHMS–RHIC Experiment are included, too.

Taking into account the fact that some information on the collision dynamics and the thermalisation degree is obtained from the spectral shapes of the interesting physical quantities and their dependencies on rapidity we used the dependence of the average transverse momentum on the rapidity densities. The different lengths of the “plateaus”in the mean transverse momentum dependence on the rapidity densities could justify the assumption of the effect of the hot and dense nuclear matter on the behaviours of the different interesting physical quantities.



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The values of the energy and baryonic densities – over 10 normal values - as well as the agreement between the experimental values on participants and phenomenological model estimations, represent a support for the estimated parameters of the nuclear matter in Au-Au collisions at $\sqrt{s_{NN}} = 200\,GeV$, as well as for the possibility to evidence such a transition in these collisions.

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GAMMA-SPECTROSCOPY OF Ca ISOTOPES

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In a recent study [1] we found in the $^{32}S+^{24}Mg$ system an *enhanced* population of the deformed $K=4^-$ band in ^{48}Cr in the binary fusion-fission case of emitting ^{8}Be from the compound nucleus ^{56}Ni as compared to the uncorrelated emission of two α- particles from the compound nucleus formed in a fusion-evaporation reaction. In order to establish this effect and to extend it to the comparison between the binary emission of ^{12}C and the uncorrelated emission of 3 α-particles in 4N-nuclei, we performed an experiment bombarding a thin ^{24}Mg target with a 139 MeV ^{28}Si beam from the XTU tandem accelerator at LNL. To identify the γ-rays from the different deformed bands in the nuclei of interest, events with at least two γ-rays registered in the Ge-detector array GASP were recorded. To distinguish between the different reaction mechanisms the emitted light particles where detected in the Si-detector ball ISIS. The procedure to distinguish fusion-fission and fusion-evaporation reaction channels is described in detail in Ref [1]. The crucial point of that kind of analyzing γ-particle coincidences is that the level scheme of the investigated nucleus has to be well understood. Since the main focus of interest is on ^{40}Ca, which can be populated by the binary channel $^{28}Si+^{24}Mg\rightarrow^{52}Fe\rightarrow\ ^{40}Ca+^{12}C$ as well as by the evaporation channel $^{52}Fe\rightarrow\ ^{40}Ca+3\alpha$, the first step was to obtain detailed information about the level scheme of ^{40}Ca.

From this experiment 19 new levels and 25 new transitions for ^{40}Ca for excitation energies up to 21 MeV were found, but no connecting transition between the positive and negative parity bands. The assumption of two steep, well separated valleys with large values of β_3 deformation of opposite sign would explain, why there are no decays between negative and positive parity states, in opposition to the case in heavy nuclei [2].

Another nucleus of interest for the investigation of deformed bands populated in different reaction mechanisms is ^{42}Ca, which can be obtained via the exit channels $^{42}Ca+^{8}Be+2p$ and $^{42}Ca+2\alpha+2p$. We expect a structure related to ^{40}Ca based on 6p4h and 10p8h configurations. From this experiment 6 new levels and 6 new transitions in ^{42}Ca for excitation energies up to 13 MeV were found.

The analysis of the population of the different bands in the different reaction channels for ^{40}Ca and ^{42}Ca as well as for ^{44}Ti is still in progress.

[1] S. Thummerer et al., J. Phys. G 27 (2001) 1405
[2] P. A. Butler and W. Nazarewicz, Rev. Mod. Phys. 68 (1996) 350

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COMPUTER SIMULATION UPON THE INTERFERENCE FIELD IN FRAUNHOFER DIFFRACTION

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In order to allow a better understanding of optical theories and phenomena, a theoretical study via computer simulation of Fraunhofer diffraction on a grating is presented. The flux density in the interference field of diffraction grating (with the number of apertures N, the constant grating d and the aperture width a) can be expressed as function of the product between grating function and aperture function.

Computer simulation allows to observed: the distribution flux density in Fraunhofer diffraction for one aperture; the dependence of grating function on the diffraction angle for a given incident angle; the dependence of the product between grating function and aperture function on the number N and the ratio d/a.

Using computer simulation the students can pursue: the narrowing of central maximum with the increasing of aperture width; the variation of the number of main maximums inside the central maximum with the variation of d/a; the secondary maximums number variation with the total number of apertures N.

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SELECTION RULES FOR SPHERICAL HARMONIC OSCILLATOR

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Selection rules in dipole approximation were derived for a spatial oscillator, using spherical coordinates. The results were used to determine the energy spectrum of charged spatial harmonic oscillator in constant electric field, using second-order perturbation theory. Comparison with the exact result confirms the correctness of the derived result.

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PHYSICS EDUCATION FOR FUTURE TECNOLOGY

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Physics is a backbone of technology. Physics is important for physicist, Engineers, Biologist & Medical science. Our aim is to bring together different agencies such as Education, Research and Industries on common platform for better quality. Continuous interaction between Education, Research and Industries is important for future plan and demand. Because future technology is depend on creative ideas and application of pure science.

