## Theoretical Study of Electron Affinities for Selected Diatomic Molecules

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It is very important to have accurate values of electron affinities (EAs) for various chemical systems because knowledge of them is necessary in solving of many problems in plasma physics and chemistry. However, experimental data are rather difficult to obtain for many molecular species. On the other hand, theoretical methods give diametrically different results. In this work we tested various approaches to calculations of electron affinities for homonuclear and heteronuclear diatomic molecules.

The EAs were computed as differences in total energies of fully optimized neutral and negatively charged diatomic molecules, i.e. $C_2$, $O_2$, $F_2$, $Cl_2$, OH, LiF, NaF, CH and CN. All computational studies are performed with the Gaussian 03W computational package. Results of Hartree-Fock and hybrid DFT methods: BVP86, B3LYP, PBEPBE, MPW1PW91, HTCH and THCTH with 6-311G++(2d,2p) and 6-311G++(3df,3pd) basis sets and high levels of ab initio computational studies with the quadratic complete basis set (CBS-Q) were compared with experimental data. Our results show that it is not possible to select one of the most efficient approaches to EA calculations for all studied molecules. Generally, the HF/6-311G++(3df,3pd) method underestimates EAs, in particular, for OH molecule, where it gives negative values (-0,27 eV). All DFT methods slightly overestimate electron affinities with the exception of B3LYP, B3PW91, MPW1PW91 and PBE1PBE for OH, where we obtained 1.75, 1.65, 1.54 and 1,53 eV, respectively, in comparison to 1.83 eV experimental value. For the $F_2$ molecule CBS-Q method was the best – we obtained 3.04 eV with comparison to experimental 3.08 eV.

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## PIC/MC Simulation of Charging of Dust Particles in Low-Temperature Plasma

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Dusty plasma is defined as plasma containing nanometre- or micrometre-sized particulates (dust grains). Since 1990s many scientists have been interested in studying of dusty plasma and in the last decade the papers concerning dusty plasma become one of the most cited in scientific articles and the number of contributions increases exponentially.

It is well known that the particulate immersed into a low-temperature plasma charges negatively because of the higher mobility of electrons. Its surface charge is a crucial quantity influencing other processes. There are several models describing the charging process. Nearly all of them are based on the fluid modelling technique, comparing the continuum fluxes of charged species to the particle surface. The computations can be performed relatively quickly, but under simplifications affecting the precision of calculations, especially for low-pressure plasma.

In this study we have applied less frequent approach – the models based on the particle (PIC) simulation. Although this approach does not provide the most effective way in the computational point of view, this technique allow us to describe satisfactorily all important fundamental processes during the charging of the particulate.

Presented results were obtained by simulations of micro-sized particles in low-temperature argon plasma at low pressure. In the first part we focus on charging of particles in plasma bulk in dependence on various parameters (plasma temperature, pressure, ...), in the second one the particle charging in the plasma sheath is considered. The collision cross-sections of the most frequent processes (elastic scattering, excitation and ionisation) are considered in dependence on energy. The motion of particles is studied by Verlet's algorithm, the collisions of particles are simulated by the Monte Carlo method.

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## Diagnosis of Xe Plasmas Using a Collisional-Radiative Model

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As a rare gas, Xe presents an outer shell structure consisting of two *s* and six *p* electrons. These outer electrons are easily ionized due to the presence of ten 4*d* electrons lying just lower in energy, a structure which is absent from the Ne and Ar atoms. Although its use is hampered by its scarceness in nature, Xe has a number of interesting properties such as high atomic weight, low ionization potential and chemical inertness. Consequently, Xe has been used in a number of applications, including adoption as a plasma thruster propellant (note the parallel use of In as a propellant, with an iso-electronic sequence to which Xe VI belongs), in lighting (because of the rich $5s^2p^6$ spectrum) and as a puffing gas for diagnostics in Tokamaks (especially in the divertor region, although Ar could be preferred because of the transmutation risks).

Non-intrusive emission spectroscopy is largely used in plasma diagnostics, because it allows for the evaluation of the local temperature and density, and provides information on the constituents and most important processes encountered in the plasma. The satisfactory application of such diagnostics requires a full Collisional–Radiative (C-R) model that takes into account all of the species present, both neutral and ionized, together with their excited state level structure. All contributing processes, notably transition probabilities between the levels, electron collision excitation, de-excitation and ionization and re-combinations (Radiative, di-electronic) need to be taken into account through their respective reaction rates. Hence, considerable amounts of Xe atomic data are required for modeling and optical diagnostics. We have evaluated a large amount of such data, which we have subsequently used in building a C-R model for the optical diagnostics of various Xe plasmas. A Maxwellian distribution was used throughout this work as a first approximation for the calculation of the reaction rates, which are entering directly into the second members of the statistical equations.

We report here on the characteristics of this model as applied to the diagnostics of a low temperature Xe plasma produced in a hollow cathode with dielectric barrier, available at the LPGP laboratory. Comparisons of the theoretical spectra generated from our model with the experimental data obtained at LPGP have been used to validate the Xe I and II atomic data and the theoretical approaches adopted. They also allowed for a systematic study of the Xe I and Xe II spectra, which lead to identification of many observed lines in the spectral region of 200 to 1000 nm, with evaluation of their energy levels and of the corresponding transition probabilities. These lines belong to the main Xe I and Xe II multiplets, with exclusion of the resonant ones which are typically present in the far UV region.

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## Investigation of Dust Particles in Collisionless Plasma Sheath with Arbitrary Electron Energy Distribution Function

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Dust particles often appear in industrial plasmas as undesirable product of the plasma-wall interactions. Large particles of several micrometers in diameter are concentrated in a thin layer (the sheath) above the lower electrode of the rf driven parallel plate device, where the electric force is strong enough to compensate particle’s gravity. The key parameter characterizing dust in the plasma is its electrical charge. Present-day theories as well as experiments are not fully successful in determining its value. Moreover, the theoretical uncertainties are significantly increased in the plasma sheath. Common model of dust charging in the plasma sheath supposes the Maxwellian electron energy distribution function (EEDF) in conjunction with a flux of cold ions satisfying classical Bohm criterion at the sheath edge. In this paper we generalize this model of plasma sheath and dust charging to arbitrary EEDF with adapted Bohm criterion. We limit our considerations to collisionless or slightly collisional plasma, where the EEDF inside the sheath is expressed through the EEDF in the plasma bulk. This is of practical importance as the EEDF in the plasma bulk can be determined experimentally.

Derived theoretical formulas are incorporated into complex numerical models, describing collisionless radio frequency (rf) or direct current (dc) plasma sheath together with particle’s quantities (electrical charge, various kinds of forces, oscillation frequency, balancing radius). It is investigated how these quantities are sensitive to various optional parameters characterizing plasma or particular model. For instance we compare balancing radii and resonance frequencies of dust particles levitating above a planar rf electrode for different EEDF’s in argon plasma. Although all distributions are chosen with the same plasma density and electron effective temperature, the balancing radii and resonance frequencies of particles confined in the sheath are noticeably different.

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## Spectroscopic Investigation of Back-Corona Discharge on the Fly-Ash Layer

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Back discharge is one of the major problems in electrostatic precipitators and other particle charging systems. Back discharge decreases the efficiency of electrostatic precipitators. During this discharge, the particles of fly-ash deposit on the collection electrode are remitted to the flow. The physical background of this type of discharge is the subject of the present paper.

The back-discharge denotes the effects which take place at passive electrode in a discharge system coated with a dust layer of high resistivity. In the case of electrostatic precipitators such a layer is formed by charged-particle deposit. The discharge processes close and within this layer have an important effect on ionization and recombination processes near discharge electrode and in the drift space between the electrodes. The results of spectroscopic investigations provided information on ionization, recombination are dissociation processes which take place in this type of discharge. The emission spectra were taken from two discharge zones: near the needle electrode and close to the crater formed in the layer. The discharge was generated in point-plane electrode geometry in ambient air at normal temperature and atmospheric pressure. Three forms of back discharge for positive and negative polarities were investigated: glow, streamer and low-current back-arc.

The discharge spectra in the spectral range of 250-600 nm have been measured. The light spectra measured for the back discharges were compared with those obtained for corona discharge generated in the same electrode configuration but with dielectric dust removed. In normal condition, the emission spectra were dominated by the gas compounds, air in the case of our experiments, (molecular nitrogen, nitric oxides). But in back discharge, atomic lines emitted by the chemical compounds of the fly ash were also identified.

Visual forms of discharge were recorded with digital camera and referred to current-voltage characteristics and emission spectra.

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## The Influence of Electrode Gap Width on Plasma Properties of Diffuse Surface Coplanar Barrier Discharge in Nitrogen

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Fast in-line plasma processing of materials often requires generation of highly non-equilibrium homogeneous plasma with as high as possible power density. The plasma source that can fulfill these requirements is the diffuse coplanar surface barrier discharge. The diffuse coplanar surface barrier discharge (DCSBD) has unique properties such as the generation of thin diffuse layers of macroscopically stable and uniform non-equilibrium plasma at atmospheric pressure with high power densities.

There are numerous parameters that can affect plasma properties of the DCSBD. Previously the influence of surface emitting layers on parameters of DCSBD has been reported. In this work the influence of inter-electrode distance (electrode gap width) on plasma parameters of DCSBD is presented. The ignition and extinction voltages as well as space profiles of rotational and vibrational temperatures were studied.

Discharge was excited under atmospheric pressure in pure nitrogen. The frequency of applied high voltage was 35 kHz. The electrode system arrangement enabled us to change the inter-electrode distance in the range from 0.01 to 5 mm in continuous way. Within this range following sequence of distances was selected: 0.5, 0.8, 1.2, 1.7 and 2.2 mm.

Electrical parameters as applied voltage and discharge current were measured by fast digital storage oscilloscope LeCroy WaveRunner 6100A. The discharge spectra were recorded by HORIBA Jobin-Yvon FRH 1000 spectrometer equipped with CCD and iCCD detectors. The quartz optical system enables us scanning (profiling) of discharge plasma in axis perpendicular to electrode orientation.

The changes of ignition and extinction voltages with respect to inter-electrode distance were followed up and it was found out that the ignition voltage increases linearly with the inter-electrode distance. The extinction voltage also increases but with much less rate. Using space-resolved optical emission spectroscopy the spatial profiles of vibrational temperature of second positive system of nitrogen ($\Delta\upsilon = -2$) and rotational temperature of R1 rotational branch of second positive system of nitrogen ($\Delta\upsilon = 0$) were obtained. In addition to these measurements the effects of inter-electrode distance change on spatial and temporal distribution of DCSBD plasma were investigated. The time-space intensity maps of second positive and first negative systems of nitrogen were integrated from the spectra. Analyzing the temperature profiles and time-space intensity maps different regimes of the discharge can be distinguished.

