GDAŃSK
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CONFERENCE
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PHYSICAL SOCIETY

Second Conference on the

ELEMENTARY PROCESSES IN ATOMIC SYSTEMS

Gdańsk, Poland, 2-6 September 2002
Gdańsk University of Technology

BOOK OF ABSTRACTS

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Compiled by E. Ptasińska-Denga and R. Szmytkowski

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FOREWORD

The CEPAS conferences have been established as a new series of bi-annual international meetings that focus on all aspects of processes and phenomena stimulated by interactions of electrons, positrons, ions, atoms, molecules, photons and other constituents of matter with gaseous, liquid and condensed matter at low and intermediate energies. The 2nd CEPAS conference organized in Gdańsk, follows the first conference hosted by the Institute of Electron Physics in Uzhgorod, Ukraine. The conference is designed to be a forum for specialists working on elementary processes in matter from Eastern and Central Europe, the European Union and other parts of the world. Special attention is paid to encourage the participation of young researchers.

This book contains the abstracts of fifteen invited lectures. It also contains the abstracts of more than ninety contributed papers from research institutions in many European countries and also in Armenia, Australia, Canada, India, Israel, Japan, Korea, USA and Uzbekistan. These contributed papers will be reported in posters sessions. Ten of these papers have also been selected for oral presentations.

The Gdańsk University of Technology is proud to host this conference and we hope that it will stimulate and promote new research initiatives. We also hope that all conference participants will enjoy visits to the picturesque Old Town of the City of Gdańsk which celebrated its millennium five years ago. We acknowledge that the conference was granted sponsorship from the European Physical Society.

Mariusz Zubek
Conference Chairman

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INVITED LECTURES

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LOW ENERGY ELECTRON – MOLECULE COLLISIONS

M. Allan,* T. Skalický and S. Živanov

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Structures due to motion of the nuclei were discovered in cross sections for electron-molecule collisions long ago and their shapes were related to the autodetachment widths of the resonances [1]. Structures of vibrational origin were subsequently predicted theoretically and observed in cases where the large width of the resonance could have been thought to prevent them (H_2 [2], HCl [3]). A variety of structures has been discovered more recently. Step-like structures are observed even above dissociation limit (HCl, HI). Narrow structures were observed at energies below the dissociation threshold. They may be due to cusps, but high resolution work has demonstrated that they lie below vibrational thresholds in some cases where they must be due to vibrational Feshbach resonances (HF [4], CH_3I [5]). At higher energies in HF [6] and in HCl [7] and HBr [8] the vibrational Feshbach resonances broaden and become boomerang oscillations. Very narrow structures due to outer well resonances are superimposed on the boomerang structures in HCl [7]. Nonlocal resonance theory succeeded in describing all the structures in hydrogen halides [8], as well as structures in the associative electron detachment [9]. Pronounced selectivity was observed in the excitation of Fermi-coupled vibrations near threshold in CO_2 [10, 11], at energies where cross section enhancement is attributed to a virtual state – albeit without structures. Recently, however, narrow structures turning gradually into boomerang oscillations were discovered even in the virtual state region of CO_2, in the excitation of certain higher-lying Fermi-coupled vibrations [12].

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I-2

NEGATIVE-ION STUDIES IN STORAGE RINGS

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Heavy-ion storage rings are used for studies of atomic, molecular and cluster ions (see e.g. Ref.[1]). In this contribution the focus will be on studies of negative ions which have been studied rather intensively at the storage ring ASTRID in Aarhus, Denmark (an early review is provided in Ref.[2]). In the talk, examples of research performed on negative ions will be discussed. This includes lifetime measurements of metastable electronic states, slow isomerization processes, scattering experiments with free electrons, and the formation of shortlived doubly-charged negative ions. As a new activity, we are studying absorption properties of negatively charged (de-protonated) biomolecules in the visible region[3]. These studies are performed at the new and smaller electrostatic ion storage ring ELISA[4]. It is demonstrated that the storage ring technique with long storage times and suitable particle detection is ideal for studies of the photophysics of chromophores. The absorption band of the anion chromophores of the Green Fluorescent Protein (GFP) will be discussed as an example. Our gas-phase absorption measurements are compared with absorption profiles of the chromophore ion inside the protein and of chromophores in liquids. In the protein, the chromophore is covalently attached to an α-helix that runs up the axis of a hollow cylinder formed by eleven β-strands. The cylindrical shape of the rigid β-can protects the buried chromophore, and based on the new absorption data it is argued that the absorption characteristics of GFP is mainly ascribed to intrinsic chemical properties of the chromophore. Absorption measurements with model chromophores of mutated GFP proteins are currently being performed in our laboratory to investigate to what extent these findings apply to other systems.

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I-3

INTERACTION OF SLOW HIGHLY CHARGED IONS WITH SURFACES

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The large potential energy stored in highly charged ions is liberated when these ions recombine near a solid surface. In such collisions short-lived multiply-excited neutral particles are formed with a large fraction of electrons bound in high-n states while inner shells stay transiently empty („Hollow Atoms“). For certain target species the potential energy deposited at the surface causes a novel form of ion induced sputtering which in analogy to the usual kinetic sputtering has been termed "potential sputtering" [1].

Since during the last two decades intense sources for slow, highly charged ions (HCI) have become available, the possibility of using potential sputtering for surface modification and nanofabrication has captured the imagination of researchers. Applications have been envisioned, ranging from information storage via material processing to biotechnology. Compared to kinetic sputtering (i.e. sputtering of target atoms due to momentum transfer in collision cascades), which unavoidably causes unwanted radiation damage in adjacent regions, potential sputtering holds great promise for a more gentle nanostructuring tool. A profound understanding of the mechanisms responsible for the conversion of projectile potential energy in such collision processes is therefore highly desirable.

Potential sputtering phenomena have been reported by several groups for a variety of insulator target surfaces as, e.g., alkali-halides, SiO_2, UO_x, GaAs, mica and hydrocarbon-contaminated surfaces (see, e.g., [1 - 5] and references therein). These investigations have in common that a dramatic increase of the total sputter yields, the secondary ion emission yields and/or the size of single ion - induced surface defects have been observed with increasing projectile charge state.

We summarize the present status of this field and discuss the mechanisms leading to potential sputtering.

This work has been carried out within Association EURATOM-ÖAW and was supported by Austrian FWF.

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I-4

Dissociative Electron Attachment and Charge Transfer in Condensed Matter.

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Experiments using energy-selected beams of electrons incident from vacuum upon thin vapour deposited solids reveal that the interactions of low energy electrons with condensed atoms and molecules have much in common with those observed in gas-phase collision physics [**1**,**2**]. For example, scattering cross sections at low energies are dominated by the formation of negative ion resonances (or short-lived anionic states) and molecular damage can be affected via dissociative electron attachment (DEA). In the condensed phase however, DEA is modulated by a variety of *extrinsic factors* that can either affect electrons prior to their interaction with the target molecule or fragment species after dissociation. *Intrinsic factors* such as polarisation, that alter the energy, lifetime, etc., of transient anions, also modify stable anion production via DEA. Recent results have uncovered the intrinsic role of charge exchange between anionic states of target molecules and their environment in determining cross sections for electron driven processes

In this contribution we will review studies in which charge transfer is observed to occur. For rare gas solids, we show how electron exchange between negatively charged excitons and either a metal substrate or co-adsorbed molecule can enhance the desorption of metastable atoms and/or molecular dissociation. We will demonstrate how transient electron capture by the 'surface electron states' of a substrate and subsequent electron transfer enhance the effective cross sections for certain electron attachment (and DEA) processes. We will devote attention to the analogous case of DEA to molecules (e.g., CF_2Cl_2, 5-halo-uracils) condensed on water ice, where electron exchange between pre-solvated electron states of ice and transient molecular anions can increase DEA cross sections.

This work is supported by the Canadian Institutes of Health Research.

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I-5

PHOTOEXCITATION AND PHOTOIONIZATION SPECTROSCOPY OF ATOMS AND MOLECULES

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Photoexcitation and photoionization spectroscopy of atoms and molecules probes the initial and final states of the ionized target regarding its electronic but also geometric structure.

This field has recently evolved in three main directions, if the spectroscopy of ions and clusters are considered to be separate subfields:

i) The analysis of the photoionization and photoexcitation processes by „complete" experiments in order to achieve an approximate description in terms of transition matrix elements, including relative phases. During the last years, there has been significant progress especially in atomic photoionization [1], whereas molecular photoionization is still in its infancy [2].

ii) The study of many-electron emission processes regarding the nature of the electron correlations governing them. Photo double ionization of helium is a prominent example for these studies because it is a show case for the three-body Coulomb problem [3]. Considering the decay of core-excited and core-ionized states the simultaneous emission of two Auger electrons has just recently been observed by electron-electron coincidence spectroscopy, thus complementing the photo double ionization studies.

iii) The scattering of the photoelectron on its way out in many cases serves as a fingerprint of the geometric structure of the ionized target. Localized inner-shell electrons probe the conformation of the nuclei in a molecule, whereas delocalized valence electrons cause a sort of diffraction, which images the delocalized electron clouds in reciprocal Fourier space. Examples for both behaviors are presented and discussed.

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I-6

PHYSICAL PROCESSES IN LASERS ON SELF-TERMINATING TRANSITIONS

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Gas lasers oscillating on transitions emitting from the upper resonant to the lower metastable levels are known as the lasers on self-terminating transitions (STT). Comparatively simple but effective pumping scheme used in these lasers is based on the dominating efficiency of excitation of the atom (or ion) resonant levels by electron impact on the front of the high-voltage pulsed discharge. Although it is more than 35 years ago as the first Mg-vapor laser of this class was invented and elaborated, there still are not resolved some principal aspects touching both the physical processes in these lasers and some practical applications.

As mentioned above, although the main pumping scheme seems to be rather simple, this simplicity is delusive. A large quantity of physical phenomena do not allow one to obtain limiting lasing parameters predicted by theoretical calculations. In this context are discussed the discharge nonuniformities, gas temperature and metastable level population relaxation during interpulse period. It is shown that all these parameters are closely connected. The question concerning the prepulse electron concentration and influence of its value on laser parameters is also discussed (known discussion between G.Petrash and S.Yakovlenko).

Sometimes the influence of these parameters is surprisingly unpredicted. It has been shown that in Bi-vapor laser the pumping mechanism is not traditional and not similar to that in the ather STT lasers. In Bi-vapor laser, the upper resonant level is excited predominantly due to dissociative excitation of bismuth dimers by electron impact.

The most impressive results in the field of STT lasers were obtained during last period using so-called HyBrID technology. CuBr compound in this laser is produced directly in a discharge tube when Ne + HBr mixture is pumped through the tube. So, in discharge new kind of particles are present (hydrogen, halogens). Influence of these particles on processes during the current pulse and interpulse period is discussed. An Cs admixture, which resonance level is in resonant coincidence with Cu atom metastable level energy, influence on lasing properties of Cu-vapor laser is also discussed.

STT lasers have extremely high amplification. A Unique tool – coherent brightness amplifiers of image - were designed using this property. In combination with the Cu-vapor laser in green and the Au-vapor laser in red, an effective blue STT laser can be useful to elaborate the color projection systems with brightness amplifiers of images. However the Bi-vapor and the Fe-vapor blue lasers tested till now do not satisfy the average power and efficiency requirements.

Suggestions for new blue STT lasers using titanium and indium atoms self-terminating transitions are discussed.

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I-7

THRESHOLD PROCESSES IN PHOTOIONIZATION OF ATOMS AND MOLECULES

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In threshold photoionisation the target is ionized just above a reaction onset. Photoelectrons are produced with energies that are typically in the range from zero to a few meV and these are detected by analysers tuned to these low energies. Threshold photoelectron studies have been applied to both single and double photoionisation. They are important because they give both dynamic and spectroscopic information. They also have a number of experimental advantages.

Close to threshold, different ionisation processes become important. For example, in photodouble ionisation, the low energy electrons move only slowly away from the ion core allowing ample time for electron correlation effects to become dominant. Also, close to threshold, indirect processes are often important. Here photoionisation proceeds via a highly excited state in a two-step process. This highly excited state may decay to the final ion state with the emission of an autoionisation electron which will be detected if it has sufficiently small energy. These indirect processes compete with the direct one and indeed can become dominant. In the case of molecules, for example, this can lead to the observation of vibrational excitation well outside the Frank-Condon region. All of this all means that threshold photoelectron spectra are invariably very different from conventional photoelectron spectra and so provide much new information.

On the experimental side, the threshold technique offers the advantages of very high resolution (~ meV) and simultaneously very high detection efficiency. This means that they can give state spectroscopic information at the level of individual rotational levels. This very high resolution is also well matched to the high photon resolution provided by current synchrotron radiation sources. The very high detection efficiency facilitates the use of coincidence techniques that are required for the study of double ionisation, where both photoelectrons are detected simultaneously.

Recent experiments will be described illustrating the techniques and the kinds of information that can be obtained from threshold photoionisation studies.

I-8

SCATTERING OF POSITRONS AND POSITRONIUM BY ATOMS AND MOLECULES

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Interest in collisions involving positrons (e^+) and positronium (Ps, the bound state of a positron and an electron, e^-) remains strong as new experimental techniques and theoretical methods are enabling increasingly stringent tests of the understanding of basic atomic and molecular collision phenomena, as well as of fundamental antiparticle-matter interactions. Current topics of research include positron-induced ion production (comprising ionization with and without Ps formation, annihilation, etc), positron impact excitation (vibrational and electronic) and positronium scattering. The status on available experimental cross-sections for positron and positronium collisions will be reviewed, including recent advances in the investigation of positron impact ionization (with and without Ps formation), excitation and annihilation. In the case of Ps projectiles, the status on measurements of the total and break-up cross-sections in collision with simple atomic and molecular targets will be reviewed. Comparison with theories shall be made wherever possible. The interested reader is further referred to recent works[1,2,3,4].

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I-9

ELECTRON DRIVEN REACTIONS IN CLUSTERS

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Mass spectrometric studies of spontaneous (metastable) decay reactions and of dissociative reactions of mass-selected cluster ions induced by photons, electrons or surface collisions have provided a wealth of information about structure, stability and energetics of these species and the dynamics of the corresponding decay reactions. Surprisingly few studies, however, have been reported concerning measurements of the kinetic energy release distribution (KERD) for the decay of metastable, weakly bound atomic (rare gas) or molecular, cluster ions.

The most common mechanism that drives unimolecular, metastable decay of atomic cluster ions is vibrational predissociation in which the excess energy is statistically distributed over all energetically accessible degrees of freedom, usually limited to atomic vibrations. However, unimolecular dissociation may also be driven by mechanisms that involve non-statistical, localized storage of excess energy. For example, large amounts of energy can be stored in electronically excited states in rare gas clusters: one characteristic features of these exciton-driven decays is the large amount of energy that is abruptly released within the metastable time window as shown here for the first time.

Using a high resolution two sector field mass spectrometer of reversed geometry we have measured metastable fractions and mass-analyzed ion kinetic energy (MIKE) peaks for metastable (spontaneous) and electron-induced decay reactions involving monomer evaporation and fission reactions of atomic and molecular cluster ions produced by electron impact ionization of neutral cluster beams. Additional information about the production of these ions as a function of cluster size has been obtained by studying the ionization thresholds using a high resolution electron monochromator.

Both, average kinetic energy release, <KER>, data derived from the peak shapes and the time dependence of the metastable fractions show a characteristic dependence on cluster size yielding immediate information on the metastable fragmentation mechanism when going for instance from the dimer to the dekamer ion. Moreover, the <KER> data contain information about the transition state temperature and thus one can use finite heat bath theory to calculate the binding energies of the decaying cluster ions allowing informative comparison with (i) previous results based on gas phase ion equilibria measurements where available and with (ii) the corresponding bulk value. The recent addition of a third sector field and a high performance electron gun enables also studies of the time dependence of the kinetic energy release distribution (KERD) and in conjunction with model calculations for these KERDs to obtain information on the dynamics of the underlying decay reactions.

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I-10

AUGER PROCESSES IN ELECTRON IMPACT EXPERIMENTS

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The Auger electron spectroscopy is a very effective tool for the study of materials. Although that tool is rather old, the application of the recent experimental and theoretical methods can still lead to new results.

In the lecture we concentrate to the line shape of the Auger peaks ejected after electron impact inner shell ionization. The line shape is affected mainly by the post-collision interaction (PCI) i. e. the Coulomb interaction of the four charged particle in the final state: the scattered electron, the ionized electron, the Auger electron and the target ion. For non-coincidence experiments, when the scattered and the ionized electrons are not detected, the peak shapes can be obtained by integration of the triply coincidence peak shapes [1] over the non-measured quantities.

We have carried out a set of calculations on the peak-shapes of argon $L_{2,3}M_{2,3}M_{2,3}$ Auger electrons at 300 eV, 500 eV and 2 keV primary electron energies at different Auger emission angles [2]. We determined the required cross sections for secondary electrons by the classical trajectory Monte Carlo method and, for high impact energy (2 keV), by the continuum distorted wave method, too. After the numerical integration the Auger peak-shapes were evaluated in the same way as the experimental spectra, so we could compare our calculations and experiments. The energy- and angular dependence of Auger peak shapes will be discussed in the lecture. Here we stress that the angular dependence of the Auger peak asymmetry has maximum, when the energy of receding three electrons is comparable, thereby the relative velocities strongly depend on the orientation of velocity vectors.

In complex spectra, when the Auger peaks strongly overlap, the knowledge of the exact line shape is essential. As an example of this problem we show the evaluation of the Kr $L_{2,3}M_{4,5}M_{4,5}$ Auger spectrum [3].

Among the diagram lines of Auger spectra we can often observe satellite lines of different origin. One of these types will be examined in details, it is the so-called resonant Auger process after deep inner shell electron impact excitation [4].

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I-11

Fragmentation and ionization induced by high energy particle collisions

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The interaction of molecules and clusters with fast projectiles like protons electrons or He atoms often leads to ionization and/or fragmentation of the large collision partner. Such processes play an important role in technical and natural plasmas. In addition damage of living cells upon the exposure to ionizing radiation on a microscopic level is also based on ionization and fragmentation of the DNA. In different laboratories specially designed instruments were used to investigate the inelastic interaction of clusters and molecules with various projectiles. These experiments have provided new information about structure, stability and energetics of these species and the dynamics of the reactions involved.

In Lyon high-energy collisions (60 keV/amu) of hydrogen cluster ions with a helium target were completely analyzed on an event-by-event basis. By selecting specific decay reactions it is possible to start after the energizing collision with a microcanonical cluster ion ensemble of fixed excitation energy and to derive corresponding temperatures of the decaying cluster ions. The relation between the temperature and the excitation energy (caloric curve) exhibits the typical prerequisites of a first-order phase transition in a finite system, in the present case signaling the transition from a bound cluster to the gas phase.

In Giessen fragmentation of fullerene ions C_{60}^{z+} (z=1 ... 3) induced by electron impact was studied quantitatively for the first time. The cross sections for the loss of a C_2 fragment indicate the presence of two different processes. At low electron energies the projectile electron leads to the direct excitation of the giant plasmon resonance. At electron energies larger than 100 eV the fragmentation of the fullerene ions can be described as an unsuccessful ionization. Only this second part of the cross section shows a dependence on the charge state z of the precursor ion.

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I-13

DYNAMICS OF IONIZATION PROCESSES STUDIED WITH THE COLTRIMS METHOD — NEW INSIGHT INTO e–e CORRELATION

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Many-particle dynamics in atomic and molecular physics has been investigated by using the COLTRIMS method. The method and its application are discussed. The COLTRIMS technique visualizes many-particle fragmentation processes in the eV and sub milli eV regime and reveals — like the bubble chamber in nuclear physics — the complete momentum pattern in atomic and molecular particles reactions. New data on e–e correlation in He are presented. Particularly the asymptotic regime of the He ground state wave function is explored, where all long range correlation is hidden.

I-13

High Resolution Studies of Electron-Ion Recombination

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Cooler storage rings are excellent tools to study recombination of electrons with ions. This process has several important astrophysics and plasma-physics applications, besides being of fundamental interest. It is the proposed mechanism for antihydrogen production in a trap filled with antiprotons and positrons. The most fundamental process is radiative recombination. When recombination proceeds via a doubly excited state in the $Z^{(q-1)+}$ intermediate system (in dielectronic recombination), then the cross section shows strong resonant-like structure. Accurate measurements of these resonances in scattering of electrons at ions can be used for critical tests of calculations.