"To live effectively is to live with adequate information"_ Narbet Wainer.

The success of every system is depend on Man, Machine and Material. We can provide quality information through e-environment to related workforce, because quality is the essence of the output. Education of physics leads to higher possibility of application of knowledge and fundamental ideas . Ratio between theory and practical components should properly maintained. Content of syllabus must be related with environment and need for future technology. Need based physics education is important.

In present paper we have discussed application of physics in higher education such as Engineering and Medical Science for better quality for future technology under e-environment. We have also discussed knowledge management for "Learner"

Keywords : e-environment, Knowledge Management (KM), Learner

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YOUTH EXPEDITION FOR OBSERVATION OF THE TOTAL SOLAR ECLIPSE IN BULGARIA ON AUGUST, 11TH, 1999

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The expedition about the total solar eclipse was organized by the "Physics"and "Natural Sciences"Departments at the University of Ruse. The observational tasks were synchronized with The National Program held by The Bulgarian Academy of Science and Sofia University.

The preliminary organization included:
Specifying of the observational tasks and development of methods for their execution
Selection of observational points
Preparation of observational devices
Development of a training manual for the observational teams

The expedition took place on August, 9th, 10th, 11th and 12th, 1999 at two separate locations: *Base 1* at Vetren village and *Base 2* at the airport of the town of Silistra.

The following observational tasks were completed:
Drawing of the solar crown
Measuring of the meteorological parameters
Precise timing of the moments of contacts
Photometrical measuring of the solar crown

The stated observational tasks were shared between 4 teams. The total number of people at *Base 1* were 37, and that at *Base 2* – 21. At both locations participated students as leaders of the youth teams.

As a result the following parameters and actions were taken:
The precise moments of the 4 contacts at both observational points
The fixed temperatures and level of humidity in the period 9am – 2.45pm local time
10 drawings of the solar crown were made
Pictures of all the stages of the eclipse were taken, as well as pictures of Baily's bead formation and the diamond ring

The results from the specified tasks are shown in a computer presentation and are also published on a specialized Internet site.

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EXTRACTING BIOCHEMICAL AND MORPHOLOGICAL INFORMATION FROM FLUORESCENCE SPECTRA OF DISEASED TISSUE BY CHEMOMETRICAL TECHNIQUES

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Diagnostic techniques based on optical spectroscopy offer the possibility to distinguish between disease and non-disease tissue in various suspicious body sites and have the potential to reveal biochemical and morphological properties of tissue. Relevant mathematical and statistical tools need to be used for extracting full information from analytical data and exploit full potential of analytical method. It is shown that tissue classification based on chemometrics and fluorescence methods has a high predictive ability and might be used for tissue diagnostics. Spectra underlying features, like the number of fluorescent chemical species present, can also be extracted by the methods. Furthermore the species can be identified and concentration of each species in tissue can be calculated, thus providing insight into the spectral features that contribute to the classification and are responsible for absence or presence of disease in tissue.

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NONLINEAR PROPERTIES OF THE PROTEINS MAIN CHAIN ATOMIC VIBRATIONS

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The temperature factors series of protein backbone atoms were analyzed by fast Fourier transform, detrended fluctuation analysis, return maps and correlation dimension. The spectral analysis revealed the presence of a long-range correlation characterized on average by a power law P=1/f7/4. The mean value of the scaling exponent was about 4/3. Beyond this range, the scaling exponent decreased significantly. The majority of the analyzed proteins showed return maps characterized by a concentration of the trajectories similar to an attractor. The series of data revealed the presence of a strange attractor having an average dimension of 4.34, which seems to be of deterministic origin. The scaling exponents appeared to be sensitive to the conformational changes of proteins.We also propose an Iterative Correlator with Random Seeds as a method to generate series characterized by a low dimensional attractor (D»4.65) and scaling properties described by a power law P=1/fa where 0<a<2. The method proved to be useful for describing the nonlinear properties of the atomic vibrations in the main chain of proteins.

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STIMULATION OR INHIBATION OF BIOSYNTHESIS OF BETA-CAROTENE BY IRADDIATION WITH GAMMA RAYS OF CALENDULA OFFICINALIS SEEDS

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β-Carotene is one of the carotenoidic pigments which have many biological functions. In plants, carotenoids are essential in photosynthesis where they function as light-quenching and photoprotectors. Carotenoids have a role in pigmentation of flowers and fruits. Next to chlorophyll, carotenoids are the major components of the complex pigment-protein from the thylacoide membrane, and some of them, such as β-carotene, were for a long time considered to be protecting the cell membrane against destructive events caused by the over excitement of the chlorophyll. The most known role of β-carotene is that the precursor of vitamin A.

It is important to see what is the effect of iraddiation with gamma rays of *Calendula officinalis* (marigolds) seeds. Could it be a stimulation or a inhibation of beta-carotene's biosynthesis?