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## Non-Maxwellian Electron Distribution Function in He/Ar, He/Kr and He/Xe Low Temperature Plasma

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Influence of inelastic processes on electron energy distribution function (EEDF) in low temperature plasma was observed many times. Production of fast electrons in Penning ionization and non-Maxwellian EEDF were observed in various experiments. Bi-Maxwellian EEDF and depletion of fast electrons due to inelastic collisions were also observed very frequently. In majority of these experiments EEDF were measured in non-isothermal plasma with electron temperature $T_e > 1$ eV. Only very exceptionally EEDF was measured in low temperature - thermal plasma with $T_e$ ~ 300 K. Experimental studies of EEDF in well-defined conditions in low temperature Flowing Afterglow plasma using Langmuir Probe (FALP experiment) are reported. EEDF were obtained from the retarding region of the probe characteristic using Druyvesteyn formula. The EEDFs were measured in pure helium with small admixtures of atomic reactant gases (Kr, Ar and Xe) at medium pressures ($p_{He}$ ~ 1600 Pa) during late afterglow (35 to 95 ms after the discharge) in nearly relaxed thermal plasma ($T_g$ ~ 250 K). The influence of fast electrons produced in interactions of helium metastable on body and tail of EEDF was observed in pure Helium afterglow. If reactant gases (Ar, Kr, Xe) were added we have observed the influence of Penning ionization and the influence of formed excited ions. Molecular $H_2$ (or $D_2$) was added together with Kr to the afterglow to measure EEDF in the plasma governed by a recombination of $KrH^+$ (or $KrD^+$) ions. Due to superelastic collisions the EEDF in the plasma is clearly non-Maxwelian.

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## Measurement of Fundamental and Higher Harmonic Frequencies as Tool to Control RF Sputtering Deposition Process

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Deposition of thin films by reactive magnetron sputtering is nowadays largely used process to prepare wide range of compound thin films. Oxygen or nitrogen gas is routinely added to the deposition process in order to let grow the oxide or nitride thin films. Adding the reactive gas to the deposition chamber may result in processing stability problems. Reactive magnetron sputtering controlled by flow of the reactive gas exhibits hysteresis behaviour. Increasing the flow of the reactive gas results firstly in enhanced gettering of the reactive gas in the growing thin film and the compound fraction on the target remains low – process runs in so called metallic mode. However, when the growing thin film reaches its gettering capacity, the target erosion rate steeply drops. In this case, it is told that transition from metallic to compound mode takes place. In order to retrieve the reverse steep increase of the target erosion rate it is necessary to decrease the reactive gas flow substantially. Since the optimal experimental condition for the thin film deposition lies very close to the transition from the metallic to the compound regime a continual monitoring of the deposition process is desirable. The most common markers used in industrial application are the following: bias on the cathode, partial pressure of the reactive gas, intensity of atomic lines and/or intensity of molecular spectral bands.

In this work, we propose other very sensitive method to control whether a radio-freguency (RF) sputtering deposition processes runs in a pre-adjusted experimental conditions. Due to the non-linearity of sheaths, RF discharges are sources of higher harmonic frequencies of electric voltage and current. Since the amplitudes of the harmonics are sensitive functions of plasma parameters, they can be used as a simple diagnostic tool for RF plasma processes. Therefore, one may expect that the abrupt change of all processing parameters during the transition from the metallic to the compound regime (such as formation of compound layer on the target, changes of plasma composition followed by change in plasma conductivity etc.) should affect the sensitive amplitudes of the harmonics. The proposed method includes identification of sensitive harmonics by harmonic analyses of discharge voltages and regulation of reactive gas flow according to variation of amplitude of selected harmonic frequency.

The frequency spectrum of the cathode voltage and of the voltage on an uncompensated probe immersed in the plasma was measured in order to test the performance of the proposed method. The experiment was performed sputtering titanium target in argon gas with small admixture of nitrogen or oxygen. The outputs were compared to other quantities usually used for process monitoring. It has been proved, that some of the harmonics are extremely sensitive markers of the transition between two regimes of interest.

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## Probe Measurements on Plasma Pencil Discharge

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This paper deals with the topic of the double probe measurements on plasma pencil discharge. At first the experimetal setup is described. Later the results of our measurements are discussed. All measurements were carried out in the outer zone of discharge. No measurements in the core of discharge were possible. We carried out the measurements at various distances from the core, beginning at the distance of 1 mm, because it was impossible to carry out the measuremets in distances shorter than 1 mm. For all these distances we established dependence on discharge output. The smallest discharge output was 50 W, the greatest one 150 W.

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## Non-Local Equation for Source of Ionization in Hollow Cathode

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To simulate an influence of pendulum effect in hollow cathode configuration on a current-voltage characteristic it is proposed to consider plane glow discharge in one-dimensional space configuration with two plane parallel cathodes and one plane anode in the middle. Pendulum effect could be switched on or off, with consideration for the anode to be transparent or not for fast ionizing electrons. On a basis of a stationary kinetics equation for ionizing electrons an integral equation for a source of ionization is derived. For hollow cathode discharge configuration (HCD) it is

$$S(x)=\sum_k N\sigma_{ion}(w_k(x,-v_{ec}))+\sum_k N\sigma_{ion}(w_k(x,v_{ec}))+$$
$$+\int_x^{x_c} dx' S(x')\Bigg(\sum_k N\sigma_{ion}(w_k(x,V_0(-x',0)))\theta(t_k(x,V_0(-x',0))-T(-x',0))+$$
$$+\sum_k N\sigma_{ion}(w_k(x,V_0(x',0)))\theta(t_k(x,V_0(x',0))-T(x',0))\Bigg),\quad 0<x<x_c.\quad HCD$$

Here $S$ is a number of ionization acts per unit of electron path, which corresponds to one cathode electron; $x_c$ is a width of cathode-anode gap; $N$ is gas density; $\sigma_{ion}$ is a cross-section of electron impact ionization; $w_k(x,v_0)=m_e v_k^{\,2}/2e$, $t_k(x,v_0)$, $k=1,...,K$ are values of electron kinetics energy and time of motion for spiral electron phase trajectory in anode distance $x$ with initial velocity $v_0$ in the cathode; $v_{ec}$ is a velocity of monochromatic cathode electron beam; $V_0(x,v), T(x,v)$ are initial velocity and time functions for phase point $x,v$; $\theta(z)=0,\ z\le 0;\ \theta(z)=1,\ z>0.$ First two terms describe a contribution into ionization of cathode monochromatic electrons only, next integral term describes ionization with secondary electrons. When anode is not transparent for fast electrons – simple glow discharge configuration (SGD) – this equation has simplified form

$$S(x)=N\sigma_{ion}(w(x,-v_{ec}))+\int_x^{x_c} dx' S(x')N\sigma_{ion}(w(x,V_0(x',0))),\quad 0<x<x_c.\quad SGD$$

If one guesses local dependence $\sigma_{ion}(x)=\sigma_{ion}(w(x))$ by neglecting a dependence on second argument, $V_0(x',0)$, the equation can be simplified further:

$$\frac{dJ_e}{dx}=-\alpha(x)J_e,\quad J_e(x)=J_{ec}\left(1+\int_x^{x_c} dx' S(x')\right),\ \alpha(x)=N\sigma_{ion}(w(x)).$$

It is well known continuity Townsend equation from local Engel and Shtenbek cathode dark space theory. Thus, equations presented give non-local extension of classical ionization theory.

Local theory cannot be used for description of hollow cathode electron oscillations. The non-local equations derived can be used as a component in self-consistent problem for field equations to calculate a current-voltage characteristic and to show how it changes in both cases – in presence or absence of anode transparency.

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# Pre-sheath Formation in an Oblique Magnetic Field: Fluid Model and PIC Simulation

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Pre-sheath formation in front of a floating electrode immersed in a magnetized plasma with the magnetic field at an oblique angle to the wall is studied with a one-dimensional fluid model. The model equations are integrated numerically in order to find the space profiles of the potential, density and ion velocities for various densities and angles of the magnetic field. The results are compared to the profiles acquired from the particle-in-cell computer simulation. We have used the BIT1 code, which is an upgrade of the XPDP1 code developed at the University of California at Berkeley. The theoretical model is collisionless with isothermal ions and we have therefore adapted the simulation input parameters in this manner. Individual simulation results were, qualitatively in accordance with the theoretical grounds as well as the analytical model. But a problem occurred due to parameters yielded from the simulation being in absolute SI units. Because of the different particle densities in the steady state at different input parameters of the simulation, it was not possible to make a good comparison with the results of the analytical model and even between simulation results themselves. Consequently we had to normalize the simulation results to evaluate the solutions correctly. The inter-comparison of the simulation results was in good qualitative agreement with the theoretical predictions. After a correct normalization we were able to make a quantitative comparison of the results obtained from the PIC simulation with the results obtained from the analytical model.

The results confirmed our expectations. The effect of the magnetic field is easily recognizable in the simulation results as well as in the numerical results. The formation of the magnetic pre-sheath depends on the density of the magnetic field as well as on the angle of the applied field. For intermediate angles and higher densities of the field we were able to identify a well defined Chodura layer, where the ions reached supersonic speeds in the direction of the applied magnetic field. We could also notice the effect of the magnetic field on the thickness of the magnetic pre-sheath in our simulation results. We could not confirm the effects of the magnetic field on the sheath formation with the analytical model, because the fluid set of equations only treats the quasi-neutral pre-sheath.

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## Optical Spectroscopic Investigations of Heterogeneous RF Plasma at Low-Pressure

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The low-temperature plasma decontamination and sterilization of surfaces has received a great attention in recent years, especially in the medical praxis or pharmaceutical industries, but also in microelectronics and in thin-film production. Ordinarily, the plasma in a low-pressure rf discharge in rare and molecular gases is used for surface treatment and usually it contains finely dispersed liquid or solid particles (CDP). The presence of CDP can substantially change the plasma properties and lead to a number of new effects. In this paper spectroenergetic properties and thermodynamic parameters of a heterogeneous rf plasma are investigated by optical spectroscopic methods.

A capacitively coupled RF discharge was operated on frequency of 5.28 MHz between two parallel plate electrodes with diameter of 120 mm, separated by a distance of 20 mm [1]. The gas pressure was varied between 0.3 and 1 Torr. The experiments were performed in helium, air and He+$CO_2$ mixtures. The supplied full specific RF power was in the range 0.1 - 0.9 W/cm$^3$. The plasma parameters are investigated at presence of $Al_2O_3$ grains (radii 1–2 μm) and samples with microorganisms (gram-positive S.aureus, gram-negative E.coli bacteria, as well as fungi C. albicans) in the discharge chamber. Emission spectra of plasma were recorded in the range of 250 - 1100 nm by means of lens spectrograph, equipped with a CCD camera, with the spectral resolution of 0.6 nm. The gas kinetic temperature of plasma was deduced from the $\Delta V= -3$ sequence radiation of the second positive system of $N_2$, recorded with unresolved rotational structure.