We present our latest results on recombination at very low relative energies between electrons and ions done at the CRYRING heavy-ion storage ring at MSL in Stockholm. This electron cooler has an adiabatically expanded electron beam that gives electrons with mean transversal velocity component of 1 meV and longitudinal component of 0.1 meV. New data on the enhanced rate coefficient is shown. Then we will concentrate on recent measurements of dielectronic recombination resonances with Li-like, Na-like, and Cu-like ions, where from the spectra of resonances very accurate values for energy splittings are derived for crucial tests of relativistic, correlation[1], hyperfine interaction, and QED effects[2]. We will see that, and how the presently most accurate data on level splittings and QED effects in heavy, highly-charged atomic systems is obtained by recombination, thus by electron scattering, instead of conventional photon spectroscopy.

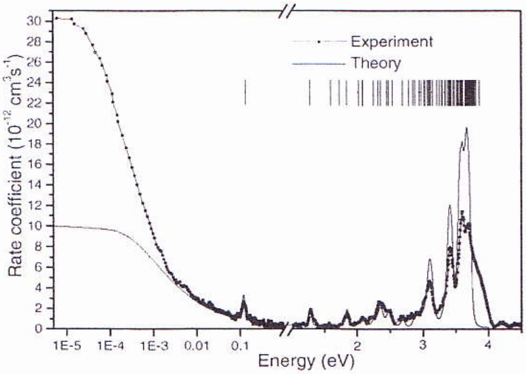

Figure 1: Comparison of the experimental recombination rate coefficient for Be^+ with a calculation [1] in relativistic many-body perturbation theory.

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I-14

Studies of physical processes in the Earth's atmosphere

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Investigation of properties of the atmosphere are of great importance. Besides recognition of mechanism leading to the formation of either the local weather or global climat changes, the knowledge of physical and chemical parameters of the atmosphere is important for understanding the processes of pollutions emission, their propagation and transformation (imission), as well as their influence on living organisms, especially for the human health.

In the atmospheric research the optical methods has been always widely used. In nowadays various methods of laser spectroscopy improve these opportunities. During the lecture we will present application of Cavity Ring – Down Spectroscopy for monitoring of atmospheric trace gases. This technique, characterized by extremely high sensitivity, can replace in the future some standard methods used for detection of the atmospheric compounds.

The possibilities of the remote investigation are of great interest for the atmospheric researchers. Here the lidar techniques provide the unique opportunities of measurements. The most simple, single wavelength lidars, are suitable to search distribution of aerosols in the atmosphere. Measurements of depolarization of the laser light scattered in the atmosphere can inform about the presence of nonspherical aerosol particles. The lidars working on two wavelengths (DIfferential Absorption Lidar - DIAL) are used for selective detection of the atmospheric pollution. Finely the lidars working on many wavelengths provide opportunity to investigate the size distribution of the aerosol particles. During the lecture our achievements obtained by means of the lidar techniques will be shown.

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I-15

ELECTRON – MOLECULE COLLISIONS CALCULATIONS USING THE R-matrix METHOD

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Electrons collisions with molecules can result in the excitation of both nuclear and electronic motions. Considerable work has been performed using the R-matrix and other methods studying these processes in the low energy regime, where many of the cross sections are dominated by resonances. Recent examples of calculations include:

- Electron impact dissociation studies of water [1] which are important for models of radiation damage in biological systems.
- The study of electron collisions with atmospherically important Cl_xO_y radicals [2-4].
- Electron impact dissociation data for H_2 and isotopomers, which required the formulation of the double differential cross section for this process [5] and the probable identification of the source of 'cold' H atoms at the edge of fusion plasmas [6].
- Electron impact rotational excitation of molecular ions, we have considered all astrophysically important diatomic ions [7] and symmetric top molecules [8], including the first ever calculations on electron collisions with the key H_3O^+ ion [9].
- Electron collisions with plasma etching gasses, in collaboration with the experiments of Dr Nigel Mason. The first ever results have recently been obtained for collisions with CF_2 radical, which show a clear pathway for dissociative attachment [14], and calculations on collisions with CF_3 have started.
- Dissociative recombination (DR), calculations performed in collaboration with Suzor-Weiner's group in Paris, obtained quantitatively correct results afor the DR of NO^+ at low energies and explained the behaviour at higher energies [15], both for the first time. Work on dissociative recombination of CO^{2+} is underway.

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POSTER SESSION A

A-1

INTERFERENCE EFFECTS IN THE TWO-COLOUR EXCITATION OF THE SODIUM ATOM

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Abstract

The steady state of the density matrix is analysed for the two colour light beam resonantly coupled to the different transitions between the lower $S_{1/2}$ and upper $P_{1/2}$ sodium hyperfine levels, $F=1$ and $F=2$. Particularly, the populations, the contributions to the transition dipole moments and the Raman coherences have been calculated for various beam intensities and detunings. The EIT resonance has been found to be entirely due to the collisional destruction of the ground state Raman coherence and the power broadening. Therefore, the corresponding profile is very narrow for the weak field, as compared with the spectral line shape. In the case of sufficiently strong coupling beam the dynamical Stark effect is dominant. We have found that the position of the EIT resonance does not depend on the field intensities of the coupling and probe beams.

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A-2

BOOMERANG STRUCTURES IN CO_2

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Vibrational excitation in CO_2 has two distinct energy ranges: a $^2\Pi_u$ shape resonance around 3.6 eV, where boomerang structures have long been known [1], and a virtual state at energies near threshold. Pronounced selectivity was observed in the excitation of Fermi-coupled vibrations in the virtual state range – albeit without structures [2, 3]. This poster reports structures of vibrational origin in the virtual state region of CO_2. They appear in the excitation of certain higher-lying Fermi-coupled vibrations involving stretch and bending [4]. The lowest two structures, at 0.45 and 0.53 eV, are narrow, higher lying structures are broader, boomerang-like, and extend up to about 0.9 eV. A possible explanation is that the virtual state, a 'state on the verge of being born', becomes 'truly born' at a bent and stretched geometry of the CO_2 and the observed structure is a consequence of the reflection of the nuclear wave packet on this potential surface. An alternative explanation would involve metastable vibrational levels of the well known bent and stretched A' valence state of CO_2^- (the lower branch of the $^2\Pi_u$ shape resonance) which could be coupled to the virtual state scattering by tunneling. The A' state of CO_2^- is generally thought to be at higher energies, though.

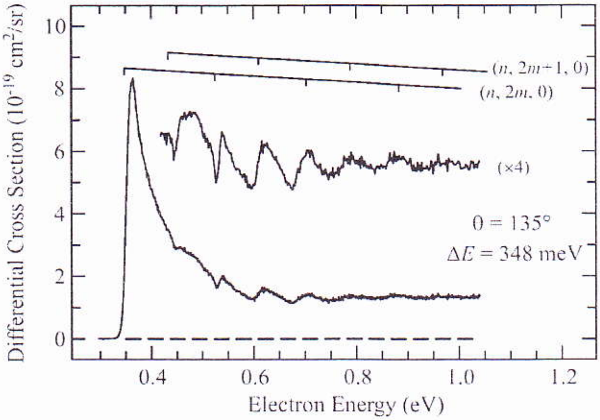

Figure 1: Cross section for exciting the topmost member of the Fermi triad $(m, 2n, 0)$ with $m + n = 2$. Selected vibrational thresholds are indicated by grids.

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A-3

ON THE CONTRIBUTION OF COSTER-KRONIG TRANSITIONS IN ATOMIC SHELLS TO THE BROADENING OF EMISSION LINES OF X-RAY PHOTOELECTRON SPECTRA OF METALS

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Broadening of emission lines in X-ray photoelectron spectra of solids is determined by different mechanisms of vacancy relaxation in the internal sell of atomic core. In the case of metals, the presence of the conduction zone causes the formation of new decay channel of the internal vacancy, channel being connected with the energy transfer to the electrons of conduction zone. In this paper the contribution of Coster-Kronig transitions with the formation of the hole in conduction zone to the whole broadening of atom level in metal has been considered. Calculations were carried out for Na (L - L V), K (M - M V), Zn (M - M) both in the Hartree-Fock approach, and with the account for multi electron correlations in RPAE approach both in the skeleton, and in conduction zone of metal. It has been shown, that in Li the wideness of 2S level in respect to the L - L V transition accounted for 70% of the whole wideness , in K - 50% of the wideness of emission band of M level, but in Zn this value accounted for ~ 2% of the whole wideness of M level. The conclusion has been made, that in Li and Na the calculated wideness of core levels coincidences with the whole non-irradiation wideness, but in Zn small value of calculated M - level wideness is connected with the fact, that besides of the mentioned (M - MM) decay channel there is the possibility of the expulsion of Auger-electrons from 3d(M) shell (Super-Coster-Kronig transition M -M M). In this case M - M V decay channel is practically closed and the whole wideness of M level is determined by the (M-M M) transition (the yield of fluorescence in Zn is ~ 1%).

A-4

COHERENT RESONANCES IN DEGENERATE TWO-LEVEL SYSTEMS IN Cs

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The phenomenon of Coherent Population Trapping (CPT) [1] has attracted increasing attention recently due to its applications in magnetometry, lasing without inversion, cooling of atoms, slowing of light, etc. It is observed mainly in alkali atoms when coupling the two ground-state hyperfine (hf) levels to a common excited level by means of two coherent radiations as a decrease in fluorescence around the two-photon Raman resonance condition.

It has been shown [2] that interesting coherent effects are observed also at a single hf transition, involving as lower levels the Zeeman sublevels of one of the ground hf state. In this case not only decrease in the fluorescence (Electromagnetically-Induced Transparency – EIT), but also increase (Electromagnetically-Induced Absorption – EIA) can be observed depending on the degeneracy of the ground and excited states. EIT resonances occur for $F_g \rightarrow F_e = F_g$-1 transitions and EIA resonances – for $F_g \rightarrow F_e = F_g$+1 transitions.

Our results show that in a vacuum cell, where there is overlapping of the hf transitions within one fluorescence line, starting from a single ground hf level, the sign of the resonances is determined by the degeneracy of the levels of the hf transition which is closed or which has the highest probability and suffers lowest losses towards the other ground level, not-interacting with the laser field. Single-sign resonances have been observed over the whole Doppler profile of the fluorescence lines of the D_2 line of Cs (Fig.1).

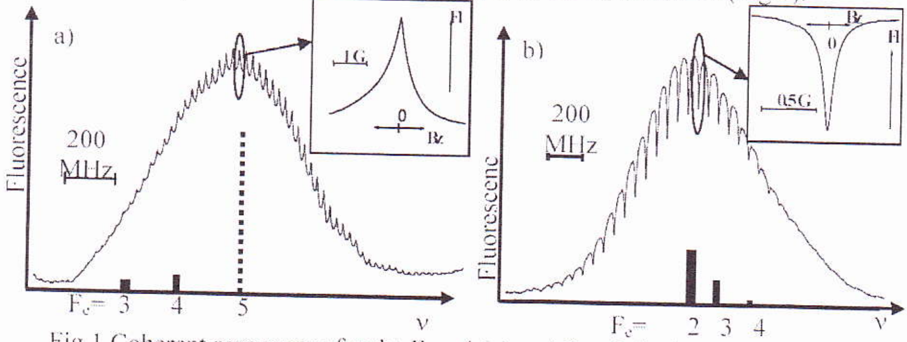

Fig.1 Coherent resonances for the $F_g = 4$ (a) and $F_g = 3$ (b) fluorescence lines

Results on the behaviour of these resonances in dependence on the parameters of the light field and transition irradiated will be presented.

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A-5

TOTAL CROSS SECTION FOR ELECTRON SCATTERING BY CH_4 , C_2H_6, CF_4 AND C_2F_6 MOLECULES IN THE ENERGY RANGE 200 – 1400 eV.

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The total electron scattering cross section of CH4 , C2H6 , CF4, and C2F6 molecules have been measured for 200 – 1400 eV electron energies using the electron beam attenuation through a gas cell. The intensity of the primary beam and the attenuated beam were measured using a double focusing electrostatic analyzer with energy resolution 0.75 eV (FWHM) or better and an angular acceptance of 1.2 x 10-5 sr. Measured cross sections have been compared to the existing theoretical predictions. The correlation between the total electron scattering cross section and the number of electrons in the target molecule is discussed.

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A-6

Temperature dependence in dissociative electron capture by 1,4-chloronitrobenzene

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Illenberger at all[1] have found unusual temperature dependence in dissociative electron attachment to 1,4-chlorobromobenzene. The effect found was explained by the temperature dependent population of the relevant normal modes containing the C-Cl and C-Br stretch vibration[1]. Following to this interesting result we studied the same molecule of 1,4-chloronitrobenzene which has positive electron affinity EA=1.234 eV[2].

Electron attachment to 1,4-chloronitrobenzene in the energy range 0-5 eV leads to three negative ion (NI) channels: M , NO_2 , and Cl . Intensity of the molecular NI decreases dramatically with temperature increasing. On the contrary, the intensity of the NO_2 and Cl ions is increasing with temperature. Moreover low energy resonance (~0.5 eV) shits left rapidly, but high energy resonance (~3.4 eV) keeps its energy. In contrast to the case of 1,4-chlorobromobenzene the ratio of NI intensities Cl :NO_2 ~2:1 in the low energy region ~0.5 eV, and 1:2 at the energy ~3.4 eV is practically constant, see figure.

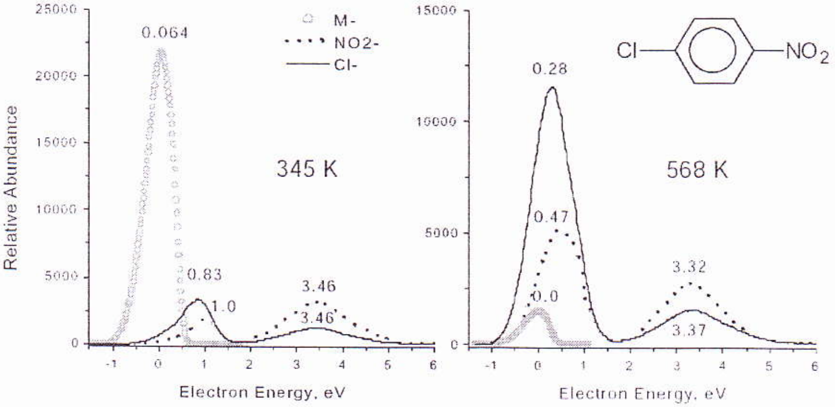

Figure. Temperature dependence of the curves of NI effective yield.

Data obtained allows to conclude that there are essential differences between temperature behavior of 1,4-chlorobromobenzene[1] and 1,4-chloronitrobenzene in dissociative electron attachment.

This work was sponsored by the Russian Foundation for Basic Research, Grant 00-02-16578.

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A-7

EFFECT OF ELECTRON IRRADIATION UPON PHOTOLUMINESCENCE OF $CdS_{1-x}Se_x$ MIXED CRYSTALS

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Mixed $CdS_{1-x}Se_x$ crystals are well known luminescent materials, the character of their luminescence strongly depending on the preparation conditions and external factors. The effect of electron irradiation upon the photoluminescence (PL) has been reported only for CdS. Hence, the studies of mixed $CdS_{1-x}Se_x$ crystals would provide new information on their luminescent properties as well as on the radiation defects formation mechanisms.

Intentionally undoped $CdS_{1-x}Se_x$ crystals were irradiated at 77 and 300 K with 10-MeV electrons up to the fluence $\Phi=10^{18}$ cm^{-2}. PL spectra were measured at 77 K from the polished crystal faces on a LOMO DFS-24 monochromator using an Ar^+ laser (λ = 476.5, 488.0 and 514.5 nm) for excitation.

In sulphur-rich $CdS_{1-x}Se_x$ crystals the intensity of so-called "green" (in terms of CdS) PL band, attributed to the transitions in donor-acceptor (DA) pairs with the participation of shallow donors (V_S, Cd_i) and deep acceptors (S_i), increases by factor of 5 to 10 at irradiation with $\Phi=5\times10^{17}$ cm^{-2}. Comparison of the obtained results with those for neutron-irradiated CdS, where the considerable decrease of the green PL is explained by the effect of electric and elastic fields of neutron irradiation-induced defect clusters upon the radiative centres, as well as effective drain for the impurities included into the recombination centres, enables us to conclude that, contrary to neutrons, 10-MeV electrons, similarly to lower-energy electrons, result in formation of isolated defects (vacancies, interstitials) but not their clusters in CdS.

The dose behaviour of "orange" (in terms of CdS) PL band strongly depends on x. While for the crystals with lower Se content, where it is attributed to the recombination through (Cd_i–Cu_{Cd}), (Cd_i–Ag_{Cd}), (V_S–Cu_{Cd}), (V_S–Ag_{Cd}) DA pairs, its intensity somewhat increases with irradiation, for Se-rich samples irradiation results in the PL band at 1.65 eV decreasing in intensity by more than by order of magnitude for $\Phi = 10^{18}$ cm^{-2}. Such radical difference in the dose behaviour of the "orange" PL band indicates that at $x \approx 0.5$–0.6 the nature of the corresponding recombination centres is changed from the neutral complexes to single-charged acceptors, evidently Cu_{Cd} and Ag_{Cd}, and strong decrease of the PL band intensity with irradiation can be explained by the fact that the radiation-induced chalcogen vacancies and Cd interstitials form complexes with the present single-charged acceptors, these complexes being responsible for the recombination processes with lower energy.

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A-8

CONTROLLED MODIFICATION OF MOLECULAR NANOFILMS BY LOW ENERGY ELECTRONS

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The interaction of electrons with molecules at low energies (e. g. below the threshold for dissociation into neutral particles) can induce selective bond cleavage via dissiociative electron attachment. In the first step a transient negative ion is formed by resonant attachment which dissociates into a neutral radical and a negatively charged fragment. In the case of halogenated compounds the cross section for such reactions can be very high and exceed the geometrical cross section by orders of magnitude [1].

We have applied the technique of low energy electron interaction to thin molecular films to study chemical reactions induced in the energy range 0-15 eV. This is done in an UHV arrangement consisting of an electron monochromator, an cryogenically cooled surface and a mass spectrometer to detect ions ejected from the surface. Electron initiated reactions within the molecular film can be followed by the infrared-reflection-absorption-spectroscopy (IRRAS) technique [2].

In the case of of $C_2F_4Cl_2$ molecular clorine (Cl_2) can by senthesized by low energy electrons. The cross section for the reaction strongly depends on the primary electron energy and exhibits a resonant like behaviour with a peak near 8 eV and another peak below 2 eV. While above the threshold for electronic excitation (≈ 6 eV) many different reaction routes are possible, at low energies dissociative electron attachment is the only possible initial step [3].

We demonstrate that by irradiation of a $C_2F_4Cl_2$ surface with electrons at energies below 2 eV the surface is completely transformed into Cl_2 (and further yet unidentified products). This is due to the fact at those energies the educt is decomposed but not the products.

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A-9

CLEAR EXPERIMENTAL EVIDENCE FOR P-WAVE THRESHOLD BEHAVIOUR IN ELECTRON ATTACHMENT TO CHLORINE MOLECULES

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One of the open problems in low energy electron attachment studies is the threshold behaviour for the anion yield in cases for which, based on the symmetry of the involved anion resonance state, s-wave electron attachment is forbidden. Two important such cases are the molecules F_2 and Cl_2. As shown in Fig. 1 for Cl_2, anion formation near zero energy is expected to proceed by p-wave attachment ($\sigma(E) \propto E^{1/2}$) via the lowest anion state with ${}^2\Sigma_u^+$ symmetry, as predicted for both F_2 and Cl_2 by theoretical calculations [1-4]. In contrast, previous experimental studies indicated s-wave threshold behaviour [5]. With the aim to clarify the problem we have measured, using the laser photoelectron attachment method [6, 7] and chlorine molecules in a seeded supersonic beam, the energy dependence of the cross section for dissociative electron attachment (DA; Cl^- formation) over the range 0-195 meV with an energy width of about 1 meV. Our data provide the first clear experimental evidence for p-wave behaviour of a DA cross section near zero energy and are in good overall agreement with the theoretical predictions (see Fig. 2: full line).

This work has been supported by the Deutsche Forschungsgemeinschaft and by the Zentrum für Lasermesstechnik und Diagnostik (Universität Kaiserslautern).