This paper presents results of irradiation of seeds of marigolds. It was carried out irradiation of seeds at 8 different doses (1 kRad, 3 kRad, 5 kRad, 10 kRad, 20 kRad, 50 kRad, 100 kRad, 500 krad), one set of seeds being unirradiated for comparison. The plants have been grown in the same conditions of light, temperature and humidity. The identification of β-carotene was realized through thin layer chromatography (TLC). The chemical concentrations of β-carotene in leaves and stalks of marigolds had been determined by Varian spectrophotometer. Quantitative determination of β-carotene was carried out through spectral analysis using a standard spectrum of carotenoids and chlorophyll a and b.

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FORMATION, INTERACTION, AND FUNCTION OF MEMBRANE TUBES

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Biological membranes often form highly dynamic tubular networks. Their exact role is not known, however, they are most probably involved in the transport and sorting of proteins and lipids. The formation and motion of membrane tubes are thought to involve motor proteins that are able to pull on the membrane as they move along the cytoskeleton. We study the theoretical aspects of the formation and interaction of membrane tubes, and we also investigate their possible role in protein and lipid segregation. We show that the force needed to form a tube changes non-monotonically with its length. In experiments bundles of tubes can often be observed. We show that there is an attractive interaction between tubes that would lead to their coalescence, and we propose a mechanism that explains the formation and existence of bundles. We also show how the coupling between the concentration of the proteins and the mean curvature of the membrane can lead to pearling instability along the tubes, and that a coupling between the concentration and the Gaussian curvature is required to induce segregation.

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THE INFLUENCE OF LOW INTENSITY MICROWAVES ON SOME BACTERIA GROWTH DYNAMICS

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It was searched for the action of low intensity microwaves (power density 10 mW/cm2,frequency of about 10.75 GHz)on growth dynamics in two microbial cultures: Staphylococcus aureus ATCC-6538 (Gram positive bacteria) and Escherichia coli ATCC-10536 (Gram negative bacteria). It was evaluated the number of living cells/ml using a JASCO spectrophotometer for measurements carried out la 3, 6 , 9, 12, 24, 36, 48 and 72 hours in samples and controls. The results obtained revealed a stimulatory effect of microwaves on cell multiplication in both tested bacteria all over the experiment. Statistical computation showed different mathematical functions for experimental graphs approach. Logarithmic function was found to fit to E. coli growth (correlation coefficient equal to 0.978)while exponential function was found to approximate S. aureus dynamics (correlation coefficient equal to 0.758). A low thermal effect could be the main cause of such behavior, as expected. However, a non-thermal effect could also be involved in the dynamics of these pathogen microorganisms.

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APPLICATIONS OF BACTERIORHODOPSIN AS ACTIVE MATERIAL IN INTEGRATED OPTICAL DEVICES

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Coupling of optical data-processing devices with microelectronics, as well as sensory functions, is one of the biggest challenges in molecular electronics. Suitable nonlinear optical (NLO) materials with high stability and sensitivity are intensively researched. In addition to organic and inorganic crystals, biological molecules have also been considered for use in optoelectronics, among which the chromoprotein bacteriorhodopsin (bR) has generated the most interest. bR, isolated from the outer cell membrane of *Halobacterium salinarum*, is the simplest known ion pump and one of the best characterized membrane proteins. Upon illumination it pumps a proton from the cytoplasmic side of the membrane to the outer space, while undergoes a cyclic series of spectroscopically different conformational states.

The big difference between the absorption spectra of the BR_{568} ground state and the so-called M_{412} intermediate state (subscripts denote the maxima of their spectra) is associated with a difference in the refractive index of the corresponding states, as can be calculated using the Kramers-Kronig relations.

The light induced refractive index change of thin purple membrane films containing oriented bR molecules has been measured by the OWLS (Optical Waveguide Lightmode Spectroscopy) technique. It is found that the value of the refractive index change is comparable to, or even exceeds that of the commonly used NLO crystals, which gives the possibility of using it as an active material in integrated optical devices.

The concept of an integrated optical light-driven light-switch utilizing the high sensitivity of the OWLS technique and the outstanding nonlinear optical properties of bacteriorhodpsin is demonstrated. Our results show a promising way to combine molecular electronics with integrated optics in order to develop future all-optical devices.

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CHEMILUMINESCENT AND PHOTOMETRIC REGISTRATION OF ANTIOXIDANT ACTIVITY OF SOME DRUGS

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We studied antioxidant activity of some psyhotropic drugs (chlorpromazine, chlorprothixene, levomepromazine, promethazine, trifluoperazine and thioridazine) in the range of concentration of 10^{-7} - 10^{-4} mol/l. We applied luminol-dependent chemiluminescence to test the ability of these drugs to scavenge the biologically relevant oxygen-derived species: hydroxyl radical, superoxide radical, hypochlorous acid) in vitro. The ability of drugs to interact with those radicals was determined by suitable set of photometric methods: deoxyribose assay, NBT test, taurine chloramine formation. We found that the phenothiazines (chlorpromazine, levomepromazine, promethazine, trifluoperazine and thioridazine) were powerful scavengers of hydroxyl and superoxide radicals. Chlorprothixene had no scavenge activity to superoxide radical. The all drugs showed a moderate scavenger effect on hypochloric anion.