The differences are discussed in the emission intensity of recorded molecular bands, and in the temperature profiles measured in pure gas plasma and in the heterogeneous plasma.

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## Probe Measurements in the Plasma of an Inductively Coupled RF-Plasma Brigde Neutralizer

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For many applications of surface processing the neutralization of an ion beam current on the target is necessary. Particularly the charging up of isolating surfaces has to be compensated by supplying a sufficient amount of electrons onto the surface. During operation of an ion thruster for spacecraft propulsion charged particles are ejected. The remaining opposite charge leads to a charging up of the spacecraft. In order to keep the spacecraft nearly at ground potential, the excess charge has to be removed from the spacecraft. Usually a neutralizer is employed to deliver an electron beam, which fulfils the above-mentioned tasks. Recently a cathode less inductively coupled 13.56 MHz radio frequency plasma bridge neutralizer (rf-PBN) has been presented for this purpose.

This rf-PBN is composed of a 1.3 cm in diameter and 2.5 cm long ceramic tube located in the centre of a cylindrical coil. The ceramic tube is closed at one side by a thin ceramic plate with a small hole for electron extraction and by a metallic plate as plasma anchor at the reverse side. This little plasma chamber was located in a big vacuum vessel. The plasma generated in the chamber was investigated by means of a Langmuir probe.

The measurements were performed using a cylindrical probe made of tungsten the symmetry axis of which coincided with that of the plasma chamber. The probe diameter was 0.1 mm and the length was 1.5 mm. The probe shaft was low-capacitively mounted at a movable carriage inside the vacuum vessel. The probe was introduced into the plasma chamber through the electron extraction hole. So spatially resolved probe measurements in the chamber were possible. The grounded plasma anchor was used as a reference electrode. A passive rf-compensation was accomplished by inserting a set of inductors self-resonant at 13.56 MHz into the probe circuit between probe shaft and grounded wall of the vacuum vessel.

Internal plasma parameters were determined in xenon and argon plasmas at rf-powers between 40 and 160 W and gas fluxes between 0.2 and 5.0 sccm. In xenon plasmas the electron temperature ranged from to 2.1 eV to 3.2 eV, the electron density from $8*10^{17}$ $m^{-3}$ to $4.8*10^{18}$ $m^{-3}$. In argon plasmas electron temperatures between 3.3 eV and 5.4 eV and electron densities between $5*10^{17}$ and $4.8*10^{18}$ $m^{-3}$ were measured. The thermal electron currents inside the plasma determined as product of the current densities to the probe at plasma potential and the area of the electron extraction hole agree well with the extracted electron currents measured earlier in xenon as well as in argon. Thus it is possible to extract the maximum amount of electrons from the neutralizer in its actual design.

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## Computational Study of Plasma-Solid Interaction in Argon Plasma with Inclusion of Magnetic Field

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The understanding of processes in the boundary layer between plasma and immersed substrates is very important in probe diagnostics and in plasma chemical technologies. Some of modern plasma based technologies employ magnetic fields; therefore the movement of charged particles in these fields are of scientific interest. In the last few years, the behaviour of the sheath region has been a topic of many investigations. The sheath structure and the sheath formation have been analyzed by many authors experimentally and theoretically and due to the complexity of the studied problems the computational approach is now being widely used.

In the presented contribution two groups of techniques of computational physics were used for the study of the sheath structure in DC glow discharge in argon plasma – fluid modelling describing macroscopic plasma phenomena and particle modelling providing more detailed insight into the plasma processes.

The contribution is focused both on the problems of computational physics and on the problems of physical processes taking place in the sheath and presheath region. A comparison of different computational methods is given with attention to efficiency of computer codes in two dimensions. Another point of interest is the inclusion of external magnetic field into the models and its effect on the sheath structure. Some of these results can be used after the modification for collisionless plasma for the discussion of plasma diagnostics in high-temperature plasma, too.

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## High Level Ab Initio and DFT Calculations of Dissociation Energies of Small Protonated Water Clusters

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Protonated water clusters $H^+(H_2O)_n$ are considered to be primary ions in the positive ion chemistry of the lower atmosphere. Hydronium ions are present in interstellar gas and molecular cloud, near the Galactic centre. Recently, $H_3O^+$ ions have found large applications in a new-generation, high-sensitivity mass spectrometers using a ‘‘soft’’ ionization i.e. the proton transfer for studies of complex molecules, mainly of biological interest. Hydrated ions and ionic water clusters are the topic of increasing interest, which are intensely studied in many laboratories. However, a rather serious span on experimental values of dissociation energies exists. The geometrical optimizations and calculations of total electronic and zero point vibrational energies of protonated water clusters $H^+(H_2O)_n$ with n to 4 were performed by the Hatree-Fock/6-311G(3dp,3pd) method, complete basis set-QB3 and hybrid density functional methods B3LYP, BVP86, B3PW91, MPW1PW91, PBEPBE, PBE1PBE, HCTH, THCTH and TPSSTPSS in the Gaussian 03W computational package. Dissociation energies were calculated for reaction $H^+(H_2O)_n \rightarrow H^+(H_2O)_{n-1} + H_2O$. Results are compared with experimental average data from NIST Standard Reference Database Number 69.

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## Spectroscopic Study of the Decomposition Processes of Acetylene in the DC and Middle Frequency Nitrogen Plasmas

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The acetylene ($C_2H_2$) – nitrogen ($N_2$) low pressure plasmas were frequently applied to deposit the carbon nitride (CN:H) thin layers by the PACVD methods. Here, optical emission spectroscopy (OES) and actinometry techniques were employed to study the direct current (dc) and middle frequency (100 kHz) glow discharges, generated in the $C_2H_2$-$N_2$ mixture. The spectral diagnostics of generated glow discharges as well as the decomposition processes of acetylene were examined. Both plasmas were excited between two circular plane Armco - steel electrodes in a Pyrex glass chamber. High energy species, including CN, CH, H, C, $N_2^+$, $N_2$, N, were identified in plasma phase. The emission intensities of main species were measured versus various experimental parameters. Optical actinometry technique was applied to evaluate the relative concentrations of the species in the reactive mixture. The effect of pressure and working gas composition on the plasma processes were investigated.

The spatial distributions of the emission intensities of the species between two electrodes in the both glow discharges were recorded. The excitation, vibrational and rotational temperatures were determined to compare excitation conditions in the examined plasmas. Plasma processes and plasma non-equilibrium phenomena were discussed. Additionally, the FTIR and X-ray powder diffraction techniques were employed to analyze the structure of solid materials, resulted from the decomposition of acetylene in the nitrogen plasma.

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## Transient Spark in $N_2/CO_2/H_2O/CH_4$ Mixtures at Atmospheric Pressure

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We have investigated a novel type of streamer-to-spark transition discharge named the transient spark (TS), operating above the liquid water in $N_2/CO_2/H_2O$ and $N_2/CO_2/H_2O/CH_4$ mixtures at atmospheric pressure. Although the applied voltage is DC, TS has a pulsed character with very short (~100 ns) high current (~1 A) pulses, with repetitive frequencies of some kHz. Thanks to the very short spark pulse duration, given by the small internal capacitance of the discharge system and the limiting series resistor, the plasma cannot reach LTE conditions.

The electrical and optical properties of TS were studied as functions of the frequency and the gas composition by electric measurements and optical emission spectroscopy. Infrared Absorption Spectroscopy was used to analyse gas samples, and solid deposits from electrodes. Liquid samples were analysed by High Performance Liquid Chromatography (HPLC) and Proton-Transfer-Reaction Mass Spectrometry (PTR-MS).

The emission of $N_2$ 2nd and 1st positive, $N_2^+$ 1st negative, CN violet and red, OH (A-X) and NH (A-X) systems, as well as atomic N, O, H, and C lines was detected. The non-equilibrium character of TS was confirmed by comparisons with calculated vibrational (3000-4000 K) and rotational (500-1500 K) temperatures.

In $N_2/CO_2/H_2O$ mixtures, the most remarkable changes in the chemical composition of the treated gas were the decomposition of $CO_2$ and the production of CO as the main intermediate product. The production of CO was most probably crucial for the synthesis of organic species detected by PTR-MS and HPLC in the liquid samples.

In $N_2/CO_2/H_2O/CH_4$ mixtures, the $CH_4$ was quickly converted partially to various organic species, CO and $CO_2$. The amount of $CO_2$ increased with increasing input energy density. The production of organic species resulting from the partial oxidation of $CH_4$ was confirmed by all applied techniques.

These obtained results may help us gain a better understanding of the plasma chemistry induced by TS leading to the decomposition of $CH_4$ and other organic species (syn-gas production from $N_2/CO_2/H_2O/CH_4$ mixture or from real exhaust gases), as well as of the synthesis of organic species from inorganic $N_2/CO_2/H_2O$ mixtures. Formation of organic species in a completely inorganic $N_2/CO_2/H_2O$ atmosphere is a significant finding for the theory of the origins of life.

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## Numerical Modelling of Dielectric Barrier Discharge in Nitrogen with Hydrogen Admixture

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Non-thermal discharge plasma at atmospheric pressure is widely used in multiple technological applications. The numerical modelling has very important role in understanding of the physical background of experiments. Numerical calculations of characteristics of the homogeneous dielectric barrier discharge in nitrogen at atmospheric pressure between parallel-plate electrodes were performed by means of one-dimensional fluid model. The hydrodynamic set of equations was solved using the fractional-step method. The modified second-order total variation diminishing scheme was used for treating of advection term. This algorithm allows the simulation with high gradient of particle density in reasonable time and it is easy to convert the algorithm to two-dimensional model.

The development of external quantities (i.e. external current, gap voltage) during the discharge is shown. The simulated data for ignition voltage are in very good agreement with measured data. Our simulations also give a qualitative explanation for discharge current profiles in pure nitrogen and in nitrogen with small admixture of hydrogen, however the quantitative comparison is not very good. The spatio-temporal development of electron, ion and metastable densities is also presented.

The influence of different processes on surface of dielectrics is discussed. It is shown that the desorption of electrons from charged dielectrics (proposed by Golubovskii) leads to the discharge current course which is not in the agreement with the experimental data. The influence of different surface processes on the shape of discharge current is also studied and the results are presented.

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## Numerical Modelling of a Planar RF Electrode in the Low-Temperature Argon Plasma

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The one-dimensional hybrid model of a planar RF electrode immersed into low-temperature argon plasma is presented in our paper.

The hybrid model consists of two parts – particle model, which simulates "fast" electrons, while fluid model simulates "slow" electrons and positive argon ions. In the particle model the positions and velocities of "fast" electrons are calculated by means of deterministic Verlet algorithm while the collision processes are treated by the stochastic way.

For the solution of fluid equations, for "slow" electrons and positive argon ions, the Scharfetter-Gummel exponential algorithm was used.