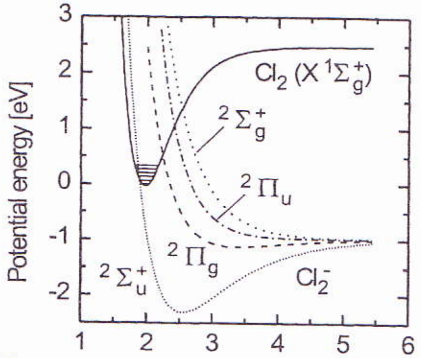

Fig. 1

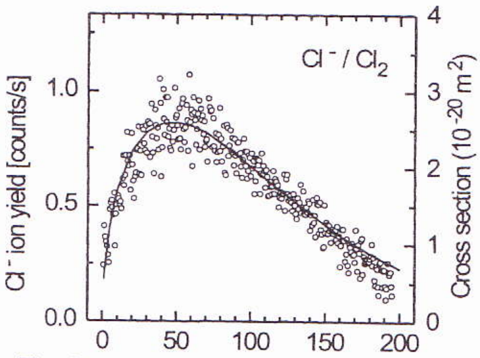

Fig. 2

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A-10

EXCITATION OF THE nP → $5S_{1/2}$ SERIES IN DENSE GA VAPOUR VIA ENERGY-POOLING IONISATION

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We have recently reported on the high efficiency of the Energy-Pooling Ionisation (EPI) mechanism in a dense Ga vapour by measuring its cross section [1]. We have anticipated that it may influence the population redistribution by way of direct recombination in the low plasma produced, eventually followed by cascade transitions, and we have already observed fluorescences arising from the 4D levels [2]. Here we report on the presence in the fluorescence spectrum, of the nP → $5S_{1/2}$ series with $9 \le n \le 26$, when Ga vapour inside a quartz cell at a temperature larger than 900°C, is resonantly excited by low power laser pulses at 403.4 nm corresponding to the $4P_{1/2} \rightarrow 5S_{1/2}$ excitation. An example of the fluorescence spectrum with only the strongest line is reproduced in figure 1. Analyses of the fluorescence intensities as function of the laser power density, P_L, and of the $5S_{1/2}$ level atomic density, demonstrate the nP levels to be populated via EPI. The effect of the presence inside the cell of a few torr of buffer gas, which eliminates all the fluorescences for $n \ge 12$ due to competitive effects such as the collisional population redistribution, will also be discussed.

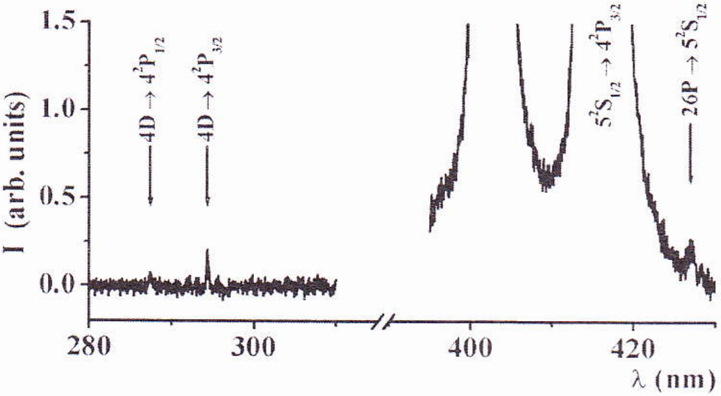

Figure 1: Portion of the fluorescence spectrum from Ga vapour inside a quartz cell following resonant excitation at 403.4 nm. T = 1050°C, $P_L = 80\ kW/cm^2$

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A-11

QUENCHING OF RADIATION TRAPPING IN A DENSE Ga VAPOUR IN A QUARTZ CELL INDUCED BY ATOM/SURFACE INTERACTION.

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When Ga vapour is kept in a quartz cell and its temperature is raised up to 1100°C, an unexpected behaviour of the radiation trapping is observed. In the first place it is strongly reduced; it reaches a maximum around $T = 1000°C$, corresponding to an atomic density $\cong 10^{13} cm^{-3}$, and at the highest temperature it is totally quenched so that the effective lifetime of the first excited state of Ga ($5S_{1/2}$) drops back to the natural value (6.2 ns) as is shown in figure 1. This behaviour persists independently on whether cells with or without buffer gas are used, whether different kind of buffer gas is used and whether the resonant transition is saturated or not. In our experiment such manifestation cannot be attributed to the "collisions of the second kind" nor to the 3-level scheme of the Ga system as was the case for In. We will show that this unusual behaviour is due, besides to the Energy-Pooling Ionisation (EPI) effect, which we have demonstrated to be very efficient in Ga vapour for $T \geq 1000°C$ [1], to the formation of fluorescent centres inside the quartz lattice in the interaction between Ga atoms and the fused silica structure. This interaction manifests when the temperature is raised above 900°C and is of great interest not only for fundamental physics but also for practical applications as it could give rise to new active materials for lasers as well as to applications in the realisation of optoelectronic devices.

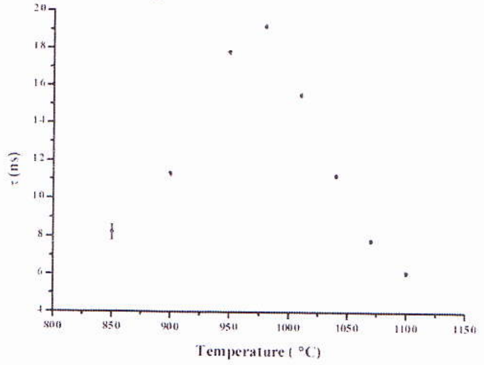

Figure 1: Effective lifetime (τ) of the $5S_{1/2}$ level of Ga versus temperature in a quartz cell with Ga + 10 torr Ne.

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Threshold Phenomena in Strong Laser - Atom Interactions

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It is well-known in general multichannel scattering theory that interchannel couplings cause particular, non-analytic behaviors (Threshold Anomalies, TAs) in the cross sections of open channels at the opening (or closure) of a given channel as the parameters of the problem are varied [1]. While the existence of TAs is a very general phenomenon that follows from general analyticity arguments, the actual magnitude of TA effects depends significantly on the dynamical details of a given problem. We demonstrate that the influence of TAs (i.e., purely quantum effects) changes significantly the general features of laser-atom processes in a nonperurbative regime when the interactions of a bound electron with the atomic core and the laser field have comparable magnitude, i. e., for intermediate values of the Keldysh parameter, $\gamma \sim 1$.

Our considerations are based on the exact solution of the complex quasienergy problem for an electron in a short-range (δ-model) potential subjected to a strong monochromatic laser field. We present essentially exact results for the intensity dependence of above-threshold ionization (ATI) and high harmonic generation (HHG) rates, $\Gamma^{(n)}$ and $I^{(n\omega)}$, in the plateau domain [2, 3]. Our analytic results for ATI and HHG amplitudes reveal the expected branch-point singularities (which are typical for a short-range potential [1]) at the ATI thresholds, and our numerical results show that the closure of a lower order, n_0-th, ATI channel with increasing intensity affects drastically $\Gamma^{(n)}$ and $I^{(n\omega)}$ in a broad interval of n with $n > n_0$. In agreement with general theory, for moderate laser intensities TAs are most pronounced at the closure of even-n_0 channels. All 4 types of TAs predicted for a short-range potential near the thresholds of S-wave channels [1] can be found in the ATI and HHG spectra. However, the most interesting are cusp features which lead to broad, resonant-like enhancements of ATI [2] and HHG [3] rates in the plateau region. TAs offer a clear theoretical explanation for enhancements of high-order ATI peaks that have been seen in recent experiments for rare gases.

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A-13

INTERACTION OF ENERGY TUNABLE ELECTRONS WITH ORGANIC COMPOUNDS IN THE GAS PHASE

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Growing interest to the studies of interaction of electrons with organic compounds is caused by their wide application in microelectronics, radiation chemistry, biology, and medicine. Inelastic scattering of electrons with molecules is known to result in excitation of electronic states in a wide spectral range, and give the unique possibility of direct population of optically forbidden states. In the gas phase at low pressure the secondary collisions of electrons with molecules and effect of surrounding are practically excluded. In this report the studies of electron energy loss spectra (EELS), excitation functions, and fluorescence spectra for polyacenes, polyphenyls, oxazoles and oxadiazoles, indole, carbazole, dibenzofuran, dinaphthofuran, 8-azasteroids, and organic europium complexes in the gas phase are presented.

A special electron spectrometer with full energy resolution of electron beam of about 0.3 eV and tuned energies in the range of 0-200 eV was used for spectral and luminescent measurements of organic compounds in the gas phase. Monokinetic electron beam of 1.5 mm in diameter is formed by electron gun consisting of heated oxide cathode and electron-optical system. The current of electron beam did not exceed 10 μA. The organic vapour density in the collision cell was less than 10^{-3} Torr in order to escape multiple collisions and secondary processes. Electrons scattered at an angle of ninety degrees relatively to incident beam was registered by 127° electrostatic Use-Rozhanski analyzer and channel electron multiplier. The registered radiation was detected in the direction perpendicularly to the electron beam propagation.

As opposite to optical absorption spectra, in EELS of all compounds under study there is a band connected with singlet-triplet transition S_0-T_1 and for some molecules the transitions into higher triplet states are observed at low incident electron energies. The cross section of these transitions strongly depends on electron energy. The singlet-singlet transitions in a range of 2-12 eV (up to S_0-S_5) as well as into super excited states are registered for different initial energies of exciting electrons. EELS of polyphenyls are more similar to those of benzene than that of polyacenes. The addition of heavy Br atom into ligand of europium complex results in growth of a relative intensity of singlet-triplet transitions. The essential change of fluorescence spectrum of carbazole with incident electron energy was found. The excitation functions of benzene, naphthalene and biphenyl have a pronounced structure. For more complex molecules they are structureless. Using excitation functions the excitation thresholds are determined. The shortwave fluorescence band for pyrene was found to be formed by direct S_2—S_0 transitions. The formation of excitation functions can be described by the contribution of manifold singlet excited states.

For some compounds (1,4-bis[2-(5-phenyloxazolyl)]benzene and Eu-complex) the dependences of elastic and inelastic transitions cross sections on incident electron energy are measured. These data are compared with those in Born approximation and exact calculations. The elastic scattering cross section value is in good agreement with geometrical dimensions.

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A-14

ENERGETICS AND STRUCTURES OF SMALL ALUMINUM CLUSTERS

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Voter and Chen version of an Embedded Atom Model, parameterized by fitting to the experimental data of both diatomic molecule and bulk aluminum simultaneously, has been applied to study the locally stable structures, energies and growth patterns of small aluminum clusters, Al_N, in the size range of N=2-13. Using molecular dynamics and thermal quenching simulations, the global minima and the other locally stable structures have been distinguished from those stationary structures that correspond to saddle points of the potential energy surface. Large number (10.000) of independent initial configurations generated at high temperatures were used to obtain the number of isomers and the probabilities of sampling different basins of attractions, for each size of the clusters. Their energy spectra have been analyzed. Comparisons have been made with the results of previous calculations used electronic structure and empirical potential methods. It has been found that the lowest energy structures are not always the most probable isomers for each size at low temperatures.

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A-15

MOLECULE-SURFACE INTERACTION: DISSOCIATIVE CHEMISORPTION OF A D_2 MOLECULE ON RIGID LOW-INDEX Ni SURFACES

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Kinetics of the reactions of nickel surfaces with a deuterium molecule are studied. Dissociative chemisorption probabilities of the D_2 molecule on the rigid low-index Ni(100), (110) and (111) surfaces have been computed by a quasi-classical molecular dynamics computer simulation technique. The interaction between the D_2 and Ni atoms was modelled by an LEPS (London–Eyring–Polanyi–Sato) function (energy surface) [1]. This analysis includes the chemisorption probabilities as functions of the relative translational energy of the D_2. The role of the surface topology was examined. An indirect mechanism which involves formation of molecular adsorption as precursor for the dissociative adsorption in the low collision energy region (less than 0.1 eV) is observed. Results were discussed by comparing with the other similar theoretical and experimental studies [2-3].

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A-16

REACTION DYNAMICS OF A Ni_{20} WITH D_2: DEPENDENCE ON INITIAL ROVIBRATIONAL STATES OF THE MOLECULE

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In order to investigate the dependence of cluster reactivity on initial rovibrational states of the molecule, the $Ni_{20} + D_2(v,j)$ collision system has been studied using quasiclassical molecular dynamics simulations. The clusters are described by an Embedded Atom potential, whereas the interaction between the molecule and the cluster is modeled by a LEPS (London-Eyring-Polanyi-Sato) potential energy function [1]. Reaction (dissociative adsorption) cross sections are computed as functions of the collision energy for different initial rovibrational states of the molecule. Initial vibrational excitation of the molecule increases the reaction rate more efficiently compared to the initial rotational excitation. Thermal rate constants are also presented and the results are compared with those of other studies available in the literature[2-3].

This work at Argonna was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Contract W-31-109-ENG-38 (J.Jellinek).

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A-17

CORE-EXCITED NEGATIVE ION RESONANCES IN STRONTIUM

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The electron impact excitation functions of the low-lying $4p^5n_1l_1n_2l_2n_3l_3$-autoionizing states (AIS) in strontium atoms have been measured in the near-threshold energy region. The measurements were performed on apparatus described in details earlier [1]. The excitation functions (EF) were obtained as the impact energy dependences of normalized line intensities in the ejected-electron spectra measured at an observation angle of 75^0 and at the incident electron beam energy spread of 0.15 eV. Taking into account the multichannel decay of the atomic AIS in strontium, only lines arising from the transitions to the ground ionic state $4p^6 5s$ were used for obtaining the functions. Figure 1 presents the EF for six lowest AIS with the excitation thresholds at 20.98, 21.12, 21.38, 21.62, 21.82 and 22.06 eV. Two features characterize the measured functions: the sharp rise of the cross-section just above the excitation threshold of the levels and a "fine" structure *a-g*. Note that the latter has not been observed in the earlier measurements [2] performed with the 0.3 eV energy resolution. Both observed features manifest undoubtedly the presence of the strong resonance processes in the $4p^6$-excitation of strontium. Similarly to the recent results on electron impact excitation of the outer p^6-subshell in alkali atoms [3,4], one may suppose that the negative-ion resonances are responsible for the presence of the structure *a-g*. Features *b, c, g* are also present in the EF of the low-lying AIS reflecting the population of these states due to the multichannel decay of the high-lying negative- ion resonances (resonance cascades). Such process has been observed earlier for lithium atoms[5].

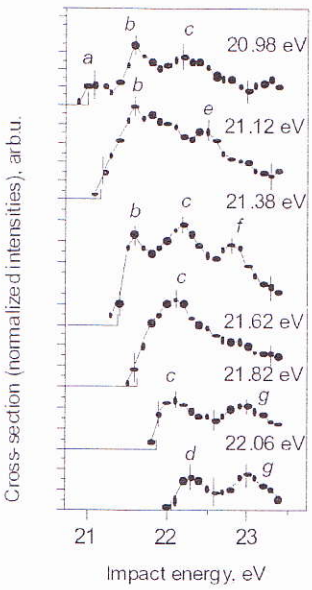

Figure 1: The EF of the $4p^5n_1l_1n_2l_2n_3l_3$ states in strontium atoms.

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A-18

LASER-INDUCED EXCITATION AND IONIZATION PROCESSES IN LASER ABLATION PLASMAS

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The success of pulsed laser ablation for thin film deposition and nanopowder synthesis has launched an effort to develop effective methods for the manipulation of laser ablated plume parameters. In the present paper laser-induced resonance ionization of ablated atoms were studied in order to clarify a possibility of enhancement of relative ionic content of the plume.

The Nd-YAG (1064 nm, 10 ns, 1–5 $\mathrm{J/cm^2}$) laser radiation or its second harmonic in combination with excimer XeCl (308 nm, 10 ns, 1 $\mathrm{J/cm^2}$) laser radiation at different temporal delays between pulses were employed for ablation. The laser beams were focused on the surface of the aluminum sample placed in the chamber under vacuum or gas (air, helium) environments. In another part of experiments the plume produced by the first ablation pulse was probed by the radiation of the excimer XeCl laser and elementary processes accompanying the interaction of the excimer XeCl laser pulses with aluminum plume have been examined.

The plume parameters were controlled using laser-induced fluorescence (LIF) and time-resolved optical emission spectroscopy (OES). The plasma emission spectra (300-700nm) were recorded and compared for different ablation regimes (single pulse and double pulse in coincidence and in sequence at various delays between pulses and laser fluences). The major species including neutral, ionized and some molecular species were identified. The particulate within the plume were observed by using Rayleigh scattering method.

The experiments demonstrated increased plasma emission, higher degree of atomization and a higher proportion of ions in dual-pulse ablation regime compared to the plasma produced by one laser. The optimal pulse separations were found both for atomic and ionic lines. The results of spectroscopic measurements were confirmed by ion probe analysis of the ionic content in the plume. Probe measurements revealed a strong enhancement of photoelectron emission from the preliminary irradiated target surface. The interpretation of results is based on the wavelength dependence of laser-plasma (inverse bremsstrahlung absorption and photoionization) as well as laser-surface interaction processes.

The enhancement of ionization was also observed when the plume (not the target) was irradiated by 308 nm XeCl laser pulses. Relaxation dynamics of the excited atomic states of aluminum after action of the excimer XeCl laser radiation on the Nd:YAG laser-ablated plume were found to be dependent on the distance from the target, XeCl laser pulse delays and the ambient atmosphere pressure. The results indicated that the resonant two-photon photoionization of the Al atoms was the most probable mechanisms for the formation of ions and excited aluminum atoms in the decaying laser ablation plasma.

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A-19

MC simulation of swarm parameters in nitrogen

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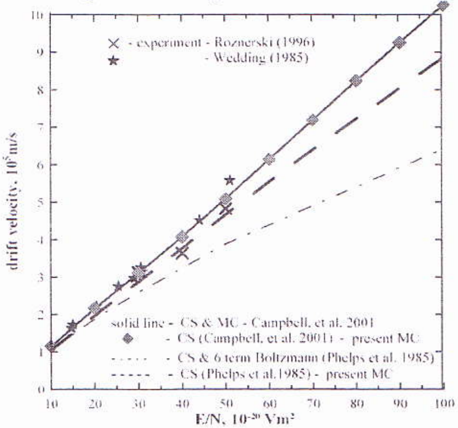
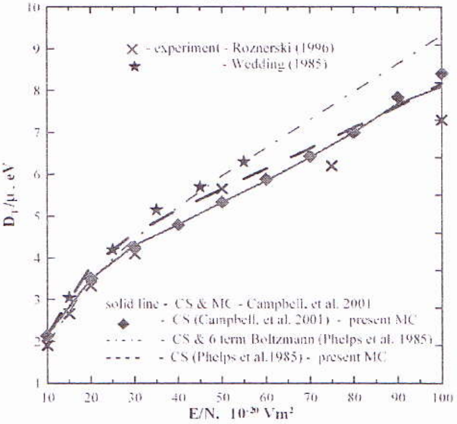
The fundamental importance of nitrogen, both from theoretical and practical point of view, has led Campbell *et al.* (2001) [1] to revisit the problem of determination of integral cross sections (CS) for that molecule. The derived integral CS for inelastic collisions were incorporated into a set of cross sections compiled by Ohmori et al.[2]. An isotropic MC algorithm was applied in order to calculate transport parameters. Good agreement with measured values was found, in contrast to the striking discrepancy with the high-energy results of Phelps and Pitchford [3]. This is an important issue because the CS [4] constitute the most popular CS set for nitrogen in the use today.

However, the calculations using Boltzmann equation in 2-term approximation [5] did not confirm the large discrepancy for CS sets [1] and [4]. Further, it was found that the conclusions of Campbell *et al.* (2001) regarding the usefulness of the cross section set [4] for electron transport calculations are based on a misleading comparison. The swarm parameters calculated by Phelps and Pitchford [3] for a pulsed Townsend experiment were related to the experimental [6,7] and the Monte Carlo simulation [1] results for time-of-flight technique (TOF). Our simulations - using an isotropic MC modeling of TOF experiments - confirm the usefulness of CS set [4].





Acknowledgement.

Authors acknowledge the reception of CS set [1] from Dr A.M. Nolan. We appreciate very much discussions and introductory results of Boltzmann analyses in 2-term approximation provided by Prof. A.V. Phelps.

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A-20

ELASTIC ELECTRON SCATTERING FROM WATER AT BACKWARD ANGLES

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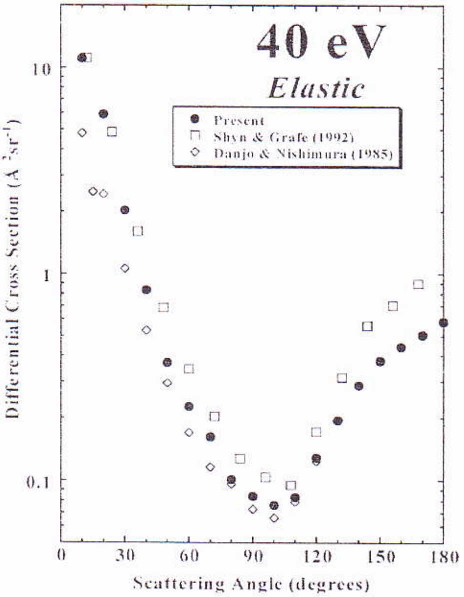
Absolute differential cross sections for elastic scattering of electrons from water vapor have been measured for electron energies between 4 and 50 eV and for scattering angles between 10 and 180°. Previous results [1-4] showed discrepancies and were limited to the angles up to 165°.