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PROCESSING AND MAGNETIC PROPERTIES OF BIOCERAMICS

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Bioactivity of ferromagnetic glass-ceramics originates from the calcium phosphate that forms apatite in a physiological environment. Their magnetic properties have been shown to be effective in hyperthermic treatment of animal bone cancer. Correlations between processing, structure, and magnetic properties are presented. A series of samples in the system 45(CaO, P_2O_5) $ySiO_2$ xFe_2O_3 were synthesized with varying the processing parameters. X-ray powder diffraction reveals a strong effect of the processing parameters on the qualitative and the quantitative composition of the samples. They all are multiphase systems of 3 or 4 phases. The major phase is calcium phosphate, while hematite and/or magnetite determine their magnetic properties. Magnetic measurements illustrate a strong dependence of the saturation magnetization and hysteresis loss of the biomaterial from the processing parameters. A systematic study of the physical properties in series of ferromagnetic bioceramics is in progress.

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LOW INTENSITY MICROWAVE EFFECT ON DEHYDROGENASE COMPLEX IN CELLULOLYTIC FUNGI CHAETOMIUM GLOBOSUM AND ALTERNARIA ALTERNATA

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Microwave exposure was carried out using 0.9 mW/cm2 power density flow and 9.75 GHz frequency, for 1, 3, and 8 hours daily, during a week. Spectrophotometric assay was used to evaluate enzymic activity of isocitratedehydrogenase, malatedehydrogenase, succinatedehydrogenase and alpha-cetoglutaratedehydrogenase in Chaetomium globosum and Alternaria alternata (fungi of biotecnological interest). Measurements were performed in mycelium at 7 and 11 days after inoculation.The activity of the four enzymes was determined both by exposure duration and culture age.

Stimulatory influence was revealed for isocitratedehydrogenase and alpha-cetoglutaratdehydrogenase in Alternaria alternata as well as for isocitratedehydrogenase in Chaetomium globosum.

Inhibitory influence was noticed for succinatedehydrogenase in Chaetomium globosum and Alternaria alternata and for cetoglutaratedehydrogenase in Alternaria alternata.

Low thermal effect as well as a putative non-thermal effect could be involved in the dynamics of these fungi, revealing new opportunities for controlling biotechnological procedures.

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ELECTRO-OPTIC SOLUTION FOR VISUAL ACUITY AND CONTRAST SENSITIVITY MODELLING

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Vision research is a relevant field to apply physics of light scattering. Opacities in the human eye lens can lead to impaired visual acuity and contrast perception, and hinder medical tests. Interference images may be used instead of incoherent light in clinical tests, but their contrast can still be decreased by light scattering.

In PLZT electro-optic ceramics, applying the electric field can induce an effective light scattering that is similar to scattering in an opaque eye lens. A model eye is set which consists of a plano-convex lens (light refraction) and a PLZT ceramics plate (controllable light scattering). The images are formed on the "retinal"plane and are observed or captured by a CCD through a microscope. Incoherent and interference patterns are imaged to approximate for clinics. Light scattering and diminishing of contrast are observed, when the applied electric field increases over E=5-9 kV/cm.

To evaluate quality changes, Fourier transformation is applied to images, and the optical transfer and point-spread functions are obtained. Transfer functions for the model could provide an additional insight in the optical part of the contrast sensitivity changes.

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METAL SURFACE ENHANCEMENT OF OPTICAL TRANSITIONS IN DNA AND LIPID: EFFECT AND MECHANISM

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The effect of surface enhanced infrared absorption (SEIRA) is well known during last 20 years. It consists in increase of the intensities of IR bands of the molecules adsorbed on metal particles or surfaces. An enhancement factor, which could be reached with SEIRA, equals to 100-1000. The interpretation of this effect similar to more known surface enhanced Raman spectra include at least 2 mechanisms such as local enhancement of external electric field near the rough metal surface due to excitation of surface plasmons and specific increase of the polarizability of the molecules at their adsorption on metal surface.

Data on SEIRA of nucleic acids deposited on the metal surface have been obtained in the experiment in FTIR reflectance mode. As metal surface, we used Au of 200-500 Å thickness on glass substrate. Roughness of Au was obtained by atomic force microscope (AFM) was about 50 Å. In our experimental conditions, the enhancement factor of SEIRA was 3-5. We used SEIRA-spectroscopy for studies of DNA and phospholipids isolated from Carcinoma Guerina cells of resistant and sensitive cancer strains of Wistar line rats and revealed some peculiarities of their structures.