Our calculations were performed for frequencies of 13.56 MHz and 500.0 kHz. Typical results of the calculations presented in this paper are total RF current and RF voltage waveforms on the planar electrode immersed into argon plasma. The next results that can be found here are the ion, electron, and displacement current waveforms on the electrode. Numerical results were compared with the experimental data measured in the hollow cathode plasma jet deposition system. Especially, the knowledge of waveform of the ion current on the RF-biased substrate is very important for experimental physicists during the deposition of thin films. The RF bias of the deposition substrate is often used to enhance the bombardment of the created films with positive ions. The ion flux and the ion energy distribution function, which can be determined from the ion current waveform at the RF-biased substrate, are important parameters that influence the properties of deposited films, such as film structure or surface morphology.

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## Mixed Water Clusters with Hydrogen Chloride and Methanol

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Water clusters have been the subject of many experimental and theoretical investigations because of their importance in understanding cloud and ice formation, solution chemistry and a large number of biochemical processes. The water clusters may adsorb plenty of organic molecules (methanol, acetone, acetaldehyde, formic acid, benzene *etc.*). Adsorption of foreign molecules is also important from atmospheric and astrochemistry points of view especially for the mechanism of catalytic depletion of stratospheric ozone or heterogeneous reactions occurring on the surface of polar stratospheric clouds. The mixed water clusters are also interesting in discussion on behaviour of low temperature plasma in the earth atmosphere. We have studied neutral pure water clusters and neutral mixed water clusters which contain hydrogen chloride $HCl\text{-}(H_2O)_n$ and methanol $CH_3OH\text{-}(H_2O)_n$, $n$ varying from *1* to *6*. Configurations of clusters have been calculated by Hartree-Fock *ab-initio* method with *6-311++G*** molecular basis set. The advantage of using this set is that calculations are relatively fast if compared to more extended basis sets (for example *D95++(p,d) set*), so numerous configurations can be easily optimized, but the precision of calculations, in terms of dissociation energies of clusters, is still high. Problem of stability of the mixed water clusters is also discussed.

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## Xe II to V Spectra in the Far UV Region

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Study of the spectra emitted by low charge-state Xe ions requires both advanced experimental techniques for the confinement of the ions in conditions minimizing the collision effects and the sophisticated analysis of the observed spectra. To develop such a study, a 1 μA beam of $Xe^+$ ions, produced by the Van de Graaff accelerator of IPNAS (Liège, Belgium), has been used. The beam was passed through a thin carbon foil. After exiting the foil, the light emitted in the far UV by the excited and ionized ions was analyzed with a CCD-equipped spectrometer. Spectra of Xe in the 30-100 nm wavelength region have been recorded at different beam energies corresponding to different excitation energies. Some spectra previously recorded, have also been used in the present study.

For the analysis of the obtained spectra a detailed **C**ollisional-**R**adiative (C-R) model of Xe plasmas, previously developed by GAPHYOR at Orsay and conveniently extended to include more resonant lines, has been extensively used. The model development required collection, measurement, calculation and evaluation of a huge amount of atomic data which are necessary to calculate the coefficients entering in the second members of the relevant Boltzmann statistical equations. By resolving the system of the statistical equations for a given electronic temperature and density we obtain the level populations of each species in conditions outside local thermodynamic equilibrium and the absolute intensity of the spectral lines.

Transition probabilities ($A_{ij}$) and electron collision excitation cross sections ($\sigma_e$) are the main parameters defining locally the relative intensities within a given multiplet. For the Xe II to V ions which are of interest here, many energy levels and $A_{ij}$ values are still missing in the literature. In order to fill the gaps, we performed calculations in *LS*, *jK* and *intermediate coupling* using *ab initio* and/or quasi-classical codes, as follows:

i) Structure and $A_{ij}$ data were obtained by using the CATS code in collaboration with the IAEA and Los Alamos National Laboratory (LANL) and the GRASP2 package in the relativistic multi-configuration Dirac-Fock (MCDF) approximation.

ii) A *Quasi-Classical Approximation* code (CbA) based on the Coulomb Approximation, developed previously by K. Katsonis was systematically used to obtain transition probabilities of multiplets belonging to neutral and ionized species of rare gases, whenever experimental excitation energies are available.

Evaluation of electron collision ionization and excitation cross sections of the Xe species involves the use of a calculational package of few body CTMC type code of GAPHYOR and the ACE code of LANL.

Spectral lines belonging to various multiplets of Xe II to Xe V ions have been studied in the region of 30 to 100 nm. In so doing, the obtained spectra are compared to theoretical spectra obtained from our C-R model. Consequently, the main resonant transitions of these species, which are present in the studied spectral region, have been identified.

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## Influence of the Wall Impedance and Self-Fields on the Cyclotron Maser Instability

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The compound influence of finite wall impedance and equilibrium self-fields on the cyclotron maser instability is investigated for a slowly rotating hollow electron beam propagating parallel to a uniform axial magnetic field. The stability analysis is carried out within the framework of the linearized Vlasov-Maxwell equation with the assumption that the beam thickness is much less than the mean radius of the beam. Stability properties are investigated for a certain choice of electron distribution function in which all electrons have a step-function in energy, axial canonical momentum, and angular canonical momentum. A dispersion relation for an azimuthally symmetric electromagnetic perturbation is obtained. It is shown that the stability growth rate decreases due to the wall resistivity and self-fields. One of the most important feature of the analysis is that in the presence of self-fields a very small increase in the wall resistivity causes an increase in the instability bandwidth in spite of the decreasing effect of self-fields on the bandwidth.

# Radial Structure of the Low Pressure RF Discharges

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The low pressure RF discharges are widely used in the microelectronics industry and plasma technologies for etching, sputtering, and deposition of thin films. The uniformity of plasma parameters across the electrode surface is of special interest for plasma technology. Therefore the investigation of the RF discharge radial structure is extremely important. This report studies the radial structure of the RF discharge glowing in nitrogen. We observed the increased discharge luminosity near the tube wall, besides probe measurements showed that in this area the electron temperature increases abruptly.

Experiments were performed at nitrogen pressure of $p$ = 0.01 - 3 Torr within the range of RF voltages $U_{rf} \leq 600$ V and the RF field frequency of $f$ = 13.56 MHz. The experiments in this study were carried out in two discharge chambers. One of them was T-shaped and served for the diagnostics of the radial luminosity. We took photos through a window at the opposite end of the horizontal part of T exposing the RF electrode and then digitized these images. In this way radial profiles of the intensity of the RF discharge luminosity were obtained. And the second chamber which served for the probe measurements consisted of two plane-parallel stainless-steel electrodes of d = 100 mm in diameter, the inter-electrode distance was $L$ = 22 mm.

We obtained the following results of the experimental measurements. The radial profiles of the RF discharge glow have an area of abruptly increased luminosity near the wall of the T-tube. At the same time via radial probe measurements in the RF discharges we observed a peak of the electron temperature near to the tube wall. Position of the luminosity peak is in a good agreement with the peak of the electron temperature. Such phenomenon can probably be observed because of the higher electron heating by the radial RF field in this area. This effect was earlier predicted in the literature using numerical simulation.

The radial effects are significant and they are caused by the positive radial electric field existence. Probably this field is caused by the ambipolar diffusion, which leads to the negative charge accumulating on the tube wall and radial sheath formation. The radial electric fields are much smaller than the axial ones. But the increase in the electron temperature near the tube wall is caused by both axial and radial electric fields. The electrons are accelerated by radial and axial forces from the radial sheath region and gain energy from the field when they drift to the center of the chamber. A rather high electric field near the tube wall is also a cause of the ion motion towards the wall out of the plasma volume. Consequently, all particles are accumulated near the boundary between the plasma volume and the radial sheath due to a comparatively low electric field in this region. This increases the ionization rate by high energy electrons here. Due to these processes we observe peaks of electron temperature near the tube wall and lower plasma density close to it.

These measurements provide better understanding of the plasma behavior in RF low pressure discharges.

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# Pink Afterglow in Nitrogen-Argon Mixtures

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Nitrogen post-discharges in various configurations have been subjects of many studies for a relatively long time. Besides various nitrogen based gas mixtures, the nitrogen-argon mixture has a special position for the use in the plasma-chemical technologies. Relaxation processes of atomic and various metastable molecular states created during an active discharge lead to the common thermal equilibrium. Besides collision processes, the light emission plays a significant role in the relaxation. Visible light can be observed up to one second after switching off the active discharge. The first period (up to about 3 ms) of the post-discharge in pure nitrogen is characterized by a strong decrease of the light emission. After that, the strong light emission at decay time of about 5 – 14 ms after the end of an active discharge is known as a pink afterglow and it can be observed in nitrogen, only. The pink afterglow is manifested by a strong increase of the pink light emission at the decay times of about 6 – 8 ms in pure nitrogen, while the yellow-orange color is characteristic for the other parts of the nitrogen afterglow. The pink afterglow maximal emission is dependent on various discharge parameters as pressure, discharge reactor wall material, discharge power, etc. The purity of nitrogen or different nitrogen contains in mixtures are other significant parameters.

The effect of nitrogen pink afterglow was studied by optical emission spectroscopy in the DC flowing regime at total gas pressure of 700 Pa and discharge current of 120 mA. Discharge was created in Pyrex tube of 14 mm i.d. The part of ±3 cm around the observation point had to be cooled down to liquid nitrogen wall temperature.

At the ambient wall temperature, the maximum of pink afterglow emission in pure nitrogen was observed at decay time of 6 ms and it was moved to the later decay times with the increasing argon percentage in the gas mixture. Simultaneously the intensity of pink afterglow decreased and at the nitrogen-argon ratio of about 1:1, the effect disappeared. At the argon concentration over 90 %, the visible light emission during the post-discharge was negligible. Another observed effect was the extension of the active discharge downstream the discharge tube with the increase of the argon presence in the gas mixture over about 50 %.

The wall cooled down to 77 K had different effects. Besides the significant increase of the nitrogen atoms recombination that increased some bands mainly of the nitrogen first positive system, the argon lines were observed during the post discharge. The active discharge extension into post-discharge region as well as the pink afterglow quenching were observed, too, because the cooling was done around the spectra observation point, only.

The kinetic model showed that the pink afterglow quenching was connected to the decrease of the v-v and pooling processes efficiency, the extension of the active discharge was done by energy transfer between argon metastables and nitrogen ground state molecules.

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## Back Discharge in Multipoint-Plane Geometry in Flue Gases

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Back discharge is a type of discharge, which occurs between charge-emitting point electrode and a plate, which is covered with a dielectric layer of high resistivity. The emitted charge accumulates on the surface of the dielectric layer until the electric field within it increases to the value which causes breakdown of the layer. The accumulated charge starts to flow throughout small breakdown channel or channels to the plate electrode. When the current starts to flow through the layer, glow discharge or breakdown streamers can be incepted in the interelectrode space. An increase of the voltage and discharge current lead to an increase of current density in these channels that causes heating of the material of the layer. When sufficiently high current flows through one of such channels, it becomes conducting due to thermal ionisation of the layer material, and back-arc discharge is generated.