The experimental system consists of a pair of hemispherical electrostatic analysers for the production, energy analysis and detection of scattered electrons. The energy resolution for the present measurement was around 50 meV. The differential measurements used the magnetic angle-changing technique of Read and Channing [5] at backward angles. This technique has been successfully used in a recent application for measuring differential cross sections of SF_6 [6].

These cross sections have been extrapolated in the forward direction to enable the integral elastic cross section to be calculated.



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A-21

DOUBLE IONIZATION DIFFERENTIAL CROSS SECTIONS OF H^-, He, Li^+ AND Be^{2+} BY ELECTRON IMPACT

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We present in this communication the results of our calculation of five-fold differential cross section (FDCS) of (e, 3e) process on He like ions (H^-, He, Li^+ and Be^{2+}). The calculation performed is in *summed mutual angle* and *constant* θ_{12} *modes* in coplanar geometry. The formalism has been developed in first Born approximation by using plane waves, Sech and correlated BBK type wave functions respectively for incident and scattered, bound and ejected electrons. The non-dipolar contribution to (e, 3e) process in *summed mutual angle mode* is found to play an important role for H^- and with the increment of nuclear charge Z, its role gets weakened. The present study shows "binary" and "recoil" peaks like distribution in *constant* θ_{12} *mode* and this distribution is found to be very sensitive to post collision interaction (PCI) between the ejected electrons and the charge Z of the He like ions. We also discuss the role of incident electron energy and momentum transfer on the ratio of the FDCS of the "binary" and "recoil" peaks and the effect of Z on it. We compare the results of present calculation with the available experimental data [1,2].

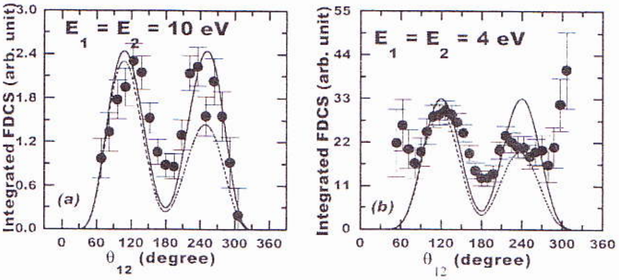

Figure : The angular behaviour of the integrated FDCS (He atom) with mutual angle θ_{12} between the ejected electrons in *summed mutual angle mode* for (a) $E_1=E_2=10$ eV and (b) $E_1=E_2=4$ eV. Solid and dashed curves represent the results of the present calculation using Sech wave function in full and accessible angular range of the experiment [1]. The other kinematical parameters are: $E_s = 5500\,eV$ and $\theta_s = 0.45$.

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A-22

A study of Th M-x-ray satellites and hypersatellites excited by energetic O and Ne ions

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The X-rays emitted from multiply ionized atoms exhibit pronounced satellite structure reflecting the distribution of spectator vacancies at the moment of x-ray emission. In the present study the satellite structure of $M_{\alpha 1,2}$ ($M_5N_{6,7}$) x-ray transition in Th excited by heavy ions, which corresponds to additional vacancies in the N- and O shell, has been measured using high-resolution von Hamos spectrometer [1] with energy resolution of about 1 eV. The measurements were performed at the Paul Scherrer Institute (PSI) using O^{7+} and Ne^{6+} ion beams of energy 376 MeV and 178 MeV, respectively, delivered by the Philips cyclotron. In these measurements despite well resolved N-shell satellites we were able to observe the structure of M-x-ray hypersatellite transitions corresponding to one additional (spectator) hole in the M-shell. The x-ray spectra measured for Ne ions show generally more prominent satellite structure, as comparing to O ions.

The measured x-ray spectra were compared with the multi-configuration Dirac-Fock (MCDF) calculations, accounting for the spectator vacancies in the N- and M-shells. The measured spectra are in reasonable agreement with predictions of the MCDF calculations. Nevertheless, the data evidence a clear necessity to include more complex multi-vacancy configurations in theoretical calculations in order to obtain a better agreement. We note that our earlier results concerning the measurements of the satellite structure of Th L-x-rays excited by energetic O ions were reported elsewhere [2].

The relative intensities of observed x-ray satellites yield an information on the ionization probabilities for the N-shells at the moment of x-ray emission. These data, after correction for the vacancy rearrangement processes (radiative, Auger and (super-) Coster-Kronig transitions), were discussed in terms of available theoretical models of the multiple ionization [3]. In this context, both a perturbative semiclassical approximation (SCA) and a nonperturbative geometrical model" (GM) are discussed. Such an analysis provides a method of testing the M-shell fluorescence and (super-) Coster-Kronig yields for multi-vacancy configurations.

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A-23

INVESTIGATION OF KINETICS OF CHEMICAL REACTIONS BY CAVITY RING-DOWN SPECTROSCOPY

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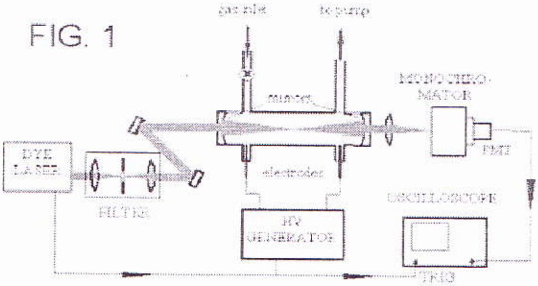
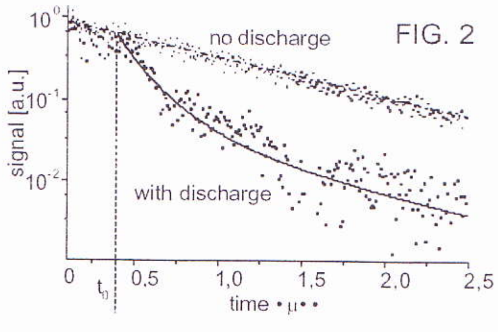
Cavity Ring – Down Spectroscopy method consists on light pulse trapping in an optical resonator filled by investigated compound. The absorption coefficient is determined by the cavity Q-factor. Here the application of this technique for kinetic studies of a decay process of CH radicals formed during a HV pulse discharge in methane is presented. The experimental setup is shown in fig. 1. The experiment was done in the cavity composed of two mirrors, which reflectivity was about 0,998. The mirrors were attached to a quartz tube filled with methane under the pressure of 270 Pa, where the pulsed discharge took place. A pulsed dye laser working at 426 nm was used as a light source. The output signal was recorded by means of a photomultiplier and a digital oscilloscope.

FIG. 1



In Fig. 2 the dashed line represents the signal when no discharge was applied. It is characterized by a decay constant of $\tau_0 \approx 1$ µs. Continues line describes the signal with the presence of the discharge, that starts at the time t_0. At this moment a decrease of the cavity Q – factor is observed, due to production of CH radicals, which absorb the light. Then, due to different chemical reactions, the CH concentration decreases, what causes increase of the cavity Q – factor. After about 2 µs, when CH radicals' concentration is negligible, both lines became parallel, since the cavity Q – factor is identical.

FIG. 2



Analyzing the signal, the evolution of CH radicals' concentration N_{CH} can be found. In this way the rate constant for the CH destruction equal to: k=1.7 10-11 was found.

This work was supported by Polish Committee for Scientific Research, grant number 2 PO 3B 03622

A-24

QUENCHING OF ^{4}He(2^1S, 2^1P) AND ^{3}He (2^1S, 2^1P) STATES BY COLLISIONS WITH Ne($^1S_0$) ATOMS

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There are no data in the literature for the process of quenching of excited ^{3}He (2^1S. 2^1P) atoms by interaction with Ne($^1S_0$) atoms while compare to interaction of the ^{4}He(2^1S. 2^1P) atoms with Ne($^1S_0$) atoms is well investigated. The excitation transfer from a metastable He(2^1S) to neon atom is one of the main processes for the inversion population in He-Ne laser. On the other hand, a significant role of ^{3}He isotope (used instead ^{4}He) in He-Ne laser (λ=6328 Å) for the increasing of the laser gain with 20-50% has been reported [1].

In the present work the quenching cross sections of ^{4}He (2^1S, 2^1P) and ^{3}He (2^1S, 2^1P) atoms by Ne($^1S_0$) atoms is reported.

A delay coincidence method is used for investigation of the He excited states quenching by Ne atoms. The mixture of He and Ne atoms is excited by pulse electron beam. From the set of the decay curves of NeI 6328 Å line one can determine the effective lifetimes of He(2^1P, 2^1S) states at different Ne atoms concentration. The corresponding cross sections could be obtained by extrapolation dependence of the effective lifetimes vs the Ne atoms concentration.

A detailed collisional-radiative model for an e-beam sustained discharge is developed. The model incorporates the most important species and reactions relevant to He-Ne mixture. The list of reactions includes about thirty points.

Our preliminary estimation about experimental quenching cross section for ^{3}He (2^1P, 2^1S) states by Ne($^1S_0$) atoms are $\sigma_{2^1P} = (2.91 \pm 0.61)*10^{-15} cm^2$ and $\sigma_{2^1S} = (1.03 \pm 0.04)*10^{-15} cm^2$; for ^{4}He($2^1$P, 2^1S) states $\sigma_{2^1P} = (1.84 \pm 0.45)*10^{-15} cm^2$ and $\sigma_{2^1S} = (8.62 \pm 0.3)*10^{-16} cm^2$.

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A-25

STUDY OF ION SCATTERING AND SPUTTERING PROCESSES AT GRAZING ION BOMBARDMENT OF CRYSTAL SURFACES

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At enough small sliding angle of incidence the focalising influencing of surface semichannels leads to the peculiar refocusing effect of reflected particles and to some peculiarities of sputtering processes.

In present work the peculiarities of ion-solid interaction processes observed at grazing ion bombardment have been considered. The refocusing effect of particles reflected from the surface semichannels of single crystals have been investigated by both computer simulation and analytical methods. The sputtering has been simulated in the primary knock-on regime. The present code is based on the binary collision approximation by using Newton equation for construction of trajectories of colliding particles. Using an universal Ziegler-Biersack-Littmark potential for description of interactions between incident ion and target atoms the trajectories of incident ions in semichannels and channels along the <110>, <100> directions of Cu(100) and GaP(100) surfaces were traced in several nearest to surface atomic layers. Both elastic and inelastic energy losses are taken into account. The inelastic energy losses are considered as local. Thermal vibrations of lattice atoms are considered as randomise on Gauss distribution. Computer code described by Pascal allows observing the dynamics of ion-solid interaction processes.

The calculation results showed that in conditions of grazing incidence the incident ions move in the surface semichannels and channels which are parallel to surface. The range of these particles in the surface channels increases considerably due to the channelling effect and achieves hundreds of Angstroms. In this case the projectiles of primary beam transfer the small portions of their energy to a great number of atoms which form channels. That is why for this case the cascade mechanism of sputtering is not observed.

The spatial, angular and energy distributions of scattered and sputtered particles as well as their yields versus the angle of incidence have been calculated. In the energy spectra the characteristic peaks corresponding to the scattering of ions by the surface atomic chains and semichannels are observed. The position and intensity of these peaks depend on the geometrical shape of surface semichannels. There is a strong correlation between the shape of spatial distributions of reflected particles and the surface structure. Analytic expressions for calculation of a refocusing energy for different shapes of semichannels formed on the surfaces of one and two-component single crystals have been obtained.

It has been shown that the possibility of preferential sputtering of one components essentially depends on the bombardment angle. At small glancing angles of incidence the preferential sputtering of heavy component atoms is possible. It was shown that in the case of grazing ion bombardment the layer-by-layer sputtering is possible and its optimum are observed within the small angle range of the glancing angles near the threshold sputtering angle. The obtained results allow to select the optimum conditions for layer-by-layer sputtering. Application of present code for investigation of diagnostics and modification of solid state surface is discussed.

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A-26

Absolute photo-absorption cross sections and electronic state spectroscopy of fluorinated selected hydrocarbons relevant to the plasma processing industry

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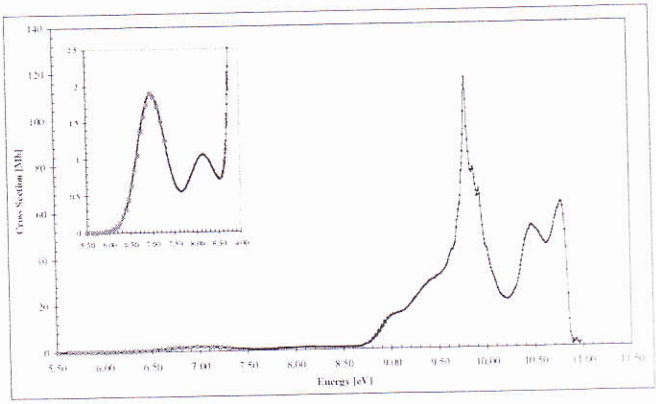
Silicon dry etching is traditionally performed using perfluoro-compounds (PFCs), most importantly CF_4, C_2F_6, C_3F_8, CHF_3, and c-C_4F_8. These species have very high global warming potentials (GWP) as they absorb strongly in the infrared and have long residence times in the Earth's atmosphere. The current generation of plasma reactors release a high proportion of unreacted etch gas into the atmosphere. CCl_2F_2 is used in reactive ion etching (RIE) of GaSb as it can be readily dissociated to produce Cl and F etching radicals. It has high GWP and is recognized as playing a significant role in stratospheric ozone depletion. The plasma processing industry is committed to the replacement of these gases with compounds of low GWP.

CF_3I is one such alternative etch gas. Due to the weak C-I bond, it should be possible to produce high yields of the etching radical CF_3 in a plasma by direct electron impact dissociation of the molecule. Furthermore, by using a combination of CF_3I and C_2F_4 in a reactor, polymerization and etching can be independently controlled through the selective generation of CF_2 and CF_3 radicals. Due to their high photolysis rates, both CF_3I and C_2F_4 are expected to have short lifetimes in the atmosphere and thus low GWP. Quantitative data is needed to model the behaviour of CF_3I and C_2F_4 both in the atmosphere and in future industrial reactors.

High resolution photo-absorption spectra of CF_3I [1], C_2F_4 and CCl_2F_2 [2] have been measured in the wavelength range 115 to 210nm (10.8 to 5.9eV). The absolute absorption cross sectional values for CCl_2F_2 are shown below. Differential cross sections for elastic and inelastic scattering by low-energy electron impact have been recorded for CF_3I [3] and C_2F_4 over a wide angular range using electron energy loss spectroscopy (EELS). Further details will be presented at the conference.

UV photo-absorption plot of CCl_2F_2:



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A-27

Ionization and fragmentation of small molecules in collisions with slow highly charged ions

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The ionization and fragmentation of small molecules, as e.g. N_2 and CH_4, was studied in collisions with slow highly charged ions utilizing a position- and time-sensitive multi-particle detector [1] which allows the coincident detection of the momenta of correlated fragment ions. If all fragments from a particular fragmentation are detected, a kinematically complete study of the molecular break-up process is possible and the dissociation energy as well as the orientation of the target molecule relative to the projectile beam can be derived for each individual event. An additional position-sensitive delay-line detector was used to determine the final projectile charge state. With this setup various fragmentation processes can be analyzed for selected charge transfer processes. Three different kinds of processes can be distinguished: target ionization and fragmentation without charge transfer, target ionization and fragmentation with electron capture into the projectile, and pure electron capture processes without free electrons. The observed spectra show fundamental differences in the fragmentation dynamics of these processes (Fig. 1).

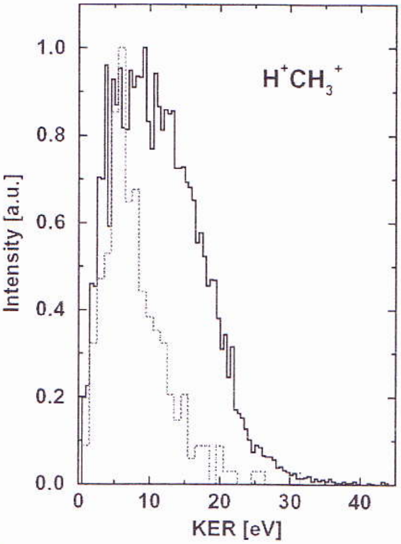

Figure 1: Total kinetic energy of coincident $H^+ + CH_3^+$ fragment ions from collisions of 43 keV He^{2+} on CH_4. Ionization and fragmentation with (- - -) and without (—) electron capture.

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NEAR-THRESHOLD PHOTODETACHMENT OF HEAVY ALKALI-METAL ATOMS

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Low-energy electron scattering by alkali-metal atoms is strongly affected by a $^3P^o$ shape resonance. Its experimental observation is very difficult because of the limited energy resolution in electron scattering experiments. Photodetachment (PD) studies of corresponding negative ions might be advantageous in this regard. However, due to the dipole selection rules, only the $J = 1$ component of the $^3P^o_J$ $(J = 0, 1, 2)$ triplet can be populated in PD experiments with a single photon. Moreover, since the $^1S \rightarrow ^3P$ transition is forbidden in the LS coupling scheme, the process indicative of the $^3P^o$ resonance becomes very sensitive to the spin-orbit interaction, and the role of the theory in interpretation of experimental data becomes especially important.

In the present work we calculate photodetachment of Rb^-, Cs^-, and Fr^- using the Pauli equation method. The Pauli equation is a weak relativistic limit of the exact Dirac equation which includes the spin-dependent potential V_{LS} added to the non-relativistic, spin-independent Coulomb potential V. For a Coulomb potential, V_{LS} contains a non-physical singularity $1/r^3$ at $r = 0$, and the Pauli equation approach breaks down. Various regularization functions have been suggested to remove this singularity [1]. Based on the exact analytic solution of the Dirac equation near the nucleus, we formulate boundary conditions for solving the Pauli equation for an electron interacting with an atom [1]. By integrating the Pauli equation using an effective potential V_{eff} that is adjusted to reproduce scattering phase shifts provided by exact Dirac R-matrix calculations, we calculated total PD cross sections. Our $^3P^o_1$ resonance contribution to the PD cross section of Cs^- agrees (in position and width) with recent experiments [2], after fine-tuning V_{eff}. For Rb^- and Fr^- the resonance contribution is much smaller than for Cs. We therefore also calculate angle-differential cross sections and asymmetry parameters which are much more sensitive to the resonant contribution than the total cross section.

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A-29

DISSOCIATIVE EXCITATION OF CARBON DISULFIDE BY ELECTRON IMPACT

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Excited atomic and molecular fragments e.g. OH, SO, CS resulted from electron- and photon-impact dissociative excitation of various molecular species play an important role in the processes occuring in the planetary atmospheres, comets and artificial plasmas. Dissociation processes in carbon disulfide (CS_2) have been investigated previously using different experimental methods which include discharge and afterglow studies [1 − 3]. Present work deals with the measurements of emission spectra and excitation functions due to the low-energy electron impact dissociation of the carbon disulfide which produces excited CS ($A^1\Pi$) fragment of the parent molecule. The measurements have been carried out by an optical excitation method using an electron trochoidal spectrometer [4] with the detection of the CS radical emission in the 240 − 280 nm wavelength region. Figure 1 presents fluorescence emission spectrum obtained at an incident electron energy of 15 eV. The spectrum has been analyzed to resolve individual vibrational lines of the detected $A^1\Pi - X^1\Sigma^+$ system and to determine their relative intensities. The dissociative excitation function measured in the electron energy range from threshold at 9.3 eV up to 30 eV indicates two dissociative processes with the second process developing above 20 eV.

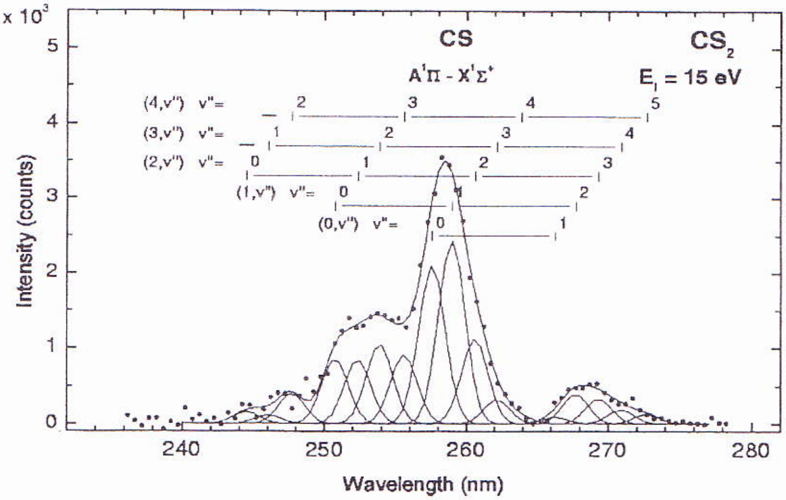

Figure 1: Fluorescence emission spectrum of CS_2 at an energy E_i of 15 eV.