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A COMPACT, HIGH RESOLUTION CAMERA FOR NUCLEAR MEDICINE

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A prototype high resolution photon imaging detector, originally intended for high-energy physics, is being further developed for biomedical applications. At its heart is an Imaging Pixel Silicon Array (ISPA) tube, a hybrid photodetector consisting of a vacuum sealed tube with a YAP:Ce (Yttrium Aluminium Perovskite doped with Cerium) scintillation window featuring an S20 photocathode deposited on its inner side, and a silicon pixel chip acting as a 2-dimensional anode plane. Scintillation light due to the interaction of photons in the crystal window generates the ejection of electrons from the photocathode, which are then accelerated by a 25 kV potential towards the silicon pixel anode, giving a spot whose centroid is used to determine with unprecedented precision the incoming photon's entrance position, and whose number is proportional to the photon energy. The anode plane contains 2048 rectangular pixels with 50 μm × 500 μm, each bump-bonded to their individual front-end electronics channel. The ISPA-tube used in this work is very compact, only 4.0 cm long by 3.5 cm diameter, with a 2.0 mm thick YAP:Ce crystal as gamma converter. With an optimal collimator, nuclear medicine images with resolution about 10 times better than a standard Anger gamma camera can be obtained with this detector. Preliminary results show an energy resolution of 22% (FWHM)) for 59.5 keV Am-241 photons and a very good intrinsic spatial resolution (below 0.5 mm) with ^{57}Co 122 keV photons.

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DO THE PROTEINS FOLD HIERARCHICALLY? RESULTS OF CLUSTERING MONTE CARLO SIMULATIONS

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A role of collective motions and clustering behavior during the folding of 2D lattice peptides was investigated. Two model peptides which have the sequences of hierarchical and non-hierarchical design were studied comparatively. Simulations were performed using two methods: conventional Monte Carlo algorithm with the fixed move set, which completely disregards collective motions, and recently described by the authors the Clustering Monte Carlo algorithm, which provides a realistic description of cluster dynamics. It was shown that the folding pathways and kinetics of hierarchically folding sequence are not described adequately in conventional MC simulations. In this case accounting for cluster dynamics provided by CMC reveals important features of hierarchical folding and dramatically increases the folding rate. Our data suggest that the methods which enables collective motions should be used for realistic description of hierarchical folding.

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LASER SYSTEM FOR DIAGNOSTICS OF LASER INDUCED PROCESSES

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Various processes and instabilities can be excited on a free surface of a melt under action on materials of an intensive laser radiation. The formed in this case structures on a surface of a melt represent significant interest for the laser technology. However direct research of surface waves in conditions of action of laser radiation with high intensity is hampered by availability of brightly flashing erosive plume above area of interaction. For an experimental research of processes in area of laser action we used experimental setup on base of solid state YAG:Nd-laser and a laser monitor on base of copper laser. The use of the laser monitor has allowed to observe of devalopment laser-induced processes on a surface of a melt through formed above action area erosive plume. For example, diagnostics of surface waves in melted material has been carried out. The researches of lead and titanium samples were made under action on their surface of a radiation from solid-state YAG:Nd-laser. Laser-induced surface waves were registered and their wavelength was determined. Obtained by means of the laser monitor computer images were processed by specially developed program. The wave structures on a surface of a melt were registered not all time of laser action. They are failed and are replaced by laminar on a surface movement of a melt from center of a cavity to its periphery or hardly turbulent movement.

Parameters of laser radiation (energetic, spectral, spatio-temporal) contain numerous information. That gives a possibility of selective influence of laser radiation on one or another processes developing under laser processing of material. Analysis and processing this information directly during the technological process will allow to control parameters of laser technological processes and characteristics of processing material.

Offered system provide the increasing of reliability and accuracy of carrying out measurements, flexibility, realisation of monitoring under control of technological process and also realisation of simple contact interface at the conservation of wide spectrum of solving problems.

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PHASE BEHAVIOR OF RAMAN SOLITARY WAVES AT DETUNING FROM RAMAN RESONANCE

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Solitary waves in stimulated Raman scattering observed as intensity spikes in a region of pump depletion. These waves can be generated both spontaneously and deterministically. Recent studies of phase behavior of spontaneous solitary waves have shown an existence of solitary waves, which were in phase, out of phase or whose phase changed the sign relative to input pump pulse [1]. But reasons resulting in generation of the solitary waves with different phase behavior remained unclear. To find out such reasons an investigation of phase structure of the solitary waves generated deterministically by optical phase shift was made. Results of the work are presented in this report. In the experiment a second harmonic of single-frequency TEM_{00} Q-switched YAG:Nd laser was used to pump the Raman medium. Stimulated Raman scattering was done in hydrogen on $Q_{01}(1)$ transition. A multipass configuration of Raman generator and Raman amplifier was used for soliton generation. The phase structure of the depleted pump pulses was investigated interferometrically using modified Mach-Zehnder scheme. Interferometric signal was obtained by superposition of the depleted and undepleted pump pulses. Solitary waves were created in the Raman amplifier through injecting of π-phase jump between the pump and Stokes fields. Such jump was realized electro-optically by Pockels cell in two different ways: either an amplitude-modulated phase shift was produced in the pump pulse or the shift was in the Stokes seed. Solitary waves, which were in phase, out of phase or whose phase changed the sign relative to input pump pulse were detected regardless of input wave on which the phase jump was introduced. Average amplitude of the solitary waves, which were out of phase, was about five times less that of in-phase solitons and twice as little than average amplitude of the solitons, whose parts were interfered with opposite signs. It has been inferred that frequency detuning from Raman resonance in the Stokes seed leading to soliton decay is also responsible for generation of the solitary waves with different phase. Numerical study shown that detuning leads to formation of phase-modulated solitary pulse. Phase shift of leading soliton edge depends on detuning and Raman gain. Modulation time is compared to soliton duration for magnitudes of detuning observed from quantum fluctuations. As a consequence phase of the solitary wave is not fixed as the solitary wave propagates in the Raman medium. At zero detuning only solitary waves, which phase coinciding with that of exciting wave, are observed. Our work shows that frequency detuning in the input Stokes pulse resulted from quantum fluctuations leads to generation of solitons with phase shifted stochastically from shot to shot.