The paper presents investigations of back discharge occurring in air and flue gases produced by the process of burning LPG or charcoal. The discharge was generated between a multineedle and plate electrodes. The plate electrode was covered with fly ash layer collected from last stage of an electrostatic precipitator. The discharge was generated at temperature ranged from 20 to 120$^o$C and at atmospheric pressure. The chemical composition of flue gases was determined using LANCOM 6500 portable monitor, based on electrochemical cells. The visual forms of the discharge were recorded with digital camera and referred to the current-voltage characteristics for various gas compositions. It was noticed that the breakdown voltage in back discharge increases with increasing water vapour and $O_2$ or NO contents. The aim of this work was to determine the effects of back discharge in multineedle-to-plate electrode configuration with fly ash dust layer covering the plane electrode on the level of the $NO_x$ and CO compounds in flue gases, leaving the discharge zone. The research is aimed at better understanding of plasma chemical process in electrostatic precipitators when back discharge occurs.

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## Electron Density Measurement Using Self-Oscillating Resonant Cavity

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The microwave interferometry and the resonator method are considered as the standard microwave techniques for the plasma electron density measurements. Although they are quite simple, certain know-how and equipment is needed.

The microwave resonator method is based on the fact that the plasma presence changes the resonant frequency of the microwave cavity. Using a swept generator, the resonant frequency can be determined by finding a resonance dip on the frequency response of the resonator. Since the finding of the dip is not instantaneous, this approach is suitable for measurements where the experimental conditions do not change in time. However, in many cases, a real-time response is required. Therefore, we propose a modification to this standard set-up.

Instead of using the relatively expensive swept generator, we integrated a Gunn diode directly into the resonant cavity. The well known feature of the Gunn diodes is their negative differential resistance, which undamps the outer resonant circuit. It means that the oscillating frequency is entirely determined by the resonator. When the resonant frequency of the resonator (microwave cavity) changes, the Gunn diode follows and produces the microwave power at the new frequency. This arrangement eliminates the swept generator and the continuous finding of the resonant dip. The output frequency of our system depends on the actual plasma density and follows very quickly its changes. The changes in the output frequency can be measured either directly (by a frequency meter/counter) or by mixing the signal with the reference oscillator. The time response of the system is fast enough to perform the real-time measurements. Effectively, we replaced an absorption measurement by the emission one, which is much simpler and cheaper.

The calculation of the plasma density from the measured frequency is straightforward and identical to the standard resonator method. It is clear that the self-oscillating system cannot provide the information about the resonant dip width, i.e. the collision frequency.

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## Optical Emission Spectroscopy of Plasmachemical Processes for Deposition of Carbon Nanotubes

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The microwave (mw) plasma torch at atmospheric pressure used for synthesis of carbon nanotubes (CNTs) has been studied by means of optical emission spectroscopy (OES). The CNT synthesis was carried out in the mixture of $CH_4$, $H_2$ and Ar with the iron catalyst either on the substrate or in the gas phase as achieved by addition of $Fe(CO)_5$ vapors. The OES showed, among others, the presence of atomic hydrogen, $C_2$ and, in the case of $Fe(CO)_5$ addition, also the presence of iron in the gas phase. The relative intensities of selected atomic lines and molecular band heads were measured in dependence on mw power and the distance from the electrode nozzle.

The OES was also used for the determination of rotational temperature, which approximates the temperature of neutral gas due to frequent collisions of the gas particles. The program DMESS that combines the simulation of rotational spectra of diatomic molecules with fitting procedure was developed in order to obtain the rotational temperature from the structure of rotational lines of given vibrational band. It is based on the least square method in which the difference between the measured and simulated data is minimized. Two methods can be used for the fitting of spectra within the program, the Nelder-Mead method (known as downhill simplex method) and the Levenberg-Marquardt algorithm. The fast Nelder-Mead method starts the fitting with the user estimated values of the parameters in order to find an approximate position of the global minimum. Then, more sophisticated Levenberg-Marquardt algorithm can be used for a more precise determination of the parameter values. The rotational temperature of thousands of degrees was determined from the Swan system of the $C_2$ molecule.

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## Characterization of Plasma Needle with Additional Grounded Ring Using Derivative Probes and ICCD Camera

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Different kinds of atmospheric pressure plasma sources have been developed for various types of applications. Advantages of working at atmospheric pressures are that expensive pumping systems are not needed, it is possible to treat samples that are sensitive to low pressures and plasma can easily be put in contact with samples that need to be treated.

Plasma needle is atmospheric pressure plasma source powered by 13.56 MHz RF generator that operates in a mixture of air and helium. Its construction makes it very useful for treating biological samples like plant tissue, for bloodless surgery, dental cavity antibacterial treatment and many other applications. The needle consist of central tungsten wire (0.5 mm in diameter) placed into a ceramic tube with slightly larger diameter and both placed into the glass tube with 6 mm diameter. Helium flows between ceramic and glass tube with typical flow rate of few hundred standard cubic centimeters per minute.

In our configuration additional grounded copper ring is added around the glass tube and close to the tip of the needle. The central wire represents the powered electrode and the grounded electrode is the treated sample. Plasma needle can operate in two different modes: bipolar mode, when surface of the sample represents grounded electrode and unipolar mode when there is no surface in the vicinity of the tip of the needle.

For the purpose of successful treatment and comparison of different treated samples with plasma needle it is necessary to characterize the plasma itself the best way possible. The standard parameters for treatment of samples are time of treatment, power transmitted to the plasma and distance of the sample from the tip of the needle. In this paper we will present some of the properties of our low temperature atmospheric pressure discharge (plasma needle). For the power measurements the derivative probes were used. The percentage of total power distributed to plasma itself was determined using derivative probes. The volume and intensity of plasma were obtained by using images taken by the fast ICCD camera.

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## Medium and Atmospheric Pressure Argon Glow Discharge with a Restricted Cathode Surface

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One approach to stabilize discharges at medium and atmospheric pressures consists of downscaling the discharge volume to (sub-)millimeter dimensions. Different geometries have been reported in literature, including schemes with micro-structured electrodes such as micro-hollow-cathodes. Arrays of discharge elements operating in parallel make up versatile plasma sources that are perspective for a wide range of applications. Still, some physical aspects of these discharges such as the pressure-size scaling and the stabilization mechanism remain unresolved.

The discharge geometry investigated in this work is an electrode-dielectric-electrode sandwich with a single bore. The exposed side of the electrodes may be covered with a dielectric to further limit the electrode surface. The dimensions are in the millimeter range and the investigated pressure range is from a few tens of kPa up to atmospheric pressure. The discharge is DC-excited and argon is used as the working gas.

It is observed that when the cathode surface is restricted to the inner walls of the bore, the discharge operates in the normal glow mode at low currents and then enters into a regime with a steep slope of the voltage-current curve. In the latter regime the discharge luminosity extends beyond the edges of the bore.

When using DC-excitation, the high power density in the discharge may lead to a fast degradation of the electrode sandwich. Therefore, a gas flow is applied through the bore. Apart from the cooling effect, the gas flow is instrumental in stabilizing the discharge and in blowing reactive species that are produced within the bore into a flowing afterglow zone.

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## Investigation of Neon RF Discharge by Means of Refined Collisional-Radiative model

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A recently developed collisional-radiative (c-r) model for neon discharge was used to investigate the plasma properties of a capacitively coupled RF (13.56 MHz) discharge in neon. By means of c-r model, population of thirty excited states of neon atom and therefore optical emission spectrum for a given electron distribution function was determined. The discharge was studied by optical emission spectroscopy. By comparison of measured and calculated optical emission spectra on the basis of least-squares method the electron temperature or electron density was determined.

The developed collisional-radiative model was refined in order to describe the studied plasma more correctly. Some important processes (as e.g. excitation transfer between 3s levels of neon atom induced by electron impact), were newly incorporated in the presented calculations. A 1/y-weighted sum of squares was used in the comparison of the spectra. Moreover, the model was modified in order to determine the emission coefficient of unit plasma volume in absolute values.

Since in previous work the measurement of relative intensities was found to be insufficient for determination of electron density, an absolute intensity measurement was performed. Jobin Yvon Horiba Triax 550 spectrometer, equipped with CCD camera, was calibrated by Oriel Tungsten-halogen filament lamp. The radiation of a defined narrow cylindrical region was taken out by means of two iris diaphragms, mounted at their common axis in front of the optical fibre. The temporal development of the plasma, important for the determination of real radiation time, was studied by Jobin Yvon Horiba FHR 1000 spectrometer with ICCD camera.

The sensitivity of the method, as well as the influence of the newly incorporated processes on the results was evaluated. Assuming Maxwellian electron distribution function, without absolute intensity calibration the method is insensitive for electron temperatures below 4 eV.

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## Electron Transport in X/$CF_4$ Mixtures (X=F, $F_2$, CF, $CF_2$, $CF_3$)

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In order to achieve high resolution plasma processing for future generations of integrated circuit technologies, the empirical development of the plasma processing tools has to be replaced by complex models based on a real understanding of the physics and chemistry of plasmas.

A description of electron kinetics in non-equilibrium plasma modelling necessarily includes calculation of transport coefficients which is based on compilation of cross sections from different sources. Requirement to establish reliable transport coefficients for $CF_4$ plasmas is especially demanding for conditions that include many reactive species.

Free radical species, such as CFy (y=1-3) and fluorine atoms, play important but complex roles plasma processing. It has always been an issue whether the presence of radicals affects strongly the transport coefficients, especially the attachment coefficient. We calculated electron transport coefficients for pure $CF_4$ and in X/$CF_4$ mixtures (X= F, $F_2$, CF, $CF_2$ and $CF_3$) for the conditions overlapping with those used in plasma technologies for semiconductor production.

For 0.01%, 0.1%, 1% and 10% of the radical species X we calculated attachment and ionization rate coefficients. In realistic plasma reactors densities of some radicals $CF_2$ were found to be of the order of up to few percent. Transport coefficients are obtained by using numerical solution of Two Term approximation of Boltzmann equation and also by using Monte Carlo simulations.

It was found that for several radicals significant effects of radicals on transport coefficients and attachment in particular could be found.

The present data may be directly implemented in codes for modelling of two frequency capacitively coupled rf plasmas as used today for etching of interconnects in dielectrics or for sources of fast positive and negative ions that are converted into fast neutrals in order to reduce charging induced damage and roughness of the treated surface. These tools will be essential in implementation of top down plasma technology for reproducible massively parallel production of nanostructures.

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## The Methods of Accuracy Increasing of Accelerator Plasma Parameters Determining by a Langmuir Probe

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The problem of plasma parameters determining for separate processes studying and for testing of the accelerator is analyzed. An opportunity to increase accuracy of electron temperature and plasma density determining by an electric probe is studied. Inaccuracies of a technique, which is traditionally used for processing of experimental probe volt-ampere characteristics, are analyzed.