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A-30

EFFECTIVE SCHEMES OF THREE-PHOTON IONIZATION OF SAMARIUM ATOM

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While studying three-photon ionization of samarium atom in the spectral range ω=17000-18450 cm^{-1} we have found a number of extremely intense maxima. A detailed analysis has shown that all of them result from two-photon ionization of even bound states and are observed exclusively in the vicinity of the frequencies corresponding to one-photon transitions from the same initial levels, as the two-photon transitions.

Fig. 1 shows a part of the measured spectrum, containing one of such maxima. A broad maximum (ω_1=18124.05 cm^{-1}) corresponds to the one-photon transition $^7F_1 \rightarrow 4f^5 5d6s^2\ ^7F°_2$ [1] while an intense maximum (ω_2=18122.05 cm^{-1}) is caused by the two-photon transition $^7F_1 \rightarrow E$=36536.7 cm^{-1} (J=1). A relatively small $\Delta\omega$=2 cm^{-1} untuning (bandwidth ≈ 0.2 cm^{-1}) between the frequencies of the one-photon and two-photon transitions is responsible for the essential enhancement of the two-photon transition at the expense of one-photon transition via the $4f^5 5d6s^2\ ^7F°_2$ state. Evidently, such enhancement is possible only in case the corresponding transitions (in our case – $^7F_1 \rightarrow ^7F°_2$ and $^7F°_2 \rightarrow E$) being allowed by the selection rules. The efficiency of Sm atom ionization at the frequency ω_2 is about four orders of magnitude higher than the efficiency of direct three-photon ionization. The maximal amplitude of the maximum is restricted by the ion signal saturation effect, related to the 100 % ionization of atoms in the interaction volume. The studies of the maximum behaviour depending on the laser light intensity and on the interaction volume have shown that without saturation the efficiency of such process will increase the direct three-photon ionization efficiency by factor of 10^6–10^7.

Thus, the considered resonant process is a relatively simple (using only one laser source) highly efficient selective scheme of samarium photoionization which can be successfully used for various applications.

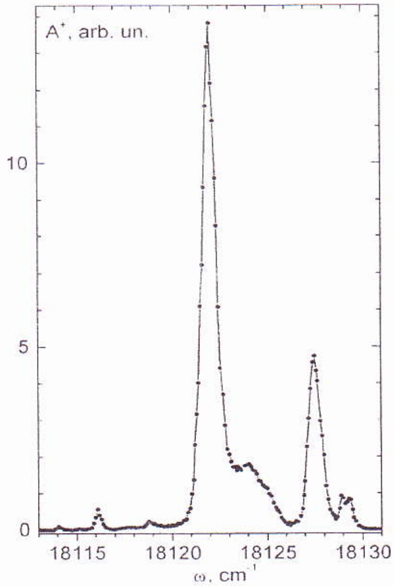

Fig.1. Three-photon ionization spectrum of Sm atom.

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A-31

DESCRIPTION OF CORRELATION IN EXCITONIC NEGATIVE ION IN Cu_2O

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M.Lampert predicted the existence of exciton negative ion in solid [1]. Variational method is usually used to calculate the energy values for ground state of such three-particle systems [2]. However this method has a known difficulty in classifying the quantum excited states. On the other hand, the hyperspherical coordinates method (HCM) (see review [3]) allows both to receive spectral characteristics and develop natural classification of excited quantum states, which are combined in series.

In the present work, HCM is used to obtain the energies of ground states of exciton negative ions for green and yellow Cu_2O lines. Thus the field of HCM application is expanded to the description of three-particle systems. The solution of nonrelativistic Schrodinger equation, which describes bound ^{1,3}S-states, is reduced to that of two boundary value problems. At the first stage the adiabatic potentials are found, which are the eigenvalues of Hamiltonian that describes the angle motion of three-particle system on the surface of a sphere in four-dimensional space and channel functions, which are also eigenvalues for this operator. At the second stage the radial equation is solved, which describes the radial motion.

To find adiabatic potentials we expand channel function by K-harmonics, which are eigenfunctions of operator of ground angular momentum for the system of three particles. The basis includes K-harmonics, which correspond to the ground angular number up to 20.

Radial equation is solved in Born-Oppenheimer and adiabatic approximations. Adiabatic approximation accounts both adiabatic and nonadiabatic potentials [4]. The ground term has only one bound state, the other are autodetaching ones converging to the excitation thresholds of lower exciton levels. As Cu_2O has two effective masses of hole [2], two types of negative ions and two series of autodetaching states are obtained differing in their reduced masses ($\mu_1=0.3895m_e$; $\mu_2=0.5561m_e$). For example, for green Cu_2O line energy value of the ground negative ion ^{1}S-state on is equal to 157 meV, for yellow line – 109 meV. Our calculations are in good agreement with results in [2].

For more complete account of correlation it is necessary to apply two-dimensional basis, which may be obtained by solving two-dimensional boundary problem [4].

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A-32

FRAGMENTATION COMPETING WITH ENERGY RELAXATION IN C AND N *K*-SHELL EXCITED $CF_3C\equiv N$

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Total photoabsorption cross sections of CF_3CN were measured in the C(1s) and N(1s) regions using synchrotron radiation at the Institute for Molecular Science. The mass spectra in coincidence with total photoelectrons were observed by use of two types of TOF-MS (time-of-flight mass spectrometer): One is a linear TOF-MS which makes it possible to derive kinetic energies and anisotropy parameters of the fragment ions in angle-resolved mass spectra [1]. The other is a reflectron type TOF-MS to achieve a high mass resolution $M/\Delta M \geq 100$ even for fragment ions with kinetic energy up to $\cong$10 eV, and gives information about site-specific photofragmentation [2].

Kinetic energy (KE) distribution of the CN^+ fragment ion showed a maximum at any excitation. However, KE distributions of the CF_3^+ ion formed in the excitation of terminal N(1s) and the central C_N(1s) electrons showed two maxima with KE $\cong$0 and $\cong$1.1 eV, while it had a maximum with KE $\cong$1.3 eV at the other terminal C_F(1s) excitation where the C_N and C_F denote the atoms forming the $C\equiv N$ and CF_3 groups, respectively. This is the first observation that the kinetic energy distribution of fragment ion depends on the site of excitation. This observation is reasonably interpreted by the consideration that the CF_3 group having vibrational modes acts as an internal energy reservoir. This is consistent with other observations made in the reflectron TOF-MS: At the terminal N(1s) excitation the large CF_3^+ ion was the main product while in the C_F(1s) region it was minor. In addition F_2^+ ion formed via excitation of bending mode was much stronger at the N(1s) excitation than at C_F(1s). That is, intramolecular energy at the N(1s) excitation flows toward CF_3 and is partly reserved as vibrational energy of the CF_3 group.

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A-33

POLARIZATION OF LYMAN-β RADIATION FROM ATOMIC HYDROGEN EXCITED BY ELECTRON IMPACT FROM NEAR-THRESHOLD TO 1000 eV

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The polarization of Lyman-β radiation, produced by electron impact excitation of atomic hydrogen, has been measured for the first time over the extended energy range from near-threshold to 1000 eV. Measurements were obtained in a crossed-beams experiment using a silica-reflection linear polarization analyzer in tandem with a vacuum ultraviolet (VUV) monochromator to isolate the emitted line radiation. Our data are in excellent agreement with convergent close coupling (CCC) calculations over the entire energy range. The data are broadly similar to the earlier measurements of H Lyman−α polarization reported from this laboratory.

This work is based upon activities carried out at the Jet Propulsion Laboratory, California Institute of Technology, and was supported by the National Science Foundation under Agreement No. PHY-9722748, the Astrophysics and Planetary Atmospheres programs of the National Aeronautics and Space Administration and by the Air Force Office of Scientific Research. Any opinions, findings, and conclusions or recommendations expressed in this publication are those of the authors and do not necessarily reflect the views of the National Science Foundation.

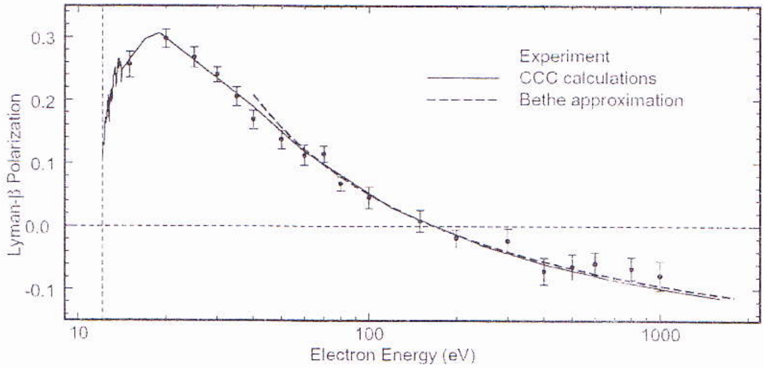

Figure 1. Polarization of Lyman-β radiation from atomic hydrogen excited by electron impact from near-threshold to 1000 eV.

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A-34

Spectroscopic and surface analysis of the laser ablation of crust on historic sandstone elements

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Pulsed laser ablation is applied for removal of the encrustation on the historic façade elements made of sandstone and results of measurements obtained by means of the laser induced plasma spectroscopy (LIPS) and also microscopic surface analysis (optical, SEM, XEDS) aimed on understanding of the underlying processes are discussed. The research is carried out for elements from the St. John's Church in Gdansk and the gotlandic sandstone under investigation represents a building material which was widely used in the past.

Experimental data known for marble, limestone and alabaster confirm that laser ablation applied for restoration purposes enables a controllable removal of the black encrustation not causing a damage of the underlying substrate (stone) due to difference in absorption [1]. From our previous work the operative range of parameters required for removal of about 0,1 mm thick encrustation by means of the Nd:YAG laser (6 ns pulsewidth, wavelength 1064 nm), i.e. energy fluence of 0.5 J/cm^2 and dose corresponding to about 15 pulses per irradiated spot for the water-moistened surface is derived, and the results are comparable with literature data known for similar materials [2]. However, there is still a lack of the sandstone case studies allowing for the process and materials diagnostic which motivates continuation of this study.

In this work the LIPS spectra are recorded for successive ablation pulses and the compounds of stone and crust such as Si(810,5; 819,6 nm), Ca(730,08 nm), Al(515,1; 670,4-686,6 nm) and K(766,5; 766,9 nm), Na(589,7 nm) are identified, respectively. The assignment of K and Na to surface degradation products is additionally confirmed by the marked decrease of the respective peak intensities for subsequent pulses while line intensities ascribed to the substrate remain constant.

The SEM images obtained for cross-sections of the sandstone samples close to the surface reveal a tight crust coverage of about 100 µm thickness composed of particles characterised by irregular shape and dimensions up to 20 µm. In some locations the quartz grains being the main sandstone component are visible. Their damage can be observed at larger magnification in the form of cracks and crumbling of the grain's surface. Below of the crust layer the absence of natural cement close to the crust-substrate interface is ascribed to prolonged interaction of the aggressive environmental pollutions. For larger depths the inter-granular spaces are filled up with crust indicating structure typical for non-deteriorated sandstone. Results of the qualitative elemental analysis obtained by means of the XEDS technique are compared with spectroscopic data and discussed.

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A-35

Complex Scattering Potential approach to calculations of e-atom/molecule total ionization cross-sections

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Electron atom/molecule total interaction in the form of complex potential ($V_R + iV_{abs}$) describes inelastic processes in the presence of elastic scattering. The complex potential generated from spherical charge density, accounts for electronic excitation and ionization of the target through the *summed-total inelastic cross section* Q_{inel} [1,2]. The calculated cross section Q_{inel} can be employed to extract total *ionization* cross section Q_{ion} at energies above the threshold (I). This is done by defining a quantity,

$$R(E_i) = \frac{Q_{ion}(E_i)}{Q_{inel}(E_i)} \; ; \qquad 0 \le R \lesssim 1 \qquad (1)$$

We represent the ratio R as a continuous function of energy ($E_i > I$) as follows.

$$R(E_i) = 1 - C_1\left[\frac{\ln(U)}{U} + \frac{C_2}{U + a}\right] \text{ where, } U = \frac{E_i}{I} \qquad (2)$$

These equations define our "Complex Scattering Potential-ionization contribution" (CSP-ic) approach. Applications of this method to molecules, radicals and dimmers/clusters will be presented in the Conference. Table 1 shows sample results.

Table 1

Target	O_2		CH_4		SiH_4		CCl_4	
	CSP-ic	Exp[3]	CSP-ic	Exp[4]	CSP-ic	Exp[5]	CSP-ic	Exp[6]
Q_{ion} (Å^2) at 100eV	2.73	2.75	3.38	4.04	5.11	5.08	13.85	14.84

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A-36

Maximum Ionization Contribution to TCS of e – Atom / Molecule Collisions; Dependence on $\sqrt{\frac{\alpha_0}{I}}$

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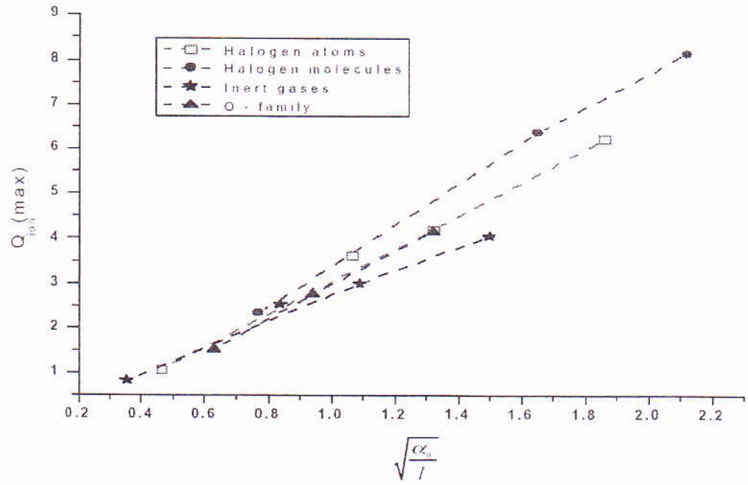
Ionization occupies an important status among the electron-stimulated processes observed with atomic and molecular targets. Calculation of total ionization cross - sections at a fundamental level is quite difficult even for hydrogen atoms. Several theories with varying degrees of approximations are in vogue today in this regard. We have recently developed CSP-*ic* [1]. In this approach total ionization cross sections Q_{ion} are obtained from the inelastic cross sections Q_{inel}. The details of calculations are given in [2,3]. The goal of the present work is to examine the dependence of the peak value of the $Q_{ion}(Å^2)$ of a target atom / molecule on $\sqrt{\frac{\alpha_0}{I}}$, where $\alpha_0(a_0^3)$, is the polarisability and $I(eV)$, is the first ionization potential of the target [4]. This dependence will be correlated to periodic properties of atoms, and the structure and bonding of selected molecules. (See sample results given below).



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A-37

THE DESCRIPTION OF THE ENERGY SPECTRUM OF NUCLEI IN THE ADIABATIC APPROACH

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The inclusion of the one sort of nucleons paring in the nuclear theory which play an important role in the formation of excited states of nuclei, and the angular and radial nucleon correlations study lead to the necessity of a method for calculating the stationary nuclear states that exceeds traditional one-particle Hartree-Fock approximations [1].

The hyperspherical adiabatic approach (HAA) was suggested in papers [2] for using for these purposes, which is yield from the framework of singlenucleon approximation. Further development and application of this approach to the study within the framework of an adiabatic multiparticle shell nucleus model of the energy spectrum of nuclei is actual. A new model is based on the assumption on the separability of the motion of the valence nucleons over fast motion on the angular variables and adiabatic (slow) motion along the hyperradius R. A convenient notion of the potential term $U_u(R)$ of nucleons is introduced. In the case of the ${}^A_Z X$ nucleus with two nucleons the nucleus description in HAA is performed in the collective variables terms whose role is played by the hyperradius R and the hyperangle α and conventional spherical angles $\hat{r}_i = \{\varphi_i, \theta_i\}$, $i=1,2$. The theoretical calculations presented in ref. [3] are well correlated with the existing experimental data of ref. [4].

A theoretical description of the energy spectrum of the deformat nuclei has been carried in ref. [5] out within the framework of the adiabatic three-particle shell model of nucleus. In the present time the theoretical calculations of the energy spectrum of the deformat nuclei such as *Zn*-64 and *Se*-74 are performing.

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A-38

THE SEMICLASSICAL ADIABATIC APPROACH TO DOUBLY EXCITED WANNIER STATES OF TWO-ELECTRON ATOM

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In Wannier states distances between each electron and the nucleus $\mathbf{r_1}, \mathbf{r_2}$ in two-electron atom are approximately equal to each other and opposite directed [1]. The two-electron wave function is expanded in a series of Wigner D-functions $D^{\pm}_{MK}$ depending on the set of Euler angles Ω in order to separate rotations of atomic frame :

$$\Psi_{LM\nu}(\mathbf{r_1}, \mathbf{r_2}) = \sum_{K=0}^{L} f_{\nu}^{I+} D_{MK}^{L+}(\Omega) + f_{\nu}^{I-} D_{MK}^{L-}(\Omega),$$
$$f_{\nu}^{I\pm} = \Phi_{n}^{I\pm}(\theta, \alpha_h, R) \tau_{n,s}^{I,\pm}(\alpha_h, R) \chi_{n,s,k}^{I\pm}(R),$$

$D^{L\pm}_{MK}$ means symmetric and antisymmetric combination of D-functions, R, θ, α_h are hyperspherical variables, $I = (L, K, M)$ and $\nu = (n, s, k)$ are sets of quantum numbers different from that by Herrick, Sinaniglu and Lin [1]. The coupled system can be reduced to separate differential equations in the case of $\mathbf{S}$- and $\mathbf{P^e}$-states .

In case of Wannier states the adiabatic approach can be applied [2]. It is assumed, that hyperspherical variables can be alligned in order of values of their time derivatives as θ, α_h and R, the θ - the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$ - can be considered as the most 'quick' variable, the hyperspherical radius R - as the slowest one. Self functions $\Phi_{n}^{I\pm}$ and $\tau_{n,s}^{I,\pm}$ can be found in analytical form. The solution of the equation relative to the R can be received in semiclassical approximation. The energy levels have been found from the numerical calculation of the Bohr-Sommerfield integral on the variable R.

The quantum defect formula for the energy of Wanier states depending on quantum numbers n, s, k has been developed.

The symmetry properties of the wave function have been considered, for example, even values of the quantum number s correspond to singlet states, odd values of s - to triplet ones.

The special atomic frame has been proposed, in this frame one can restrict the number of coupled equations, to define the exact quantum number above the number of M, and to apply the the present approach to the Stark effect for Wanier states.

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A-39

Lifetimes of the $k^3\Pi_u^\pm$ state in H_2 and D_2
Experiment and Theory

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The negative parity component of the 1s4p $k^3\Pi_u$ state in a molecular hydrogen is an unique state because strong light emission from its rovibronic levels above the first ionization and the second dissociation limit can yet be observed. This suggests that the non-adiabatic interactions of this state with the autoionization (AI) and predissociation (PD) continua are rather weak and their decay rates are comparable with the radiative decay(RD) rate. On the other hand, the light emission from the $k^3\Pi_u^+$ levels above the second dissociation limit is entirely eliminated due to strong PD effect by the other triplet plus state. In this work we investigated the competitive process among AI, PD and RD in the $k^3\Pi_u^-$ state both by experimental and theoretical methods.

We present systematic lifetime measurements for H_2 and D_2 $k^3\Pi_u^-$ rovibronic levels over a wide range of the vibrational quantum numbers υ beyond the dissociation and ionization limit and for some rotational quantum numbers N. We also present dependence of lifetimes on N for H_2 $k^3\Pi_u^+$ υ=0 level. Lifetimes were measured for radiative transition lines $k^3\Pi_u^\pm(\upsilon',N') \rightarrow a^3\Sigma_g^+(\upsilon'',N'')$ by a delayed coincidence method combined with direct electron impact excitation from the ground state of molecules and single photon counting technique[1]. The experimental results for H_2 and D_2 $k^3\Pi_u^-$ levels were overall consistent with the present theoretical results based on a precise quantum-defect calculations[2,3] of the rovibronic term values as well as RD, PD and AI decay rates for H_2 and D_2 isotopes.

The non-adiabatic AI rate was proved to be important for H_2 $k^3\Pi_u^-$ $\upsilon \geqq 4$ vibrational levels, while PD rate was found to be very small compared with RD rate for both H_2 and D_2 isotopes. The lifetimes of $k^3\Pi_u^+$ υ=0 level showed strong N dependence.