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FORMATION AND DECOHERENCE OF SCHRÖDINGER-CAT STATES IN THE MORSE POTENTIAL

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We investigate the dynamics of an initially well-localized wave packet in the Morse potential with coupling to a thermal environment of harmonic oscillators. A master equation is introduced describing the time dependence of the reduced density operator corresponding to a general anharmonic system. This equation is applied to the case of the Morse oscillator, where periodic collapse and revival in the expectation value of the displacement operator is related to the formation of Schrödinger-cat states. The environment damps the amplitude of these revivals according to the strength of the coupling, and the Schrödinger-cat states also disappear gradually. We characterize the states of the system which arise due to the effects of the environment by the aid of the corresponding Wigner function. Dissipation of the system's energy leads to thermal equilibrium as the final, steady-state solution. The time scale of decoherence is much shorter, and gives rise to states which are mixtures of localized states along the phase-space orbit of the corresponding classical particle. This behavior is to a large extent independent of the coupling strength and the temperature of the environment.

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"ANOMALIES" OF LASER-INDUCED EXPLOSIVE EVAPORATION IN LIQUIDS

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Threshold conditions of a thermal destruction of quasi-liquid bio-structures irradiated by laser pulses are explored. The work is a physical background for application of power IR lasers in surgery.

The objects of investigations were water or gel dye solutions with controlled spectral absorption coefficient and the alterations of media irradiated by YAG laser was fixed. The alterations take place as the result of formation of micro-bulbs at preliminary stage of explosive evaporation.

The experimental dependence of the initial temperature of explosive evaporation T as a function of spectral absorption coefficients of the medium (for $1<K<30$ sm^{-1}) is found. The measured volumes T is variable over thte range 95-110 ºC. These data are inconsistent with classic concept of the explosive evaporation temperature, that has order of 200 - 210 ºC for heating pule of about 100 ms.

A feature of laser action onto liquids is forming of acoustic fields formed as a result of superposition of waves created by separate spikes of running (free) laser generation. Described effect can be used for creating of effective laser surgery scalpels of new generation.

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PARAMETRIC SELF-EXCITATION OF DIPOLE OSCILLATIONS OF A MOLECULE ROTATING IN THE VICINITY OF CONDUCTING MEDIUM

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The effect of parametric self-induced excitation of dipole oscillations in a molecule rotating in the vicinity of a plane metallic surface is predicted. The rotation may be inertial or driven, say, by a rotating linear polarized laser field. The dipole oscillations are treated either in a model of two-level quantum oscillator or in a model of nonlinear semiclassical oscillator. The effect exists under the following conditions:

I) the plane of molecular rotation is not parallel to the metallic plane,
II) the distance between a molecule and the metallic plane is of the order of or much less than the radiation wavelength,
III) the rotation frequency is in Mathieu resonance with the frequency of dipole oscillations.

The phenomenon originates from the periodic modulation of the value of an image dipole which depends on the orientation of the original dipole. We find the growth rate of the parametric instability and investigate analytically the saturation stage of the instability process. We calculate the radiation losses of a rotating dipole and show that parametrically excited molecular bunches can be used as a new source of coherent radiation.

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METHOD OF INTEGRAL EQUATIONS FOR ULTRAFAST PULSES AND ITS APPLICATION TO THE OPTICAL PROPERTIES OF GaAs

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Instead of using a frequency-dependent refractive index, we propose to use the integrodifferential equation approach to describe reflection and transmission of an ultrashort pulse passing through the system`s boundary. This method, which is an adaptation of the extinction theorem for ultrafast pulses, explicitly follows time and space evolution without the slowly varying envelope approximation. When the duration of the pulse is comparable with the relaxation time, the results differ significantly from those given by the traditional method Fresnel formulas), especially if the carrier frequency is close to an absorption line. We compare the two approaches, using the data of GaAs in the infrared domain where pulses of only a few cycles are available experimentally. We also work out a method that efficiently includes the background refractive index that originates from electronic transitions.

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LYOT FILTERS OBTAINED FROM THIN CRYSTALLINE FILMS

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The article deals with the study of light filters design; there are treated the filters that are based on interference of polarized light in tiny crystalline films. A presentation of the steps that leads to a certain wavelength filter is shown in the present article, also. Four filters were obtained using crystalline films of different thickness. Maximum transmitance was detected for wavelength value of 5000Å, 5130Å, 5900Å and 6590Å respectively.