Features of probe-plasma interaction in area, where the magnetic field does not influence on movement of electrons and in area, where electrons drift in the crossed magnetic and electric fields are investigated. In both areas, based on a preliminary estimation of electron temperature and plasma density, potential distribution in a layer nearby the probe is calculated from Poisson equation. Real velocity of ions, flying from plasma into a layer nearby the probe is taken into account. The movement of electrons and ions are modeled numerically on the base of Monte Carlo method.

The special mathematical model of plasma electron components has been created to study features of processes nearby the probe in area, where electrons drift in the crossed electric and magnetic fields. Base on this model, process of electron maxwellization and electron distribution function formation (similar to Maxwellian function) was investigated and features of a probe-plasma interaction were studied.

Distribution of charge density nearby the probe is determined by the particle movement numerical modeling. It is determined, that the area of increased ion density nearby the probe is always formed. It is result of that the probe body creates "shadow" – as electrons does not pass in some area at a probe. Potential distribution and an electric field in "shadow" area are determined. This "shadow" effect influences electron movement to a probe and that is why it also influences on the electron temperature determination. Possible features of a probe orientation and possible probe designs in view of the plasma movement features, to avoid the "shadow" effect described above are analyzed.

By numerical modeling, it is determined that the electron current on a probe can be in some times less, than it is predetermined with widely used technique of probe measurement results processing. Such difference - result of "flow" of an electron stream around of a probe, which potential is less than the plasma potential and which sizes are limited. By the numerical experiment, it is possible to determine a value of this difference and then this value can be used for processing of experimental data for specification of results of plasma parameter determining.

Thus, results of an experimental research of accelerator plasma parameters can be specified based on results of mathematical modeling.

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## Two Channels of Self-Organization of Ionized Gaseous Media

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When there is lack of equilibrium, the evolution of the thermodynamic system can be described in point of form by means of the so-called non-lineary dynamic systems. Modelling assisted by high-power computers, as well as various experiments, have proved that such dynamic systems, deterministic in principle, develop through bifurcations towards states of *deterministic chaos*. However, beyond this chaos the appearance of a number of *self-organized coherences*, at an even higher level, can be noted. Such coherences are known by the name of *dissipative structures*. These dissipative structures, the internal entropy of which is extremely small, behave like real *exotic macroscopic bodies.* They are capable of consuming flows of energy-information from the ambient in order to maintain their structure at the expense of the processs of throwing out into the environment high flows of entropy. Nowadays, an ample number of examples of self-organization are known, such as the Benard cells, the non-lineary structures of electric field in semiconductors (the Gunn effect), some structures in non-lineary optics, the collective processses in chemistry such as the Belousov-Zhabotinsky reaction.

Since: coming to terms with the condition of non-lineary is easier to achieve in ionised gases under low pressure than in other media; the diversity of the instabilities of these media is impressive (today, more than 2,000 types of instabilities of the plasmas are known); the structures formed can be investigated by means of both electrical methods and optical methods (since the environment is transparent); the interactions between the microscopic components of the system are relatively simple (with a prevalence of the binary processses), it follows that the analysis of the structure, the forming and the evolution of the double layers (DLs) and of the other electric charge complex structures (CCSs) occurring in the plasma represent an ideal experimental basis for developing the physics of non-lineary processes. On the other hand, as evinced by the experiments conducted by numerous authors, a fairy large class of phenomena observed in the experimental devices for obtaining plasma can be understood phenomenologically starting from the consideration of the primary processes along the dynamics of the DL. Virtually, all phenomena implying an accumulation and an periodical emission of energy within the plasma can be understood on the basis of the DL dynamics.

In the present paper is presented an experiment whereby two mechanisms of self-organization of an ionized gaseous medium are demonstrated: one of the mechanisms is based on the long-range interactions between the constituents of the medium, while the second mechanism is essentially based on the short-range interactions. The purpose is to check whether a theoretical scenario is true, according to which, irrespective of the type of the interactions that are dominant in the system, the latter tends to spontaneously form dissipative structures when the conditions that are imposed allow it. Starting from the actual experimental situation, the existence is proved with arguments of a number of *threshold-values of the control parameter* above which these dissipative structures can be generated.

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## The Effect of Electrode Material on Ozone Production in Negative Corona Discharge Fed by Carbon Dioxide

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The effect of different outer electrode material on generated ozone concentration has been studied in coaxial negative corona discharge fed by carbon dioxide. The experiments have been carried out at atmospheric pressure and ambient temperature. The discharge reactor containing coaxial cylindrical electrode system (molybdenum inner electrode of diameter 125 µm and outer electrode of diameter 17.8 mm), were used in experiments. The 10 cm long exchangeable outer electrode was made of brass, stainless steel or aluminium. Negative corona discharge was generated in the tube. The gas was flowing from the reactor to the cell of UV spectrometer, which was used for measurement transmittance of light. Using Lambert-Beer formula the ozone concentration in the discharge gap was calculated. The electric parameters of the discharge (current, voltage) were measured as well. The dry carbon dioxide was flowing through the reactor at flow rate of 50 $cm^3$/min.

It was found out that the electrode material effect is not negligible. The ozone concentration was highest with aluminium electrode. When brass electrode was used the ozone concentration was approximately 25% lower and when stainless steel electrode was used it was approximately 65% lower in comparison with aluminium at the same amount of energy put into the gas volume.

The ozone composition is the sequence of processes that take place mostly in the volume of the gas. It suggests that the differences in the final ozone concentration in the gas mixture are caused by the ozone decomposition processes that can be both of homogenous (in the gas volume) or heterogeneous (on the walls of the reactor) nature. The heterogeneous process of ozone decomposition

$$O_3 + \text{wall} \longrightarrow O + O_2 \qquad k_{11} = ? \qquad (1)$$

depends on the material of the wall and on the dynamics of electric wind transporting ozone molecules through the discharge gap. The reason why different amounts of ozone are produced with different electrodes is the ozone decomposition in contact with the discharge tube. As the processes of ozone generation and decomposition are active simultaneously in the reactor and the rate of decomposition is various depending on the electrode material, the final ozone concentrations are different. Therefore the final ozone concentration is lowest with stainless steel electrode where decomposition rate is highest and highest with aluminium electrode where decomposition rate is lowest.

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## A Study of the Thermal Treatment for Waste Containing PCBs

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There is growing demand in public opinion on retreated from the scientific community effort that PCB-containing waste must be rapidly identified properly collected and properly destroyed in order to stem their continued migration into the general environment. PCBs are highly stable organic compound. that are either oily liquid or solid and are colorless to light yellow in color. there are no known natural sources of PCBs. PCBs don't burn early and are good electricity insulating material. they have been used widely at coolants and lubricants in transformers, capacitors, and other electrical equipment. PCBs can be released into the environment from hazardous waste sites that contain PCBs, illegal or improper dumping of PCBs waste, and leaks from electrical transformers containing PCBs. PCBs may be carried long distances in the air and they remain in the air for approximately 10days.

In water, a small amount at the PCBs may remain dissolved, but most sticks to organic particles and sediments. PCBs in water build up in fish and marine mammal and can reach levels thousands of times higher than the levels in water. One might get exposed to PCBs by using old fluorescent lighting fixtures and old appliances such as television sets and refrigerators. Animal experiments have shown that PCB mixture produce adverse health effects that include damage, skin irritations reproductive and developmental effects, and cancer. The purpose of this paper is to review the existing thermal technologies to treat PCBs presenting their limitation and some technical, environmental, social and economic criteria to choose the most proper technique. In this study we investigated both the decomposition and unintentional formation of polychlorinated biphenyl congener during thermal treatment plant such as plasma melting treatment, plasma pyrolysis - melting treatment.

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## Plasma Diagnostics of Underwater Electrical Diaphragm Discharge for Fabrics Treatment

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Underwater pulse diaphragm discharge is an effective tool in the production of hydrated electrons and hydroxyl radicals, which can be used for material surface modification (bondability, hydrophilicity, surface energy). For efficient material treatment it is necessary to identify key operational parameters controlling the discharge plasma characteristics and to establish some appropriate diagnostics methods and models for plasma characterization.

The discharge was generated in the narrow slit of 0.1×1mm positioned between two metallic electrodes at 2 cm mutual distance. Both electrodes and the slit (diaphragm) were immersed in water medium. Polypropylene nonwoven fabrics of 50 gsm and 30 mm width was fed trough the slit with an adjustable speed. The electrodes were connected to a pulsed HV power supply based on the double rotating spark gap. The maximum peak voltage was 40 kV DC. The maximum repetitive rate of pulses was 60 Hz. The duration of the electrical pulses was determined by the water conductivity. Different water based media were used in this study: deionized water + NaCl to adjust the conductivity; regular tap water; and $CO_2$ saturated mineral water.

Initially the plasma starts within the air bubbles trapped inside the porous structure of nonwovens. After the air voids are filled with water a different discharge breakdown mechanism takes place. The high intensity electrical current flowing through the narrow slit is capable of initiating the water vaporization. The discharge starts in the water vapour bubbles created by that vaporization. The discharge manifests itself as thin plasma filaments propagating along the textile surface up to the distance where the metallic electrodes are positioned. The length of propagation is given by the conductivity of water solution and amplitude of the applied voltage.

The plasma parameters - electron number density, temperature of electrons, excitation temperature, have been measured by optical emission spectroscopy completed by the voltage, and current measurement. The sampling optical fiber was installed directly in the slit to minimize the water absorption of emission light. The electron number density will be estimated preferable from spectral line profile of $H_\alpha$. Our contribution will summarize the results of our experiments.

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## Mass Spectrometry Study of the Coplanar Barrier Discharge Operating in Ambient Air at Atmospheric Pressure

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Planar barrier discharges are very promising plasma sources for surface treatment. One of them is the coplanar barrier discharge - DCSBD (diffuse coplanar surface barrier discharge). The greatest advantage of it is the possibility to generate a non-equilibrium low-temperature plasma at atmospheric pressure in ambient air. In order to understand the process of the treatment knowledge of the composition of plasma, i.e. of the active species, is needed.

DCSBD operated at atmospheric pressure in atmospheric air as a working gas. The DCSBD electrodes, consisting of 15 pairs of silver strip electrode embedded 0.5 mm below the surface of 96% $Al_2O_3$ ceramics, was energized by 14 kHz sinusoidal voltage, supplied by HV generator LIFETECH VF700. The mutual distance of the 200 mm long and 2 mm wide silver strip electrodes was 1 mm.

In this contribution the mass spectrometry measurements of the DCSBD are presented. After conditioning, the measurement by the HIDDEN EQP mass-energy analyser was done. We have made our measurements of DCSBD discharge in RGA positive mode. This means that we have used internal electron source with variable electron energy in order to be able to detect neutral species. This source allows ionization of neutral species entering the MBMS and detecting them by the EQP analyzer. The recorded positive ion signal is directly proportional to the radical number density. We have made measurements for two different powers of 300 W and 400 W and for two different distances (5 mm and 10 mm) from the orifice of the MBMS.