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A-40

Decay of vibrational breathing modes in H_3^+

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The triatomic hydrogen positive ion H_3^+ finds much attention as a benchmark system for the treatment of polyatomic ions in general. Also, it plays a central role in the chemistry of interstellar clouds by driving protonization reactions which lead to the formation of many more complex molecules. Several properties of H_3^+ are still not well studied experimentally, in particular the dissociative recombination with low energy electrons is still a controversial issue, and absolute internal relaxation rates have not yet been measured.

Using beam storage techniques and Coulomb explosion imaging we have studied the breathing mode vibrational relaxation by direct measurements of the H_3^+ molecular geometries as a function of the storage time. The molecular ions were accelerated to ~0.5 MeV/amu from a standard ion source and injected into the ion storage ring TSR. Since the formation of H_3^+ is exothermic by 1.7 eV the ions reach the storage ring with a broad spectrum of internal excitations. The observed relaxation rates for the lowest breathing excited levels were of the order of theoretical prediction, but yet considerably shorter. For comparison with theory it proved to be necessary to include rotational excitations, which have substantial influence on the vibrational lifetimes. We have used the theoretical transition probabilities of the UCL line list for H_3^+ [L. Neale, S. Miller and J. Tennyson, Astrophys. J. **464**, 516 (1996)] to develop a model for the rovibrational decay. The model shows good qualitative agreement with the experimental data and gives further hints for very long-lived highly excited rotational states in accordance with recent DR imaging measurements at the TSR (see L. Lammich et al., this conf.).

Funded by DIP (BMBF) and EU (RTN "Electron transfer reactions").

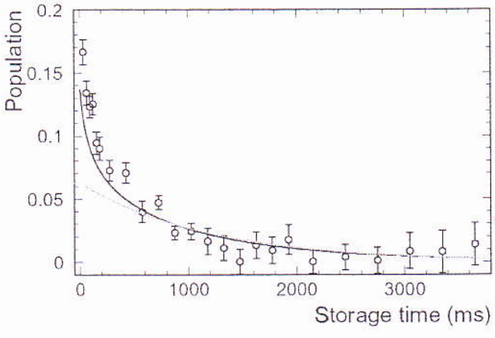

Figure 1: Population fractions for the first excited symmetric stretch mode measured with the CEI technique. The grey line represents a rotationless calculation resulting in a lifetime of 1.18 s, the black line is the outcome of a more detailed rovibrational model with an initial internal temperature of 0.23 eV.

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A-41

EXPERIMENTAL ELECTRON-SCATTERING TOTAL CROSS SECTION FOR C_4H_6 MOLECULE

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Absolute electron-scattering total cross section for 1,3-butadiene, isomer of C_4H_6, has been measured over the impact energy range from 0.5 to 370 eV by means of electron-beam transmission apparatus [1] under single collisional conditions. Preliminary results of measurements are presented in Fig.1. The obtained total cross section exhibits two distinct resonant-like maxima located at about 0.9, 3.2 eV and a very broad enhancement centred at 8.5 eV.

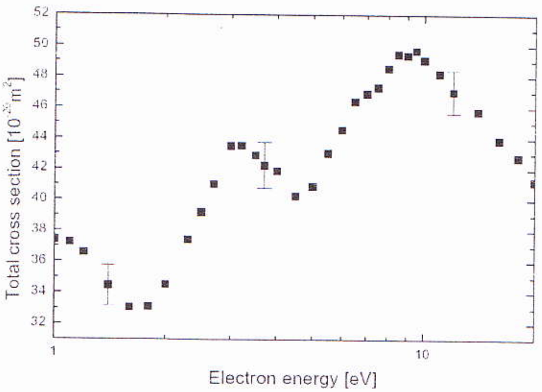

Figure 1: Total electron-scattering cross section for 1,3-butadiene (C_4H_6). The error bars at selected points represent the overall (statistical plus systematic) experimental uncertainties.

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A-42

FLUORINATION EFFECT IN ELECTRON SCATTERING

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We report the absolute total electron-scatering cross-sections (TCSs) determined in transmission attenuation experiments [1] for some hydrogenated (C_3H_6, C_3H_8) and perfluorinated (C_3F_6) molecules, over the energy range from 0.5 to 370 eV. Figure 1 presents our results along with C_3F_8 data of Tanaka [2] for the comparison. There are substantial differences in the shape and magnitude of TCS energy function for hydrocarbons and their perfluorinated counterparts. In particular, TCSs for perfluorides exhibit a very broad maximum between 20 and 80 eV.

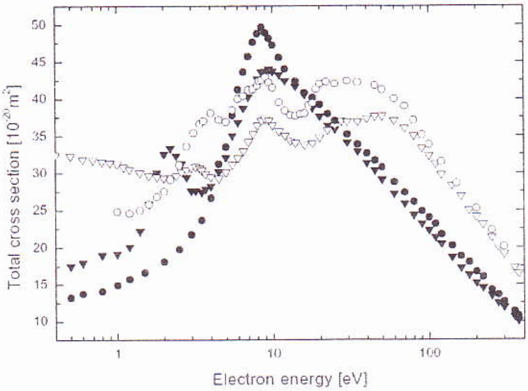

Figure 1: Comparison of electron-scattering total cross sections for propene, hexafluoropropene, propane and hexafluoropropane: (▼), C_3H_6; (▽), C_3F_6; (●), C_3H_8; (○), C_3F_8 [2].

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BREAKUP DYNAMICS IN THE DISSOCIATIVE RECOMBINATION OF H_3^+ AND ITS ISOTOPOMERS

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The dissociative recombination (DR) of the triatomic hydrogen molecular ion in the vibrational ground state with zero-energy electrons leads to two different final channels, one being the breakup into one hydrogen atom and a (possibly rovibrational excited) hydrogen molecule, the other being the breakup into three single hydrogen atoms. All emerging fragments are in their electronical ground state. This process is of large interest for interstellar ion chemistry and under intense experimental and theoretical study as a benchmark case for elementary reactions in small molecules.

The distributions of fragmentation momentum geometries and the vibrational excitation of H_2 and D_2 products were measured for H_3^+ [1] and D_3^+, stored as a fast beam in an ion storage ring (TSR, Heidelberg). The storage allows radiative relaxation of the molecules during up to 80 s before the electron interaction.

Another interesting result is the finding of an excess energy of several hundred meV in the total energy release of the three-body breakup (cf. Fig. 1). This was attributed to a very long lived rotational excitation of the H_3^+ ion, which could have strong implications on measurements of its DR rate coefficient in storage rings. Additional experiments performed on D_3^+ and D_2H^+ allow a comparison of the different isotopomers.

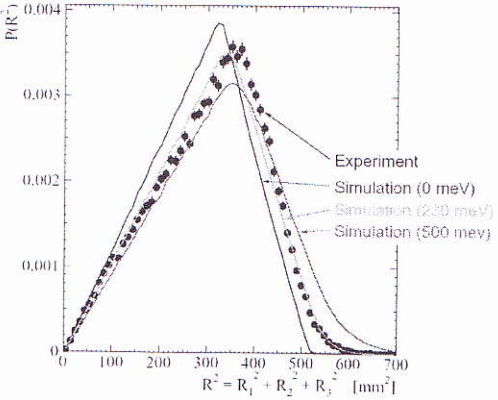

Figure 1: Distribution of 'image sizes' for the three-body breakup of H_3^+, which are strongly correlated to the kinetic energy release. Experimental data are shown in comparison to Monte Carlo simulations assuming rotational excitations of different temperatures.

Funded by DIP (BMBF) and EU (RTN "Electron transfer reactions").

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A-44

UNRESOLVED FINE STRUCTURE OF HYDROGEN BALMER LINES AND TOTAL EMISSION CROSS SECTIONS IN BEAM AND PLASMA EXPERIMENTS.

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Spectral lines of Balmer series of atomic hydrogen (H_α, H_β, H_γ...) are known to have extremely narrow multiplet structure. This fine structure is usually unresolved being masked by the instrumental, Doppler and/or Stark broadenings, and the total intensities of Balmer lines have to be measured. These intensities are widely used for plasma diagnostics and for determination of so-called emission cross sections in experiments with electron beams, but the existence of the fine structure is ignored without any argumentation (see bibl. in [1]). The aim of present contribution is to show that the ignorance may lead to significant mistakes in both: (i) the studies of the cross sections for direct (electron-atom) and dissociative (electron-molecule) electron-impact excitation processes; (ii) the spectroscopic diagnostics of ionized gases and plasmas.

The possibility of a correct account of the fine structure of Balmer lines was shown within simplest excitation-deactivation model (electron-impact excitation and spontaneous emission decay) for two simple limit cases: *the case 1* – when collisional redistribution of population density among the fine structure *nl* sublevels may be neglected (The situation may be reached in gas-beam and crossed beams experiments); and *the case 2* – when due to efficient mixing collisions, the *nl* sublevels are populated according to Boltzmann Law, being mainly proportional to their degeneracies (The situation is typical for gaseous discharge plasmas). In both cases *the total emission cross sections* (and corresponding rate coefficients) may be introduced and related to *the partial excitation cross sections*, spontaneous emission transition probabilities and the lifetimes of *nl* sublevels.

Quantitative analysis based on all available experimental and calculated data on the direct and dissociative electron-impact excitation of atomic hydrogen [1] show that:

(i) There is significant difference between the emission cross sections (as well as between the rate coefficients for Maxwellian electron energy distribution) of electron-impact excitation of the H_α and H_β lines calculated for those two limit cases (e.g., the difference exceeds an order of magnitude for dissociative excitation of the H_β line). Thus, the data on the total emission cross sections measured in beam experiments can't be used in plasma spectroscopy, where collisional redistribution of population density among *nl*-sublevels is significant.

(ii) To be able to obtain the emission cross sections and the rate coefficients for the case 2 one has to know the partial excitation cross sections of *nl* sublevels.

(iii) Nowadays, from the first four Balmer lines (relatively easily detectable) only first two lines, i.e., H_α and H_β, may be actually used in plasma spectroscopy due to the absence of data on the partial excitation cross sections of *nl*-sublevels with $n>4$.

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A-45

Electron Impact Excitation of Atoms and Molecules and Spectroscopic Determination of the Dissociation Degree of Hydrogen in Non-Equilibrium Plasmas.

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The dissociation degree of hydrogen is one of the most important parameters of hydrogen-containing plasma especially in relation to surface and volume plasma chemistry. In non-equilibrium gas discharge plasmas a calculation of the dissociation degree is too complicated and unreliable. Therefore, several experimental methods were proposed and used [1-5]. They are based on measurements of absolute [1] and relative [2-5] intensities of atomic (Balmer lines) [1-5] and molecular (Fulcher-α band system) [2-5] emissions. In a wide range of plasma conditions hydrogen atoms and molecules are excited mainly by electron impact, the atomic excited states being populated in electron-atom (direct excitation) and electron-molecule (dissociative excitation) collisions. Then, the intensities are proportional to the densities of atoms ([H]) and molecules ($[H_2]$), and their ratio $[H]/[H_2]$ (connected with the dissociation degree) could be obtained. The excitation rates depend also on the shape of electron energy distribution (EED) and electron concentration, so methods [1-2] include Langmuir probe measurements, which cannot be used in most plasma sources. This problem may be overcome by introduction of the electron temperature T_e - artificial magnitude having the sense of a parameter of Maxwellian approximation of real EED in the vicinity of an excitation threshold [3-5]. Every measured ratio of the intensities may be related to a line on the plain T_e,$[H]/[H_2]$. The intersections of more than two of such lines would give the opportunity to obtain $[H]/[H_2]$ and to verify an applicability of the method in certain plasma conditions.

The goal of the present report is to show that insufficient knowledge of cross sections for electron-impact excitation of atomic and molecular hydrogen is now "the bottle-neck" in development of pure spectroscopic (non-invasive, remote and *in situ*) methods of determining the dissociation degree. The current situation in experimental and *ab initio* studies of the electron-impact cross sections is presented and analyzed. Quantitative analysis of the intensity ratios measured in low-pressure microwave and arc discharges is discussed. It is shown that the considered problem of Plasma Spectroscopy needs help from Collision Physics by obtaining the electron-impact cross sections via: (i) CCC calculations of the direct excitation of the nl- fine structure sublevels of the hydrogen atom for $n>4$; (ii) more detailed experimental studies of the dissociative excitation of the nl- sublevels for $n>2$ and of the direct excitation of separate electronic-vibro-rotational spectral lines of other than Fulcher-α band systems of H_2 molecule.

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A-46

PARTIAL AMPLITUDES AND ZERO-RANGE POTENTIALS IN MULTI-CHANNEL SCATTERING

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A multi-center-multi-channel scattering problem is studied from a point of view of integral equations system that appears while one-particle wave function equation of the electron under action of a multi-center potential with non-intersecting ranges is considered. Spherical Bessel functions basis expansion of the potentials introduces partial l-amplitudes and radial functions $y_l(r)$. The idea of the generalized partial potentials (the class contain distributions) may be understood via integral equation with the asymptotical behavior of solutions at infinity that fit a scattering problem

$$y_l(r) = j_l(kr) - 2k \int_0^d j_l(kr_<) h_l(kr_>) U_l \, y_l(r') r'^2 dr'. \tag{1}$$

Where k is a wavenumber, $h_l(z) = n_l(z) + i j_l(z)$ and $j_l(z), n_l(z)$ are the spherical functions. The upper limit in the integral is the potential range. For the generalized zero-range potentials (GZRP) we develop [2], introducing

$$U_l = A\delta(r-0) r^S \left(\frac{d}{dr}\right)^P r^Q. \tag{2}$$

S, P, Q - some integers, that are defined by singularities of n_l and j_l, and hence define the class of the GZRP. $\delta(r-0)$ - Dirac function on $[0, \infty)$. Taking into account the zero-range character of the potential we substitute (2) in (1) and account the asymptotic of the spherical functions that yields $y_l(r) = (1 + iC) j_l(kr) + C n_l(kr)$.

$$C = -2A \frac{k^{l+1}}{(2l+1)!!} \int_0^d \delta(r-0) r^{2+l+S} D^P \left(r^Q y_l(r)\right) dr. \tag{3}$$

The condition of the $C < \infty$ fix the class of the integers S, P, Q. The asymptotical behavior at $r \to \infty$ give partial scattering amplitudes $f_l(k)$.

The approach is generalized to multi-center (with $A \to A_i, \mathbf{r} \to \mathbf{r_i}$) and multi-channel case by a matrix formulation [1] (see also [3]) in which a state vector components associated with scattering channels. The zero-range potentials naturally enter the scheme while the class potentials as operators of multiplication is widen to distributions. The class naturally contains superpositions of the potentials (2). Analog of multipolar expansion is treated similar to [2]. Spin variables, oscillations and rotations are incorporated into the scheme as in [3].

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ATOMIC FLUORESCENCE AFTER THE NEUTRAL DISSOCIATION OF THE RYDBERG STATES OF DIATOMIC MOLECULES AS A TOOL FOR INVESTIGATING THE DISSOCIATION PROCESSES IN MOLECULAR IONS.

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Recently [1-3] photon-induced fluorescence spectroscopy has been applied to study the neutral photodissociation of the oxygen molecule. It was found that during dissociation of the superexcited $O_2^* \, 2\sigma_u^{-1} \, (c\,^4\Sigma_u^-) \, n(d/s)\sigma_g$ molecular states the molecular Rydberg $n(d/s)\sigma_g$-electron is captured by one oxygen atom forming the $O^* 2p^3(^4S)\, nd/s$ excited atomic Rydberg states and leaving the other atom mostly in the $2p^4(^1D)$ state. There exists another deexcitation path: autoionization of molecular Rydberg states into different continua. These two deexcitation channels compete with each other. In the case of autoionization, Rydberg states manifest themselves only in photoabsorption spectra of molecules. In contrast, fluorescence from $O^* 2p^3(^4S)\, nd/s$ excited atomic Rydberg states is a result of neutral dissociation. Here the Rydberg electron plays a role of "inner probe" allowing one to compare the predissociation and autoionization lifetimes. Therefore the joint analysis of atomic fluorescence emission cross sections together with the absorption cross section of molecules provides information on the dissociation and Auger rates and can be a powerful tool to study the dissociation processes in molecules.

In the present work, to interpret the results of our measurements of atomic fluorescence emission cross sections of oxygen following the neutral dissociation of molecular Rydberg states converging to the $2\sigma_u^{-1} \, (c\,^4\Sigma_u^-)$ threshold [2,3], we performed extensive calculations of potential curves of molecular oxygen. The calculations were performed using the Multi-Reference Configuration-Interaction method and yield accurate potential curves for all spectroscopically observed O_2^+ states. The obtained potential curves were used then to calculate predissociation lifetimes. Comparing the latter with the autoionization lifetimes allows us to explain the main features in the observed fluorescence emission cross sections.

Ph.V.D. would like to acknowledge support by the Alexander von Humboldt foundation.

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A-48

Electron and photon induced processes in SF_5CF_3

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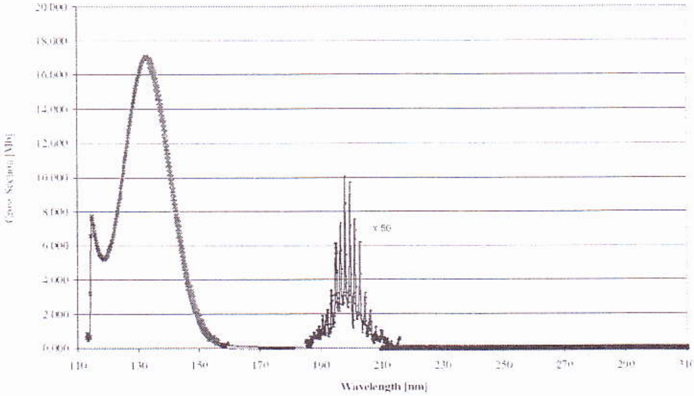
Concern for the effects of climate change has grown during the last years and many of these arise from the constant emission of pollutants. The major contributions are strong greenhouse gases compounds such as CO_2, CH_4 and N_2O. The recent International Panel for Climate Change (IPPC) report forecasts that mean global temperatures may rise by as much as 5.8°C by the end of the century [1]. However there are number of gases when although present in much smaller quantities have a significant contribution to global warming due to their large infrared absorptions.

A newly discovered totally anthropogenic origin molecule is trifluoromethyl sulphur pentafluoride (SF_5CF_3). It possesses the largest radiative forcing on a per molecule basis of all gases present in the atmosphere, 0.57 $Wm^{-2}ppb^{-1}$, according to a recent report [2]. Moreover, the levels in the atmosphere for this molecule are currently small, but growing at a 6% per year rate.

In order to understand and study the molecular spectroscopy and electron induced processes for this molecule, and determine the lifetime and global warming potential in Earth's atmosphere, we have used the electron energy loss spectroscopy technique to study the molecule in the UV/VUV region [3], high-resolution infra-red spectroscopy, and recently we measured a VUV photo-absorption cross section at the ASTRID synchrotron radiation facility, Aarhus, Denmark.

A photoelectron spectra has also been measured at the University of Liège, Belgium. Further details will be presented at the meeting.



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A-49

OBSERVATION OF ELECTRON IMPACT EXCITATION OF OXYGEN AT 180°

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Electron impact excitation of oxygen (O_2) has been observed at scattering angles of 90° and 180° in the energy loss mode. In this experiment a new conical coil system that is a further development of the magnetic angle-changing technique $[1-3]$ has been incorporated into an electron hemispherical spectrometer. Conical shaped solenoids enable cancellation of the dipole and octupole magnetic moments of the system and therefore high localization of the magnetic field (which decreases with distance as r^{-7}). In addition they give efficient pumping of the target gas from the electron scattering region. Figure 1 shows energy loss spectra recorded at an incident electron energy of 10.4 eV. Excitation of two states, the $a^1\Delta_g$ and $b^1\Sigma_g^+$ are seen in the spectra, along with excitation of vibrational levels of the $X^3\Sigma_g^-$ ground state. The $b^1\Sigma_g^+$ state, which observed at 90°, was not detected at 180° in agreement with theoretical prediction of the $\Sigma^- - \Sigma^+$ selection rule [4]. The intensity ratio of the $a^1\Delta_g$ peaks at 90° and 180° differs from that predicted by theoretical calculations presented in [5]. However, the relative intensities of the energy loss peaks of $a^1\Delta_g$ and $b^1\Sigma_g^+$ states at 90° are consistent with the previous measurements of [6].

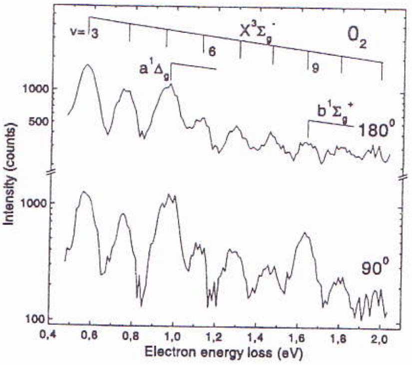

Figure 1: Energy loss spectra of oxygen observed at an incident electron energy of 10.4 eV and at the scattering angles of 90^0 and 180^0.