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SPECTROSCOPIC-ELLIPSOMETRICAL STUDY OF THE CONDITIONS OF PHOTON–SURFACE-PLASMON COUPLING IN DIFFERENT TYPES OF MULTILAYER DIFFRACTION GRATINGS

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Devices using surface-plasmon resonance (SPR) coupling in a multilayer diffraction grating on a semiconductor surface are basic components of optochemical sensors and photodetectors sensitive to wavelength, angle of incidence and polarization of light. Their sensitivity can be changed over a wide range of the light spectrum (UV, visible and IR) by variation of geometrical, structural and optical parameters of multicoated diffraction gratings.

In this paper we present results of investigations of Au-Cr-GaAs and Al_2O_3-Al-GaAs multilayer structures employing atomic force microscopy (AFM), optical and spectroscopic-ellipsometrical measurements. Fabrication of different types of the investigated structures, such as diffraction grating and bi-grating (the grating groves along two perpendicular dorections), started with manufacturing of the surface diffraction gratings on GaAs substrates by holographic technique. The microstructure and geometrical parameters of each grating were defined by means of AFM measurements. Thin metal (Al, Au, Cr) films were thermally evaporated on the corrugated semiconductor substrates. Optical and structural properties of the metal and oxide overlayers were studied by spectroscopic ellipsometry

Our special interest was focused on the study of interaction of p- and s-polarized light with the multilayer grating surface under conditions of the grating grooves being perpendicular and/or parallel to the plane of incidence of light. We have observed a splitting and/or a broadening of SPR maximum for different types of multilayer structure. We have analyzed the conditions of SP-excitation in both types of the multilayer diffraction gratings.

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NEAR-FIELD TRANSITION RADIATION BY BUNCHED ULTRARELATIVISTIC ELECTRONS

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The transition radiation by bunches of ultrarelativistic electrons which passed through the thin metallic transverse-limited disk has been considered in the near-field region. For the long-wavelength radiation both longitudinal and transversal sizes of region where radiation is formed (near-field or pre-wave region) have the macroscopic values. The most interesting case of small-size detector in the near-field region is investigated.

It is shown that in the pre-wave region the strong self-interference of transition radiation field and interference between own electron field and whole radiation field are occurred. The simple analytical formulas for spectral-angular distribution of electromagnetic energy flux in the "forward"and "backward"directions have been obtained. Both the spectral-angular density of whole electromagnetic energy flux and spectral-angular density of transition radiation are strongly depending on distance from the target. The considered interference effects can play very important role in the number of modern experiments with accelerated bunches of high-energy charged particles.

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ATOM CLUSTER IMAGING BY FREE ELECTRON X-RAY LASERS

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Linac based free electron lasers will produce extremely short (<100fsec) and intense (~10^{12} photon/pulse) hard x-ray pulses. The unique features of this beam will allow the study of the atomic structure and the different physical and chemical processes in solids at a level not accessible today. However, to understand the experimental results one has to have a detailed picture of what happens during the burst in the sample. In several suggested applications small samples containing only 10^3 - 10^6 atoms are the possible candidates. In order to have a feeling about the atomic motions, we performed model calculations on the dynamics of particles of a cluster in an intense hard x-ray pulse. The parameters of the pulse were chosen to be in the range of the planned free electron lasers. The movement of the particles was followed by non-relativistic classical dynamics. The main processes: photo-absorption, Auger process, inelastic and elastic scattering of electrons were taken in to account by their respective cross sections. Here we report our findings on all carbon atom clusters. The results show that the clusters disintegrate via Coulomb explosion, similarly to small clusters in intense laser beam. However, the dynamics of the explosion is significantly different. We analyzed our data from the point of view of structure determination. We found that the number of ionized particles increases faster than expected in previous studies. Therefore collection of useful data is possible in the first ~10% of the pulse.

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NONLINEAR INSTABILITY ANALYSIS AND IMPURITY LIQUATION FOR SOLIDIFICATION WITH A MUSHY LAYER

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The present work is devoted to the nonlinear instability analysis of exact analytical solutions obtained in Ref. [1] for the solidification with a metastable two-phase zone. This study shows that the instability may evolve in accordance with "oscillatory"scenario. It is well-known that oscillatory behavior of a solid-liquid interface is responsible for the layer distribution of impurity in the solid phase. Such a liquation changes many properties (e.g. mechanical, electrical, and so on) of solid ingots. Therefore, a calculation of liquation characteristics is very important from industrial and theoretical point of view. The nonlinear analysis under consideration helps us to find a law between the frequency and amplitudes of main harmonics. In the present study, not only the aforementioned law was deduced but also a distance between neighboring layers of impurity distribution in the solid was found.