We have recorded m/z spectra in the range from 1 to 100 amu. Also, dependence of the positive ions ($N^+$, $O^+$, $N_2^+$, $O_2^+$ and $NO^+$) on the energy of the electrons emitted from the filaments is recorded in order to see the thresholds for different reactions. When the discharge is on there is a change in number of positive ions recorded by the MBMS. With the increase of the distance between the discharge and the orifice there is a decrease in yields of measured positive ions ($N^+$, $O^+$ and $NO^+$). Also, formation of the $NO^+$ radicals is influenced by the applied power.

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## The Influence of the Surface Conditions on the RF Plasma Characteristics

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Electron emission from solid surfaces by impact of the energetic ions is one of the most fundamental effects in capacitively coupled plasma (CCP) sources, making them very useful as plasma processing devices. Depending on characteristics of the incident ions and of the surface, secondary emission of electrons and ions may be effected in various ways. The present paper deals with the effect of the electrode surface conditions: clean (atomically clean) and contaminated electrodes (standard conditions even after mechanical and chemicals cleaning) on the characteristics of an asymmetric discharge. For that purpose, we have perfomred PIC/MCC simulations of an asymmetric rf source of 27 MHz, with the electrodes made of the same material but with different secondary electron emission coefficients (SEEC) due to different surface conditions. The secondary electron emission from a surface under the action of an ion is described by the coefficient quantifying the number of secondary electrons produced at the cathode per ion usually known as the electron yield per ion and denoted by $\gamma_i$. In our simulations we have implemented a more accurate model of the secondary electron production per ion suggested by Phelps and Petrović, that includes the energy dependence of the yield.

The obtained simulation results clearly show that in the asymmetric discharge with both contaminated electrodes electron yield per ion is different for small and large electrode due to discharge asymmetry which leads to different energies of ions bombarding the powered and grounded electrodes. In the case with one clean and one contaminated electrode the discharge characteristics strongly depend upon which electrode is powered. Futhemore, analizis of the simulation results indicates that the plasma density is significantly higher in the arrangment with contaminated powered – clean grounded electrodes than in the case of clean powered - contaminated grounded electrodes. On the other hand, IEDF does not change significantly when electrode conditions are changed.

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## Electron Beam Energy Deposition in Non-Uniform Plasma of Stationary Beam Plasma Discharge

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Stationary beam-plasma discharge (SBPD) is useful as a generator of dense highly nonequilibrium plasma. It is formed as the result of non-collision electron beam-Lengmuir wave interaction. The interaction being realized in systems having plasma spatial non-uniformity reveal some peculiarities of energy deposition from electron beam to plasma. In the presented work power loss of electron beam propagating in plasma of SBPD along magnetic field was studied experimentally. Power loss efficiency data were obtained in a device having sheet-like electron beam as directly by use of calorimetric method as being derived from measured beam electron distribution function (BEDF). At the same time, plasma parameters such as plasma density and plasma electron temperature were measured. SBPD was realized at gas pressures $10^{-3}$–$10^{-2}$ torr. It appeared that experimentally obtained dependencies of beam power loss at its passage through longitudinally non-uniform SBPD-plasma on beam parameters differ significantly from that ones taking place in the case of uniform SBPD-plasma. Beam relaxation length is more large in the case of non-uniform plasma, it is enlarged at beam electrons initial energy increase. The enlarge effect becomes stronger as plasma longitudinal gradient increase. As well, power loss dependencies on beam current are not so sharp compared with the case of uniform plasma. As a result, energy deposition along the beam path becomes more uniform compared with the case of uniform plasma, length of power deposition may be enlarged significantly. All observed effects become more distinct for beams of smaller cross size. To explain the experimental results, mathematical model of beam relaxation was designed being based on the quasi-linear relaxation theory. As the theory as the developed model can be used for description of processes realized in systems of weak supercriticality where volumetric Langmuir noise density is a small fraction of thermal energy density. The model uses all basic wave processes influencing decrease of beam-plasma instability growth rate including process leading to disturbance of electron beam - Langmuir wave velocity resonance. Analytical expression was found in the result of modeling. The expression gives true description of e-beam relaxation processes within wide range of SBPD parameters such as beam energy, beam current, plasma density, plasma electron temperature as well as system parameters - magnetic field strength, plasma density longitudinal gradient, e-beam width. The results obtained show the SBPD to be a generator of uniform plasma of flexible adjusted parameters. Both experimental data and analytical expression of beam relaxation can be useful in several applications.

# Study of H and T Form of Oxygen Discharge in Silica and Pyrex Discharge Tube

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The DC glow discharge in oxygen has been studied by means of optical emission spectroscopy and double-probe diagnostics in pressure range of hundreds of Pascals. In this pressure range it is possible to find two forms of positive column. These forms are defined according to the values of axial electrical field strength. We distinguish low-gradient T form and high-gradient H form. Our investigation was focused on the variations of intensities of oxygen spectral lines and bands in the dependence on the discharge current and on the pressure with respect to the existence of the T and H form of the discharge. The influence of the discharge tube material on these properties of positive column was also investigated.

Two U-shaped discharge tubes (Silica and Pyrex glass) were used for measurements of parameters of the DC glow discharge. The tubes were equipped with two pairs of cylindrical platinum probes used for measurements of electrical field strength. Emission spectra were analyzed by means of monochromator Jobin Yvon-Spex Triax (focal length 550 mm) using plane grating (1200 grooves/mm). This arrangement allowed us to detect emission spectra in the range 200 - 1050 nm. Great attention has been devoted to the purity of the experimental system. Before each measurement both discharge tubes were heated up to 420 ºC and they were pumped for several hours. The measurements were realized in spectrally pure oxygen of Linde production (guaranteed purity 5.0) for pressure range 150 - 950 Pa and for discharge currents up to 40 mA.

First we have focused on study of range of existence of both forms. H form was detectable in the whole pressure range while T form was found for pressures above 600 Pa. Existence of particular forms was verified by measurements of axial electrical field strength. Our attention was paid to emitted radiation, i.e. to spectral lines of atomic oxygen triplet 777.2 nm and atomic oxygen 844.7 nm and atmospheric A-band of molecular oxygen.

To compare emission spectra in H and T form we have focused on the investigation of the relative intensities of studied lines and bands. H form was characterized by similar values of intensities of 777.2 nm and 844.7 nm lines while intensity of 777.2 nm line was permanently higher than 844.7 nm in T form. Therefore different ratios of atmospheric A-band intensity to 777.2 nm line and to 844.7 nm line were found in T form while similar values of these ratios were observed in H form.

It is known that material of the discharge tube can exert influence up the atomic oxygen particles density. It is caused by various re-association of the oxygen atoms on the wall. In our case it has been found that atomic spectral lines were more significant in the discharge tube from Silica. Higher ratios of intensities of molecular band to both atomic lines were then observed in Pyrex glass compared to Silica in the both forms. Increase of intensity of spectral band corresponding to molecular oxygen with increasing pressure was also observed for all conditions under which our measurements were undertaken.

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## Diagnostics of Plasma Pencil by Optical Emission Spectroscopy

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During several last years different plasma discharges with nozzle and powered by rf generator driven at frequency 13.56 MHz have been investigated. Plasma pencil is a special type of plasma nozzle working at atmospheric pressure, which is interesting for possible applications such as local treatment of surface, deposition of thin films, change surface energy, cutting in surgery, etc. Through this nozzle, which is made from quartz tube with typical inner diameter 2mm, flows working gas (argon with water vapour). The powered electrode is connected through the matching unit to the rf generator.

In this contribution, we present diagnostics of unipolar discharge channel generated by the plasma pencil at atmospheric pressure. For different electrical parameters and various construction design of the plasma pencil the parameters of the plasma channel are estimated from optical emission spectra in the spectral range 200 - 900 nm: rotational temperature from OH rotational lines, vibrational temperature from nitrogen bands as well as concentration of electrons and temperature of neutral gas from Stark and Doppler broadening of hydrogen lines, resp.

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## Optical Investigation of Small Size Atmospheric Pressure Plasma Jet Working in Argon

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Plasma processing of materials has proven its feasibility in a wide range of applications. The development of atmospheric pressure cold plasma sources is highly encouraged by the technological and financial advantages coming from the widening of the classes of materials to be processed and the use of inexpensive equipment. The determination of plasma characteristics is an important issue in order to better control the process parameters.

This work reports on the spectral investigation of a small size radiofrequency plasma jet generated in argon at atmospheric pressure. The discharge is generated in argon flow (2000 - 10000 sccm) in a small interelectrodic space at RF powers in the range 15 – 150 W. It expands in open atmosphere through a hole performed in the grounded electrode as a plasma jet. The plasma was investigated by means of Optical Emission Spectroscopy in the spectral range 200 – 1000 nm by using a typical spectroscopic setup consisting of a focusing system, a Bruker 500 IS/SM spectrograph and an CCD camera (Andor iDUS, DV420A).

The spectra show the presence of several Ar lines in the region 600 – 1000 nm, as well as the emission of molecular bands related to the impurities excitation, namely, the OH 3064 Å system ($A^2\Sigma^+$ - $X^2\Pi$) and NH 3360 Å ($A^3\Pi$ - $X^3\Pi$) system. The intensity distribution recorded along the axial direction show a very fast decrease of the Ar lines intensity (one order of magnitude during the first 0.5 mm), while the intensity associated to OH and NH emission decreases much slower.

By fitting the experimental spectra corresponding to OH bands with the simulated ones, the rotational temperature along the axial expansion direction was determined. The rotational temperatures are around 550 K in the nozzle proximity and decreases along the expanding axis. These values are compared with the temperatures measured by means of a thermocouple inserted in the jet. These small values are an indication towards the cold character of the plasma source, thus opening the way for treatment of temperature sensitive substrates, like polymers or biomaterials.

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## A study of the Plasma Distribution in the DC Plasma Jet in Argon

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Spatial variations of plasma parameters have been studied in the DC plasma-chemical jet-type reactor in argon by means of movable Langmuir probe. The reactor vessel was constructed in UHV technology in order to achieve very clean and defined experimental conditions. The plasma-jet system consisted of water-cooled titanium nozzle with inner diameter 4 mm. The plasma flow entered the cylindrical reactor vessel 30 cm in diameter and 35 cm in length. The applied diagnostics consisted of two Langmuir probes and of mass-spectrometer. One cylindrical Langmuir probe was radially movable in the plane approximately 40 mm below the nozzle exit. Second probe protruded into the reactor vessel from the top and enabled thus the measurement of the radial as well of the longitudinal variations of the plasma parameters. The experiments were performed at typically 20 Pa argon pressure, discharge current 100 mA and the mass flow of argon 30 sccm. The ultimate pressure in the reactor chamber was in the order $10^{-5}$ Pa.