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POSTER SESSION B

DIFFERENTIAL CROSS SECTIONS FOR POSITRON IMPACT EXCITATION OF HYDROGEN

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We present theoretical calculations for excitation of hydrogen atom by positron impact. In our recent work we use a *distorted wave polarized orbital* (DWPO) model and the *classical trajectory Monte Carlo* (CTMC) method to calculate the angular differential and total excitation cross sections for positron impact induced 1s-2s transitions in hydrogen (Fig. 1).

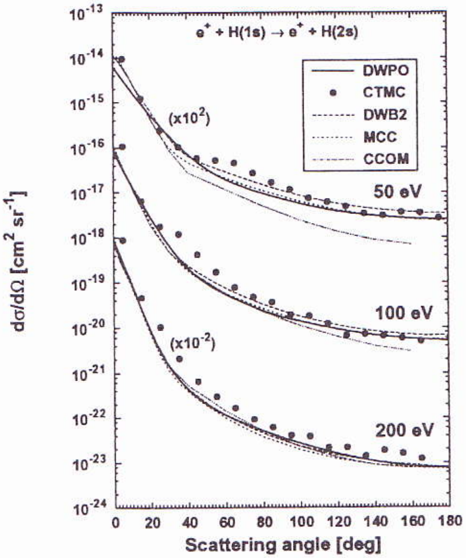

Figure 1. Differential cross sections for positron impact excitation of the 2s state of hydrogen at 50, 100 and 200 eV bombardment energies. DWB2 [1],MCC [2], CCOM [3].

In this work the cross section data obtained by various models are compared and the differences between the calculations are discussed.

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B-2

Relativistic and Nondipole Effects in Two-Photon Ionization of H-like Ions by VUV Photons

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The use in recent experiments of short, high-frequency (VUV) laser pulses produced by the high-order harmonic generation of fundamental laser beams in gases and test operation of intense free-electron lasers (HASYLAB at DESY, Hamburg) with photons of energies in excess of 200 eV stimulate the analysis of relativistic and nondipole effects in multiphoton laser-atom interactions. We present such analysis for the two-photon ionization of high-Z hydrogen-like ions with exact account for relativistic effects (using the Dirac equation for description of an electron in a point-like Coulomb field) and employing the full multipole expansion for the photon vector potential in electron-photon interaction, which we take into account perturbatively, in the second-order perturbation theory. To analyze the relativistic and nondipole corrections to the Elliptic Dichroism (ED) effect in the angular distribution (AD) of photoelectrons (i.e., the dependence of the differential cross section on the *helicity* of a photon beam, which vanishes for the case of completely circularly-polarized photons), we consider the general case of elliptically-polarized photons.

The separation of kinematical and dynamical factors in the AD is performed using an effective angular technique based on the reduction formulas for bipolar harmonics and multipole expansions of irreducible tensor sets [1]. As a result, the polarization-angular factors in the differential cross section of two-photon ionization from an arbitrary $|njlm\rangle$-state of the H-atom are expressed in an invariant form involving only scalar products of photon polarization vectors with the electron momentum $\mathbf{p}$ and Legendre polynomials of the angle between $\mathbf{p}$ and the direction of photon beam. Dynamical factors involve second-order matrix elements of the radial part of relativistic Coulomb Green function (RCGF). In calculations of these matrix elements we use a generalized Sturmian expansion of RCGF with two arbitrary parameters α and α' [2]. An appropriate choice of these parameters provides a good convergence of Sturmian expansions over a wide range of photon frequencies. The results of numerical calculations will be presented for the total and differential rates of two-photon ionization from the ground state of a H-like ion with different Z as well as for the magnitude of ED parameters in the AD.

Partial support by RFBR Grant 00-02-17843 is acknowledged.

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B-3

Influence of the Laserbandwidth on the Excitation Probability in a Two-Level System

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In connection with planned collision experiments involving vibrationally excited molecules, we address the problem of optimal excitation of molecules in a collimated molecular beam by a coherent infrared light source with sub-MHz bandwidth. Apart from the averages over the beam-divergence related Doppler profile (corresponding to off-resonant excitation) and the longitudinal velocity distribution of the molecular beam (leading to different interaction times with the photon field), we are concerned with the effects of coherent population return (CPR) [1]. Here CPR plays a substantial role, irrespective of the light intensity, for conditions such that the detuning Δ from resonance is larger than the Fourier width T^{-1} of the transform limited coherent light source (T = pulse length of interaction). As an example of interest, we consider excitation of a two-level system (e.g. HF($v = 1$, $J = 1$, $m_J = 0 \leftarrow v = 0$, $J = 0$, natural linewidth about 32 Hz) [2] with a single mode continuous wave optical parametric oscillator (OPO). The molecular beam velocity is around 1000 m/s with a velocity width (FWHM) of about 20 %. Assuming a Lorentzian OPO linewidth of 100 kHz, intensities corresponding to a Rabi frequency of $\Omega_R \approx 3\,\mathrm{MHz}$ and pulse lengths (i.e. transit times) of $T \approx 2.5\,\mu s$, numerical solutions of the optical Bloch equations with damping [3] yield single pass excitation probabilities $> 10\,\%$ (averaged over the longitudinal velocity spread) for detunings up to about 1 MHz, demanding a rather narrow beam collimation. The calculations also show that at constant Rabi frequency more efficient excitation can be achieved by using a less coherent light source (i.e. an OPO with broader instantaneous linewidth), thus yielding *excitation by decoherence*.

This work has been supported by the Deutsche Forschungsgemeinschaft through Forschergruppe *Niederenergetische Elektronenstoßprozesse* and by the European Union Research Training network COCOMO, contract number HPRN-CT-1999-00129.

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B-4

ELECTRON SCATTERING ON N_2O- FROM CROSS SECTIONS TO DIFFUSION COEFFICIENTS

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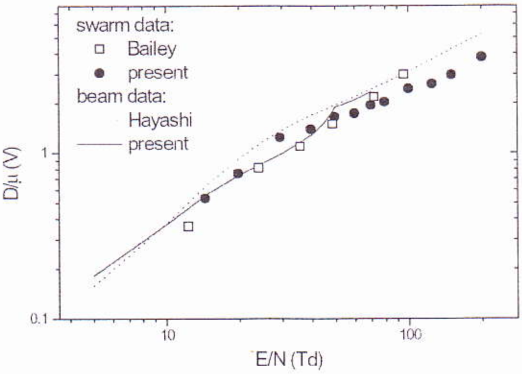
Only recently measurements of electron scattering cross sections with beam techniques in N_2O have been extended to partial (elastic, vibrational, ionization) data (see [1] and references therein). On the other hand, swarm studies on this molecule are still sporadic [2]. In this work, measurements of the ratio of transverse and longitudinal diffusion coefficients to the mobility (D/μ and D_L/μ) for electrons in N_2O are extended to intermediate reduced electrical field values - the range E/N from 15 Td to 200 Td. In this range the swarm data loose a part of their "competitiveness" with beam experiments compared to ultralow energies. However, we show that the diffusion coefficients in this E/N range remain extremely sensitive to presence of inelastic processes.



The experimental results for D/μ are in Fig.1. compared with data calculated by a numerical solution of the Boltzmann equation, in two methods and using two alternative cross section sets – a recent evaluation by Karwasz et al. [1] and a set of cross sections elaborated by Hayashi [3]. The present model shows, that high cross section values for vibrational excitation (1/2 of the elastic one) at the resonance around 2.3 eV are essential to explain observed structures in diffusion coefficients.

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B-5

Modified Landau-Zener formula for near-threshold energies

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When adiabatic potential energy curves for the relative motion of two atoms in different electronic states almost cross, Landau-Zener theory gives a formula for the probability of a non-adiabatic transition between the curves. The probability depends on the slopes of the curves and their separation at the avoided crossing, and on the velocity which is assumed to be so large that the relative motion of the atoms is essentially classical.

For near-threshold energies, close to the asymptotic value of one of the curves, the corresponding velocity is very small at large separations. Then quantum reflection [1], which can prevent the atoms from coming close to the avoided crossing, becomes a dominating effect. The probabilities for transmission to smaller separations - in either electronic state - thus vanish towards threshold, a feature not contained in conventional Landau-Zener theory. We propose a correction which takes the effect of quantum reflection into account so that the correspondingly modified Landau-Zener formula remains accurate at low energies, all the way down to threshold.

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B-6

THEORETICAL CONSIDERATION OF LIGHT-INDUCED SPECTRA IN O_2 MOLECULE IN INTENSIVE LASER FIELD

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New spectral lines of VUV absorption, and the effect of the predissociation in O_2 molecule in presence of intensive laser field of intensity $10^{13} - 10^{14}$ v/cm^2) and wave length 800-2000 nm have been considered in the model of two quasimolecular states with nonadiabatic interaction [1].

The distortion of $X^3\Sigma_g^-$ and $B^3\Sigma_u^-$ potential curves of O_2 molecule by the interaction with laser field in vicinity of the pseudocrossing point R_c has been considered in the dipole approximation. Molecular curves in the absence of laser field have been splined from CI computation [2].

The molecule-electromagnetic field interaction has been estimated in dipole approximation [1]. The dependence of the dipole matrix element between $X^3\Sigma_g^-$ and $B^3\Sigma_u^-$ electronic functions on internuclear separation R has been approximated with the aid of r-centroids approach [3] as

$$D(R) = 2.8\exp(-0.916R)\; a_o, \tag{1}$$

the expression (1) is valid in the interval of R = 2.0 - 3.0 a_0.

Vibrational wave functions in vicinity of equilibrium point of new adiabatic potential curve have been expanded into the series of harmonic oscillator functions. The positions of new vibrational levels have been found from the diagonalization of the Hamiltonian. For the calculation of predissociation probability the Landau-Zener model has been applied.

We examined the reliability of the method of estimation of values of matrix elements of diabatic interaction $D_{appr}(R_c)$ in the point of pseudocrossing R_c between adiabatic energy curves through the difference between adiabatic energies $U_a^{\pm}(R_c)$ in the case, when these energies are calculated only in few number N of points of R in vicinity of R_c and splined anywhere. $D_{appr}(R_c)$ can be estimeted by the equality: $D_{appr}(R_c) = 0.5(U_a^+ - U_a^-)|_{R=R_c}$ as if the exact diabatic interaction $D(R)$ (1) would not been known. We found, that the precision of the estimation of $D_{appr}(R_c)$ depends drastically on the number of points N especially for narrow pseudocrossings.

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B-7

ABSOLUTE DIFFERENTIAL CROSS SECTIONS FOR ELASTIC ELECTRON SCATTERING IN NEON IN THE ANGULAR RANGE FROM 130° TO 180°

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In a continuation of our studies of elastic electron scattering in the backward direction [1, 4] we have measured differential cross sections (DCS) in neon, in the angular range from 130° to 180°. Absolute DCS's for elastic scattering in neon over the full range of scattering angles are important since neon has been suggested as a secondary standard in the measurements of DCS's of other atomic and molecular species. The experimental setup was based on the magnetic angle changing technique [2, 5] which allows the collection of scattered electrons in the range of scattering angles up to 180°. The DCS obtained in Ne at an energy of 5 eV are shown in Figure 1 in comparison with the existing experimental data below 130° and with the theoretical calculations. In the angular range above 140° the present results are higher than the theoretical predictions. Using DCS of [3] which were extrapolated down to 0° together with our results in the remaining angular range, the total and momentum transfer cross sections have been obtained. Both cross sections are in good agreement with the experimental results of [3, 8].

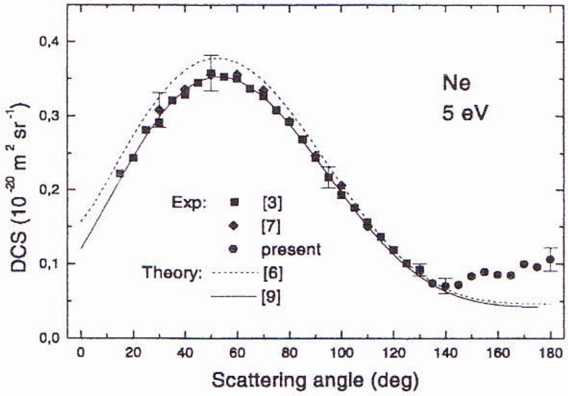

Figure 1: Differential cross sections in neon at an electron energy of 5 eV.

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B-8

D^- ion desorption from condensed CD_4, C_2D_2, C_2D_4, C_2D_6 and C_3D_8 molecules induced by electron impact.

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The processes initiated by low energy electron impact, including the desorption of anions from condensed molecules have a practical importance in many research fields e.g. plasma physics, radiation physics and astrophysics. Recent experiments indicate that electron scattering via transient anions provides an efficient pathway for secondary electron damage to DNA [1] and a plausible contributory mechanism to ozone depletion [2].

In present work we have studied the energy dependence of the electron-stimulated desorption of D^- ions for CD_4, C_2D_2, C_2D_4, C_2D_6 and C_3D_8 molecules condensed on a platinum substrate. In these experiments (see e.g. [3]) multilayer molecular films are condensed on a clean polycrystalline, cryogenically cooled ($T \simeq 20$ K) Pt foil. The thin films are bombarded with a monoenergetic (FWHM = 80 meV) electron beam (0-20 eV) produced by an hemispherical electron monochromator. The desorbed anions are mass selected with a quadruple mass spectrometer and detected by an electron multiplier. The apparatus is housed in ultra high vacuum chamber reaching a background pressure of 10^{-10} mbar which is maintained by a combination of a ion pump and closed-cycle refrigerated cryopump.

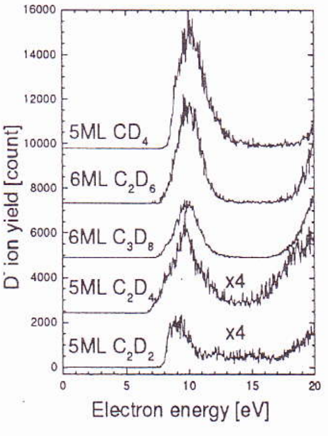

Figure 1: Comparison of D^- signal desorbed from condensed CD_4, C_2D_2, C_2D_4, C_2D_6 and C_3D_8 molecules on Pt substrate

The recorded D^- yield functions for 5-6 multilayers of CD_4, C_2D_2, C_2D_4, C_2D_6 and C_3D_8 are shown in fig. 1. For each species studied, the yield function contains a broad resonant maximum, located near 9.2 for C_2D_2, 9.7 eV for CD_4 and C_2D_4 and 10 eV in the case of C_2D_6, and C_3D_8. At higher impact energies weak D^- fluxes were recorded, which then slowly increases in intensity above 15 eV for C_2D_4, 17 eV for C_2D_6 and C_3D_8, and 18 eV for CD_4, and C_2D_2 molecule. The observed resonant structures are attributable to dissociative electron attachment process in which a temporary negative ion is created by resonant electron capture [4]. The position of resonant maxima and width of resonance peaks are very close to those observed for similar non-deuterated hydrocarbons films [5].

This work is supported by the Canadian Institutes of Health Research.

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B-9

Charge Transfer Processes in Plasma Processing

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Plasma processing is widely used to alter the properties of materials as well as to synthesize new materials. One such process is plasma polymerization. The elementary processes that occur during plasma polymerization of acetylene have been investigated and are reported here. Specifically, time of flight mass spectrometry as well as optical emission spectroscopy have been employed to detect the ions and excited species present in C_2H_2, O_2, He, Ar, and He/Ar plasmas. Mass spectra, optical emission spectra, and ion kinetic energy distributions are reported. The results show a decrease in energetic (~400 eV) ion signal with increasing pressure and a change in the ion kinetic energy distributions. This is attributed to symmetric charge transfer reactions within the plasma sheath. The results allow the extent of the plasma sheath to be made. The results suggest that symmetric charge transfer reactions are ubiquitous within plasmas and that such reactions are very important in determining the properties of the thin films thus synthesized.

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B-10

LIPS spectroscopy for contamination analysis and the laser cleaning diagnostics of historical paper documents

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Recently, a growing interest in application of the radiative techniques for restoration and analysis of documents and artefacts on paper and parchment is observed. The potential of ablative laser cleaning is confirmed experimentally and the optimal interaction parameters such as wavelength (532 nm) and energy fluences (< 1 J/cm^2) are specified [1,2]. For the laser wavelengths applied so far the degree of polymerisation of the paper substrate reveals smaller changes for irradiation at 532 nm in comparison to 308 nm due to the fact that the bond energies of main cellulose compounds are not accessible by the 2,33 eV photons [1]. It is shown that spectroscopic measurements can deliver information on the chemical composition of the substrate and the pigments applied as well as of the surface contaminants, and also their light-induced deterioration can be studied in this way [2].

In this work the LIPS spectra of historical paper documents recorded before and after the surface cleaning by means of the Nd-YAG laser pulses at 532 nm (6 ns pulsewidth) are studied. The plasma is induced by the pulsed laser beam at 532, 355, or 266 nm focused in the vicinity of the sample surface and the emission spectra are recorded. An independent experiment under similar conditions, i.e. cleaning at 532 nm and plasma excitation at 248 nm (KrF excimer laser, 15 ns) is carried out, too. In both cases the system consisting of the spectrograph (Acton Res.), cooled CCD camera (CVI) and PC-based acquisition unit is used for recording and storage of the spectra.

Results indicate that the shorter excitation wavelengths result in a more reach and intense spectral structures in the UV range which allows for a better confidence of the assignment. The appearance of the sharp emission lines at 616.4, 646.5, 717 nm (Ca I), 589.4 nm (Na I), and 766.5, 769.9 nm (K I) ascribed to the surface pollutants is reproduced for the plasma excitation at 248, 355 and 532 nm, and is in agreement with our previous measurements [2]. The effect of the gaseous environment (air, N_2, or Ar) is characterized by a slight intensity decrease of the overall spectral shape in the case of N_2.

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B-11

$M1$–$E2$ interference effect on polarization dependence of two-colour frequency mixing in Tl atoms

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Three-wave mixing of a two-colour radiation is a simplest nonlinear process which may be useful both for frequency conversion of intense laser radiation in atomic medium and for probing and determining details of atomic level structure. In free atoms this process is strictly forbidden in electric dipole approximation. The magnetic dipole ($M1$) and electric quadrupole ($E2$) interaction also cannot contribute to coherent scattering of sum- or difference-frequency photons collinearly with incident waves. Nevertheless, *incoherent collinear* scattering is possible in atoms with non-zero angular momentum in their ground state in addition to *non-collinear coherent* scattering, when one of the three waves propagates at right angle to the other two collinearly propagating waves.

The double-resonant process is the most efficient in atomic medium. The level structure of Tl atoms provides possibility for resonant interaction with incident radiation of frequency $\omega_1 = E_{6P_{3/2}} - E_{6P_{1/2}} - \varepsilon$ both in $M1$- and $E2$-approximation. The interference of contributions from these interactions provides enhancement or reduction of coherent scattering amplitude, depending on relative polarization of incident waves. This dependence may be presented by equation for the amplitude of scattering coherently photons with frequency $\omega' = \omega_1 + \omega_2 = E_{7S_{1/2}} - E_{6P_{1/2}} - \varepsilon'$, as follows

$$U = \frac{A}{\varepsilon\varepsilon'} \left\{ \left[1 + \frac{3}{5}\omega_1 R^{(2)}\right] (\mathbf{e}_1 \cdot \mathbf{e}_2)(\mathbf{e}'^* \cdot \mathbf{n}_1) - \left[1 - \frac{3}{5}\omega_1 R^{(2)}\right] (\mathbf{n}_1 \cdot \mathbf{e}_2)(\mathbf{e}'^* \cdot \mathbf{e}_1) \right\}, \quad (1)$$

where the resonance detuning $\varepsilon = \Delta - i\Gamma/2$ ($\varepsilon' = \Delta' - i\Gamma'/2$) includes real and imaginary parts of energy for excited levels (the level widths Γ and Γ').

The difference between cross sections for $\mathbf{e}_2 = \mathbf{e}_1$ and for $\mathbf{e}_2 = \mathbf{n}_1$ gives quantitative information on the value of the radial quadrupole matrix element $R^{(2)} = \langle 6P_{1/2}|r^2|6P_{3/2}\rangle$, thus providing really existing facilities for the use of the frequency mixing techniques for measuring matrix elements for electromagnetic transitions in atoms.

More efficient results may be obtained by inducing coherent collinear scattering in atoms exposed to external fields. As was demonstrated in calculations for atoms in spherically symmetric states [1, 2], a constant magnetic field induces additional resonance in the forward scattering amplitude and so is a good candidate for the use in the laser light conversion as well as in the two-colour spectroscopy of atoms.