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REVERSIBLE AND IRREVERSIBLE ABSORPTION OF GAS MOLECULES AND THE POSSIBILITY OF THE APPEARANCE OF NEGATIVE PROBABILITY AND COMPLEX ENTROPY

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Gas in a vessel containing absorber can be absorbed in two ways. Irreversible absorption is taking place when absorbed gas molecules do not go back to the medium from which they were absorbed. Reversible absorption happens when absorber returns a part of the absorbed molecules and possibly absorbs them later again. The change of the number of molecules in time, due to irreversible absorption, is proportional to the number of molecules, while in case of reversible absorption it is proportional to the mean value of the number of molecules in time. Markov's graph is given for processes described, which is used to formulate the system of integral-differential equations. That system can be reduced to one degenerated hyper-geometric equation, with Kumme's functions as its solutions. The probability of finding a particle in absorber and out of it is described using Kummer's functions. At certain choice of the parameters these probabilities may become negative which implies complex values for system entropy. In this paper I analyse the conditions when negative probability of the absorption of gas molecules may occur.

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MODE-COUPLING APPROACH FOR SPIN-FACILITATED KINETIC ISING MODELS

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The *d*-dimensional *2*-spin facilitated kinetic Ising model is studied analytically starting from usual master equations and their transformation into a Fock-space representation. The evolution of relevant operators is rewritten in terms of a projection formalism. The obtained frequency matrices and memory terms are analysed. Especially, the structure of the memory terms is approached by using the well-known factorization approximation as the standard decomposition technique of *N*-point correlation functions. The temperature dependence of the relaxation times related to the *2*-spin facilitated kinetic Ising model shows a non-Arrhenius behaviour. Furthermore, a characteristic stretched decay of the correlation function is obtained.

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WILL IT EVER DIE? FIGHTING AUTO-CATALYTIC PROPAGATING ILLS WITH FIELD THEORY

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The representation and study of complex social dynamics using statistical mechanics and field theory techniques has become recently an important subject of research.

In particular it was found that Statistical systems of discrete proliferating elements present very non-trivial phase diagrams [1]. In particular the renormalization group analysis showed that for large enough 2-dimensional systems, discrete proliferating dynamics leads always to the survival and expansion of the proliferating trend irrespective of the destruction rate enforced on the individual elements [2]. For finite (small) size systems however, this effect eventually disappears.

The discrete spatially extended character of the social interactions makes the propagation of social trends very dependent on percolation-transition effects [3].

We apply the effects 1 and 2 to the problem of stopping unwanted proliferating social ills such as smoking, drugs, violence and terrorism. According to 1), the prospects are that in a large enough world such trends can never be subdued. As a possible way of fighting them, we show that by interdicting certain sites to the propagating ill (e.g. non-smoking areas, terrorist stopping boundaries), one leads (according 2) to the splitting of the available space into disconnected finite regions in which the proliferating trend disappears according to 1).

An animated simulation movie demonstrating these effects will be presented and comparison with real life phenomena will be discussed.

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FRACTAL AND NON-LINEAR PROPERTIES OF FAST HYDRODYNAMICALS PROCESSES

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The fractal methods of processing of optical images has been developed. The local dimensions of similarity information and topological entropy of images were calculated. These parameters allow to determine the moment of change of hydrodynamical conditions of melted material movement

For study of development of processes on a surface of substance under action of powerful laser radiation we offered to use methods of the nonlinear dynamics. These methods allow to restore a phase portrait of dynamic system and determinate the character of hydrodynamicals processes on the substance's surface.

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CHAOS ENFORCED INSTANTON TUNNELING

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The influence of chaos on quantum tunneling is an important problem not only in quantum mechanics (chaos assisted tunneling), but also in quantum field theory (the search of instanton induced events in QCD). The problem is an extremely small probability of instanton tunnelings in realistic theories of particle interactions (electroweak theory, QCD). We demonstrate on the example of the model system that small perturbation leading to chaos squeezes dilute instanton gas and increases the probability of instanton tunneling.

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FADING MARKOVIAN RANDOM EVOLUTION

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Process of Markovian random evolution is studied. The process models particle's motion under a force which increases its velocity. The limit distribution of particle's position is found. Nonlinear integral and differential equations for the functionals of evolution are also found and solved.

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SCALING PROPERTIES OF EIGENVALUE SPECTRA IN ARBITRARY ONE-DIMENSIONAL QUARTER-WAVE FRACTAL NANOSTRUCTURES

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We have shown that fractal multilayer stacks, as a whole class of multilayer nanostructures, possess scalable eigenvalue spectra (optical for dielectric and electron energy for semiconductor stacks). The scaling relations have been found to match the geometrical parameters of the structure. An analytical calculation based on the generalization of the method proposed by Sun and Jaggard [D.L.Jaggard, X.Sun, Opt.Lett.,1990, vol.15, p.1428] has shown that spectral scalability directly results from spatial self-similarity of the multilayer.

Both analytically and numerically, spectral scalability was found to persist in all fractal multilayers. This means that it is a characteristic property of fractal structures, such as the presence of forbidden energy gaps is characteristic for periodic multilayers or Cantor-set spectra are specific for quasi-periodic stacks.

Additionally, it was found that quarter-wave condition, which requires all constituent layers in the structure to be of equal optical length, plays an important part in letting one observe scaling properties even in structures with smaller number of layers. Other conditions leading to more apparent scalability are investigated.

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