The plasma jet nozzle presents a hollow cathode, and as a consequence the charged particles are generated not only by gamma processes on the cathode surface, but also by so-called pendulum electrons and by intensive photo ionization. The pendulum electrons are the electrons emitted from the cathode surface that are accelerated by the cathode fall near the nozzle surface and pass through the diameter of the hollow cathode to the opposite cathode wall. There they are reflected back and after passing the diameter of the nozzle they again reach the cathode fall region, again are reflected etc. On their way through the nozzle volume the pendulum electrons intensively contribute to the ionization of the working gas that flows permanently through the nozzle and is being continuously pumped out of the reactor volume.

The probe electronics is galvanically isolated from the control computer that significantly reduces the noise. Further improvement of the signal-to-noise ratio is achieved by averaging approximately 400 data points acquired at a particular probe voltage. The probe system is controlled by using the Agilent VEE control software.

The obtained data map the plasma parameters in two dimensions - radial and axial. System is supposed to have the cylindrical symmetry. The first measurements revealed very interesting feature of the jet plasma, namely that the mean electron energy (the electron energy distribution function is not Maxwellian) reaches a minimum at the jet axis and rises with increasing radius up to a certain value that then remains approximately constant with radius. The electron density reaches maximum of the order $6\times10^{17}$ $m^{-3}$ at the jet axis and decreases comparatively slowly with increasing radius down to the limiting value of about $10^{16}$ $m^{-3}$.

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## Role of OH and H Radicals in the Production of Hydrogen Peroxide by the Pulsed Corona Discharge in Water

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Non-thermal plasma processing in aqueous solution by applying a high voltage power is considered to be an attractive method for the production of highly active chemical species directly in water. Different types of electrical discharges (AC, DC, pulsed) generated either directly in water or above the water surface are being studied as possible method for water treatment. It has been demonstrated that the pulsed high voltage discharges generate in water plasma that initiate a variety of physical and chemical effects as high electric field, intense ultraviolet radiation, overpressure shock waves and, especially, formation of various reactive chemical species such as radicals (OH·, H·, O·, $HO_2$·) and molecular species ($H_2O_2$, $H_2$, $O_2$). Among them especially ·OH radicals play very important role due to their high oxidative power capable to completely oxidize virtually any organic compound in water. It was shown that pulsed electrical discharges in water are effective at degrading a number of small organic compounds including phenols, TCE, biphenyls, organic dyes etc., since the mechanism of degradation of organic compounds was found to be attributed mainly to the oxidation by hydroxyl radicals. Consequently, the removal efficiency of the discharge can be significantly enhanced in the presence of iron due to Fenton's reaction, where hydrogen peroxide produced by the discharge reacts with ferrous ions to produce hydroxyl radicals. It has been demonstrated that production of $H_2O_2$ by the pulsed electrical discharge in water depends mainly on the applied input power and solution conductivity. General mechanism of $H_2O_2$ formation is thought to be mainly the recombination of OH radicals that are formed by electron impact dissociation of water molecules in the plasma discharge zone. However, the exact mechanism is still unknown since OH radicals can also contribute to the decomposition of $H_2O_2$ and thus decrease its production. There is also possibility of the influence of reductive species on the production of $H_2O_2$ (e.g., H, $HO_2$, $H_2$).

In the present study a free radical scavenging property of dimethylsulfoxide, phenol and potassium bromide has been used to determine the production of $H_2O_2$ by the pulsed electrical discharge in water generated in the reactor with point to plane geometry of electrodes. These substances are highly reactive with OH radicals and, thus, capable to eliminate a possible decomposition of $H_2O_2$ by OH radicals. In addition, varying their scavenging strength they are also capable to control reactivity of H radicals with $H_2O_2$. Effects of these scavengers on the production of hydrogen peroxide by the discharge in water will be presented and the role of OH and H radicals will be discussed.

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## Study of Heterogeneity in an Azimuthal Direction of Hall Accelerator Plasma Flow

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The Hall accelerator (HA) is widely used in plasma technologies in various areas of techniques: as a source of ions for surface processing and for carrying out of researches in the field of nuclear fusion, as electric propulsion system for space vehicles. At the same time HA continues to be studied by many scientists in the different countries. One of directions of HA modernization – the control over electron transfer through a discharge interval. The way of electron transport transfer in the discharge interval of HA has been investigated for many years, but full understanding of physical bases of transfer process is not achieved. In particular, large attention is paid to study fluctuations in plasma, which can play a significant role in transfer of electrons through a discharge interval.

Fluctuations of plasma are spatial plasma heterogeneity, change in time in each point. Besides, it is possible existence of plasma quasi-stationary spatial heterogeneity, caused by features of HA design. Research of such quasi-stationary spatial heterogeneity of plasma potential in an azimuthal direction has been carried out using HA models of M-70 and M-40 type (where 70 and 40 are the values, in mm, of outer diameters of discharge chamber) in various modes of discharge voltage, value of a magnetic field and using various designs of the anode-gasdistributor.

The heterogeneities of plasma luminescence in azimuthal direction of plasma flow in HA, operated in various modes have been registered. Registered plasma heterogeneities can be explained in the following way. There is a longitudinal electric field of a constant sign in the discharge chamber during all its extension. Near the apertures in the anode-gasdistributor there is an intensive ionization of the gas. The ions, which were given birth near to apertures, fly out from the discharge chamber and form streams with increased of concentration of charges. Due to the occurrence of areas of charges heterogeneities in an azimuthal direction, it is going charge polarization in these areas and, as consequence, it is possible existence of azimuthal components of an electric field. The extension of these areas is estimated as visual distance of $L \sim 10^{-2}$ m, amplitude $\delta\varphi \sim T_e$ – electron temperature, the intensity of the induced electric field $\delta E \approx \delta\varphi/L$. At the analysis of possible mechanisms of electrons conductivity, these fluctuations should be taken into account as the additional factor, which increases electron conductivity.

Analysis of results allows to formulate a hypothesis that gas ionization and formation of ion streams, directed to the discharge chamber output occur in all volume of the discharge chamber (from the anode up to discharge chamber output). I.e. the widely known mode, when the ion stream is formed in narrow area close to the discharge chamber output, is not realized, and the area with negative (back) potential drop near to the anode is not formed. It specifies separate jets of the ions, which were given birth near to apertures in the anode-gasdistributor and accelerated in a longitudinal electric field in all an extension of the discharge chamber.

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## Theoretical Study of Proton Affinity and Proton Transfer Energy for Selected Chemical Compounds

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The ionization phenomenon is one of the main problems in plasma physics and chemistry. In mass spectrometry traditional methods of ionization, like electron impact or inductively coupled plasma, lead usually also to fragmentation of molecules. In mass spectra ionized fragments of analyzed molecules usually appear. And thus identification of the parent molecule is difficult and sometimes simply impossible. The problem of gas-phase ionization without molecule fragmentation can be solved by using so-called soft ionization, for example via a proton transfer reaction from the hydronium ion $H_3O^+$ to the analyzed molecule. In this work the Restricted Hatree-Fock method with 6-311G(d,p) and 6-311G++(2d,2p) split-valence molecular orbitals basis sets, quadratic complete basis set (CBS-Q) method and different hybrid density functional theory (DFT) has been applied to geometrical optimizations and calculations of total electronic, zero point vibrational and thermal energies for small neutral and protonated organic and inorganic molecules, i.e. CO, $CO_2$, NO, $NO_2$, $N_2O$, $H_2O$, $SO_2$, $CH_3OH$, $C_2H_5OH$, $CH_3CHO$, $CH_3COCH_3$ and $CH_3COOH$. The proton affinity and proton transfer energy has been calculated at 298.15 K for reactions $M + H^+ \rightarrow MH^+$ and $M + H_3O^+ \rightarrow MH^+ + H_2O$, respectively. Present results are in good agreement with experimental results and with other theoretical data, in particular for B3LYP/6-311G++(2d,2p) and CBS-Q methods.

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# Properties of Plasma Injected in Open Magnetic Trap from Independent UHF Source

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Various ways of filling the open magnetic trap with plasma are used in different experiments on study of plasma in order to develop methods of the plasma heating and confinement, to study the interaction of electromagnetic waves with magnetoactive plasma etc. From all existing methods the UHF contactless methods are used most frequently. As a rule, the plasma formation takes place in the trap itself in the electron cyclotron resonance (ECR) regime. However, this method has various disadvantages. In particular, the range of magnetic field change in the trap is strictly limited by the existence of UHF discharge in the magnetic field; with the change of magnetic field, discharge regime and plasma parameter change and most important is that the "hot" region of the UHF wave absorption in plasma is in the trap itself, which is often undesirable. Therefore, the application of an independent "quiescent" plasma source with controllable parameters, which is far from the trap and from which the "target plasma" is injected into it, is of great interest. For this purpose side by side with other methods we have proposed the method of filling the open magnetic trap by plasma injection along the magnetic field from the separate stationary UHF source removed from the trap. In this source the plasma is formed in the ECR regime in highly nonuniform magnetic field.

We investigated the plasma properties in independent UHF source and the "target plasma" properties in the magnetic trap with a homogeneous and mirror configuration of magnetic field. The distribution of plasma particle density along the trap is measured and the dependences of density and temperature on the conditions of plasma formation in the UHF source and on the trap parameters are investigated. The spectral characteristics of plasma in the trap are investigated too. Experiments and data analysis have shown:

1. Plasma is created in UHF source of 2400 MHz / 150 W in the ECR regime.
2. The UHF plasma source can be maintained both in ECR regime and at magnetic field $H_s < H_e$. The condition of upper hybrid resonance (UHR) can be fulfilled in plasma volume.
3. One can effectively inject plasma from the independent UHF source into the open magnetic trap. The distance between the plasma source and the trap will not affect efficiency.
4. Rather "quiescent" plasma is accumulated in the trap with controllable density within the range $(2\times10^{8} \div 2\times10^{12})$ cm$^{-3}$ and electron temperature $(2 \div 3)$ eV.
5. Plasma particle lifetime in the trap is determined by classical mechanisms of particle escape at the expense of collisions. At fixed value of magnetic field in the trap it practically does not change with the variation of neutral gas pressure and reaches the value $\approx 4\times10^{-3}$ s at the strength of the magnetic field in the trap equal to 1600 Oe.
6. For relatively high pressure ($p > 10^{-3}$ Torr) particle lifetime is determined by ambipolar diffusion across the magnetic field and at low pressure ($p < 7\times10^{-4}$ Torr) it is determined by longitudinal ambipolar diffusion.
7. The energy accumulated in plasma is consumed in the trap mainly for ionization and excitation of neutral gas, as well as for heating of newly formed electrons.

A set of experimental data gives the possibility to conclude that such method of filling the open magnetic trap with plasma can be successfully used in various physical experiments.