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B-12

Spin-orbit-induced magnetic dipole effect on two-colour frequency mixing in alkali atoms

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Three-wave double-resonant frequency mixing of a two-colour radiation in alkali atoms is determined by electric quadrupole interaction with electromagnetic radiation [1]. In one of three possible routes for this process, with resonance on n_1P- and n_2P-states, a contribution of magnetic dipole interaction into the process' amplitude may appear. Specifically in heavy atoms, where the spin-orbit interaction is rather strong to mix states with different principal quantum numbers, $n_1 \neq n_2$, and equal angular l and total J momenta, the magnetic-dipole amplitude for scattering sum-frequency photons may be comparable to the electric quadrupole amplitude with the same resonance singularities. The interference between $M1$ and $E2$ processes may influence on the polarization dependence of corresponding cross section.

The amplitude for coherent scattering of radiation with frequency $\omega' = \omega_1 + \omega_2$ by atoms in $|nS_{1/2}\rangle$ state may be presented in the form:

$$U_{coh} = \frac{C}{\varepsilon_{3/2}\varepsilon'_{3/2}} \left\{ \left[1 + \frac{\varepsilon_{3/2}}{\varepsilon_{1/2}} + \frac{\varepsilon'_{3/2}}{\varepsilon'_{1/2}} \right] (\varphi + \varphi') + s \left[\frac{\varepsilon_{3/2}}{\varepsilon_{1/2}} - \frac{\varepsilon'_{3/2}}{\varepsilon'_{1/2}} \right] (\varphi - \varphi') \right\}, \qquad (1)$$

where C is a field-amplitude-dependent factor, $\varepsilon_J = \Delta - i\Gamma/2 = E_{n_1P_J} - E_{nS_{1/2}} - \omega_1$ ($\varepsilon'_J = \Delta' - i\Gamma'/2 = E_{n_2P_J} - E_{nS_{1/2}} - \omega'$) is the resonance detuning with the lower $|n_1P_J\rangle$ (the upper $|n_2P_J\rangle$) level, including the imaginary part (the excited level width Γ), $\varphi = (\mathbf{e}_1 \cdot \mathbf{k}_2)(\mathbf{e}_2 \cdot \mathbf{e}'^*)$, $\varphi' = (\mathbf{e}_1 \cdot \mathbf{e}_2)(\mathbf{k}_2 \cdot \mathbf{e}'^*)$ are the scalar products of the unit field vectors, and

$$s = \frac{5\alpha^2 Z_i \langle n_1P|r^{-3}|n_2P\rangle}{2\omega_2^2 \langle n_1P|r^2|n_2P\rangle} \qquad (2)$$

is the ratio of the spin-orbit [2] and electric quadrupole matrix elements. The contribution of the spin-orbit-induced $M1$ interaction (the term proportional to s in (1)) gives rise to the circular dichroism effect: in coherent scattering from an atom exposed to *linearly polarized incident waves* propagating at right angle to one another (with the unit wave vectors $\mathbf{k}_1 \perp \mathbf{k}_2$), the sum-frequency radiation may be *elliptically polarized* with the circular polarization degree $\xi' = i(\mathbf{k}' \cdot [\mathbf{e}' \times \mathbf{e}'^*])$ directly proportional to the spin-orbit mixing parameter s, the fine-structure splitting of resonant levels, δ and δ', the combination of level widths Γ, Γ', and detuning Δ, Δ':

$$\xi' = \frac{2s\delta\delta'(\Gamma'\Delta - \Gamma\Delta')\sin 2\theta}{(|\varepsilon|^2\delta'^2 + |\varepsilon'|^2\delta^2)(1+s^2) + 2\delta\delta'(1-s^2)\mathrm{Re}(\varepsilon^*\varepsilon') + 2s(|\varepsilon|^2\delta'^2 - |\varepsilon'|^2\delta^2)\cos 2\theta},$$

θ is the angle between polarization vectors $\mathbf{e}_1$ and $\mathbf{e}_2$. The model potential method [3] is used for numerical estimates of radial matrix elements in (2).

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B-13

Electron collisions with C_2H_4, C_2F_4 and C_4F_8

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In the contemporary technology of plasma deposition and etching, perfluorocyclobutane (c-C_4F_8) and its fragments (e.g. C_2F_4) play an important role in the preparation of silicon dioxide surfaces. To explain the complex behaviour of different components in such a gas discharge, knowledge of differential, momentum transfer and integral cross sections for scattering of low energy electrons is crucial.

The important range of electron kinetic energies in these processes spans from a few hundred meV to a few tens of eV. Experimental and theoretical investigation of these two gases has been rather limited until recently. In the most recent work, Winstead and McKoy [1] calculated *ab initio* differential (DCS) and integral cross sections for elastic scattering of electrons between 1.5 and 60 eV on c-C_4F_8 using the Schwinger multichannel (SMC) method. The only published experimental data available for comparison are those of Sanabia *et al* [2] and Nishimura [3] for the total scattering cross section.

Research on the one of the simplest fluorocarbons, C_2F_4, the fluorinated analog of ethylene (C_2H_4), extends from swarm measurements and analyses [4] to the most recent theoretical calculation of Winstead and McKoy [5]. Old measurements of relative DCS for elastic scattering at 25 eV and 40 eV by Coggiola *et al* [6] seem to be the only published experimental data to date. Therefore, there is an interest in experiments at lower electron energies, especially below 10 eV, where it is known that the ethylene cross sections are resonantly enhanced. For ethylene there are previous, relative DCS measurements [7] and several theoretical calculations using the Schwinger variational technique [8,9].

In our experiments, we are using the crossed-beam technique to measure absolute DCS for elastic electron scattering and vibrational excitation of C_2H_4, C_2F_4, and C_4F_8, at energies from 1 to 100eV, and scattering angles from 10° to 130°.

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B-14

INTERACTION OF LOW-ENERGY ELECTRONS WITH SURFACE: THE SEES AND TCS STUDY

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A detailed study of the near-surface phenomena has become possible owing to a recent development of new investigation techniques and instruments making it possible to determine the composition of a substance and its geometric and electronic structure. The low-energy secondary electron spectroscopy (based on the study of phenomena accompanying the process of interaction between the flow of slow-moving primary electrons with energy ≤ 1 keV and crystal surface) which does not destroy the sample is one of the methods to control surface roughness. In this case the observed experimental spectra of truely secondary electrons (SEES) and spectra of target current (TCS) show the totality of phenomena taking place both in the volume and near-surface layer of the crystal. The fine structure of those spectra is determined by the energy dispersion of unoccupied high-level electronic states (above the vacuum level) to which the electrons are scattered or from where they are emitted. The existing theoretical interpretation of fine structure peculiarities is not complete enough because of the variety of elementary processes taking place in a solid. The present study deals with the development of the above-mentioned methods basing on the energy band structure of crystals. As before, (see, e.g. [1-4]) during the calculation of SEES and TCS the electron scattering with a preset momentum at the crystal was considered within the approximation, when the probability of scattering was proportional to a number of finite states at a given energy level with a preset direction of quasi-momentum. The energy dependence of the band energy level broadening, the electron-electron and electron-plasmon contributions to the distribution function of highly nonequilibrium charge carriers (obtained from the solution of the kinetic (Boltzmann-type) integral transport equations describing the cascade process of the inelastic scattering of the primary electron flow [5]), the isotropic component of current from the electrons scattered on the surface were taken into consideration. In addition, it was a success for us to rather satisfactorily explain the main structure in spectra of a number of crystals. And there occurs a possibility for the experimental study of the electron dispersion in the region of energies much higher than vacuum level and for usage of the SEES and TCS data in a more perfect calculation of band structure showing which singularities of the spectra relate to some or other bands. The method being developed enables one to distinguish between the volume effects in SEES and TCS from the surface ones which are to be investigated separately [6].

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B-15

STRONG INTERACTION BETWEEN AUTOIONIZATION CHANNELS IN THE *even* $4p^4 n\ell$ SATELLITE PRODUCTION IN Kr

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The *even* satellites of the 4s-level in Kr are connected with the set of $4p^4 ns/md$ configurations. Photoionization cross sections (PI CS) for these satellites at their thresholds are strongly influenced by the doubly-excited states $4p^4 n\ell m'\ell'$ [1-3]. Calculation performed in [2,3] allowed one to understand the nature of the main features in PI CS. However, theory gave the absolute values of the satellite PI CS which are about four times larger than the experimental ones.

To understand the reason of this discrepancy in the present work we took into account the interaction between autoionization channels which in general is considered as a small one [4]. The atomic and ionic wave functions involved in the calculation were computed within the configuration interaction Pauli-Fock approach. It turned to be that autoionization channels $4p^4 n\ell\varepsilon\ell'$ interact surprisingly strong because of the large overlap of atomic orbitals entering the matrix element for the configuration interaction. As a consequence of strong interchannel interaction the channel wave functions are renormalized. This gives rise to substantial decrease of the satellite PI CS by a factor from 3 to 5 thus explaining the above discrepancy between theory and experiment.

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B-16

Investigation of electron impact induced transitions between excited lithium levels.

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Results of measurements of rate constants for transitions starting from 2P level of lithium induced by electron impact are presented. The investigations were done by the method described in [1]. Measurements were performed in heat – pipe oven containing the mixture of sodium and lithium vapours with several torrs of argon as a buffer gas.

The plasma was generated by a pulse from laser tuned to the 3S – 3P transition in sodium (589nm) [2]. After 2 μs, when the parameters of plasma were stabilized a pulse of other laser, tuned to 2S – 2P transition in lithium (670nm), produced Li(2P) atoms. Due to collisions of Li(2P) atoms with electrons the higher excited Li(nl) atoms were produced. The fluorescence from those atoms was used for monitoring the Li(nl) concentration. The fluorescence signal was integrated within a time period of 2 μs by means of the photon counting system. The k_{2P-nl} rate constant was determined in respect to the well known k_{2S-2S} rate [3,4].

The electron energy distribution and the electron temperature were retrieved from the voltage – current characteristic of the plasma probe.

Results of measurements for the 2P – 3P transition are presented in Fig. 1. The experimental error reaches about 40%. Uncertainty of the electron temperature determination is about ±10% The experimental data (circles) are compared with calculations based on close coupling approximation (solid line), done by I. Bray [3] especially for this experiment. Dashed line represents results achieved using formulas by Schweinzer et al [4].

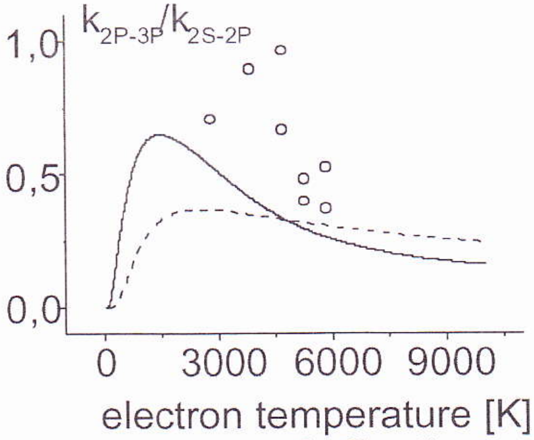

Figure 1: Rate constant for 2P – 3P trnsition.

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B-17

ELECTRON-PHOTON COINCIDENCE MEASUREMENTS OF POLARIZATION OF RADIATION FROM CADMIUM ATOMS EXCITED TO 5 $^1P_1$ STATE BY ELECTRON IMPACT

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The electron-photon coincidence technique has been used to determine the state of polarization of 228.8 nm radiation emitted by cadmium atoms excited to 5 $^1P_1$ state by electron impact. Data have been obtained for two values of electron energy and scattering angles in the range from 10° to 40°. Reduced Stokes parameters and electron impact coherence parameters (EICP), characterizing the state of the excited atoms immediately after the collision, have been extracted from the measurements and compared with results of relativistic distorted-wave approximation calculations. Theoretical predictions are in good qualitative agreement with experimental values.

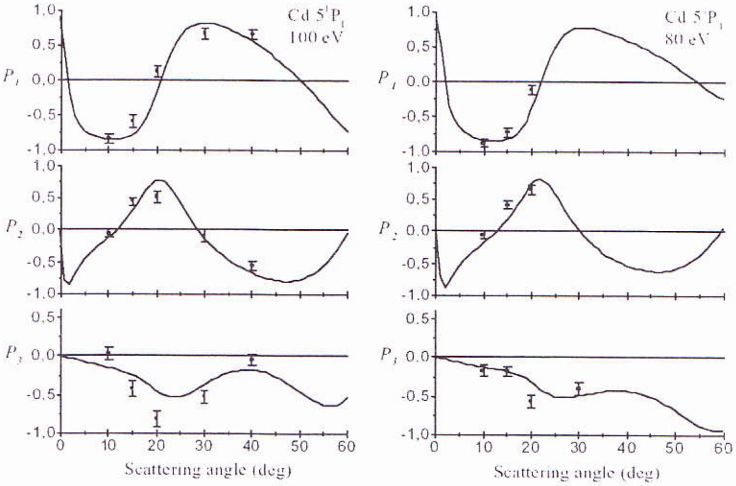

Figure 1. Experimental (■) and theoretical (——) values of polarization parameters for electron impact excitation of 5 $^1P_1$ state of cadmium atoms for incident electron energy of 100 eV (left column) and 80 eV (right column). Depolarizing effects of hyperfine interactions were taken into account in RDWA calculations.

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B-18

Electron-helium scattering within the S-wave model

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Abstract

There has been much progress in the solution of the three-body problem that is electron-impact excitation of atomic hydrogen. Hence, the next frontier in the field is the four-body problem of electron-impact excitation of helium. Interestingly, since the helium discrete spectrum contains only one-electron excitations, a frozen-core description of the target suffices for discrete excitation phenomena and ionisation leaving the helium ion in the ground state. However, ionisation processes may also leave the helium ion in an excited state, and double ionisation processes are also possible. To treat these the full four-body problem needs to be solved. We will report the first attempts to solve this problem non-perturbatively while restricting all orbital angular momenta to be zero, the socalled S-wave model.

B-19

LOW-ENERGY ELECTRON SPECTROSCOPY OF Si(100) AND Ge(100) SURFACES

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In the majority of the electron-spectroscopic methods of investigation of electronic properties of surface and bulk of solids probing is performed by photons or electrons with the energy E>100 eV, for which optical selection rules and energy and momentum conservation laws are valid. In the Institute of Electron Physics of Ukrainian National Academy of Sciences the technique of low-energy electron backscattering (LEEB) is elaborated, where probing is carried out with the beam of 0–10-eV electrons. At such energies the optical selection rules break down. Therefore in elastic and inelastic LEEB spectra both direct and indirect transitions of excited electrons between the maxima of density of electron states in the reduced Brillouin zone are revealed. Besides, the LEEB spectra provide data on electron surface states.

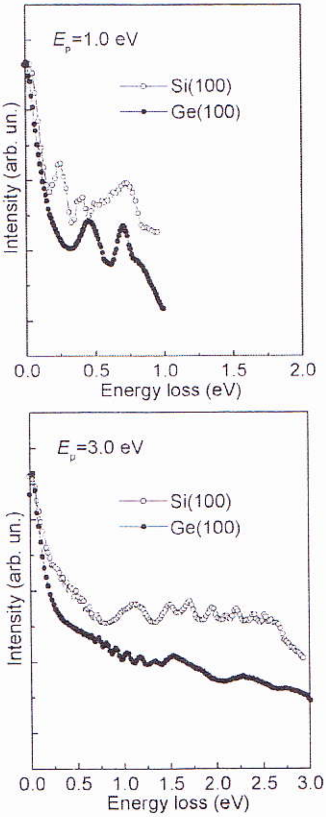

Fig. 1

Using high-resolution ($\Delta E \leq 50$ meV) LEEB technique, the studies of energy loss spectra at various energies of primary electron beam (E_p=0.1÷3 eV) for the mirror-polished Si(100) and Ge(100) surfaces were performed. The resonant character of excitation of surface and bulk electron states for the surfaces under investigation is shown – the energy loss spectra is very sensititve to E_p.

Figure 1 shows typical energy loss spectra at E_p=1.0 eV and E_p=3.0 eV for Si (100) and Ge(100).

The obtained results on the bulk electron states are in good agreement with the known experimental data, obtained by photoemission spectroscopy and characteristic loss spectroscopy techniques as well as bulk electron structure of silicon and germanium, calculated theoretically using the orthogonalized plane wave, local potential and *GWA* methods.

The presence of the known surface electron states for Si(100) and Ge(100) is confirmed, their energy position being determined more precisely. Besides, for Ge(100) a new surface electron state in the gap with the density maximum at the energy 0.18 eV above the valence band maximum is revealed.

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Multiterminal measurements as a method to determine the resistivity components in highly anisotropic media

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The resistivity and its dependence from temperature is one of the common characteristic of the solids. In case of isotropic materials a four-terminals method is commonly-used to determine it. The layered crystals (colossal magnetoresistance manganites, high temperature superconductors, etc) are available mostly in the form of thin platelets. That is why the determination of the smallest dimension's resistivity component is a difficult task.

The object of our investigation are materials with high uniaxial resistivity anisotropy ($\rho_c \gg \rho_{ab}$). We present a method for determining the resistivity tensor from a six-contacts measurement, based on analytical solutions of the Laplace's equation. To avoid measuring of vanishing voltages on the bottom of the sample the c-axis and diagonal current injections are used. The condition of the applicability of our method is high effective anisotropy ($\Gamma = \exp\left[\gamma \frac{\pi D}{L}\right] >> 1$), where $\gamma = \sqrt{\frac{\rho_c}{\rho_{ab}}}$ - is the resistivity anisotropy, L and D are the length and thickness of the sample.

Using this method allows us to measure only one sample instead of two. That could be important in case when reproducibility of samples properties is bad, even in the same batch due to somewhat different concentration of impurities or dopants. We take into account the influence of size of the current contacts and their misalignment to make the method more useful for experimental use. The rapid calculation of the tensor components and the increase of the accuracy are advantages of our analytical solution with respect to numerical calculations.

In addition, using of different current injections (i.e. diagonal and ab-plane) in same time could be the method to determinate the quality of contacts and the homogeneity of the sample.

B-21

Dynamic Hyperpolarizability of Hydrogen Rydberg Levels

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The dynamic hyperpolarizability (DHP), $\gamma(-\omega;\omega,-\omega,\omega)$, determines the atomic response to a monochromatic external perturbation (of frequency ω) in the 3rd order in the perturbation amplitude, F. Applied to atomic spectra, γ gives corrections $\Delta E_i^{(4)} \sim \gamma I^2$ to the usual (linear in the laser intensity, I) Stark-effect, $\Delta E_i^{(2)} \sim \alpha(\omega)I$, of a (non-degenerate) atomic level $|E_i\rangle$. For $|E_i| > \hbar\omega \geq |E_i|/2$, $\operatorname{Im}\Delta E_i^{(4)}$ yields the two-photon ionization rate of the $|E_i\rangle$-state, whereas for $\hbar\omega \geq |E_i|$ it gives also the linear in laser intensity corrections to the photoionization cross section (given by the imaginary part of the dynamic polarizability $\alpha(\omega)$).

We present exact numerical results for the DHP γ_{nlm} of high-lying H-states $|nlm\rangle$ as well as for the perturbation of $|nm\rangle$-levels by a laser field taking into account the terms $\sim I$ and I^2. Since even $\sim I$-terms mix degenerate l-levels of the same parity [1], we evaluate $\sim I^2$-terms by calculating "generalized" DHPs for these mixed levels. In calculations of 4th-order dipole matrix elements, contributing to the perturbation theory expression for γ, we employ an effective method based on generalized Sturmian expansion of the Coulomb Green's function [2] having two arbitrary parameters, β and β'. After explicit integration over radial variables, γ is presented as a double series of hypergeometric functions. By an appropriate choice of β and β', the convergence of this series is achieved for any frequency ω, including in the above-threshold domain, $\hbar\omega \gg |E_n|$.

For $n \leq 10$ and linear and circular laser polarizations, we performed numerical calculations of γ and $\Delta E_{nm}^{(2)}$ and $\Delta E_{nm}^{(4)}$ (taking into account l-mixing) over a wide interval of frequencies, from $\hbar\omega < |E_n|$ up to $\hbar\omega \sim 20|E_n|$. In the high-frequency limit, a part of the mixed levels clearly shows the onset of stabilization with increasing the laser amplitude F. (See Table 1 for mixed states of the $n = 5$ shell with $m = 0$ in a linearly-polarized field.) The asymptotic behavior of γ at high ω and its dependence on quantum numbers n, l, m and laser polarization are discussed.

Partial support by RFBR Grant 00-02-17843 and NSF Grant PHY-0070980 is acknowledged.

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Table 1: $\Delta E^{(2)}$ and $\Delta E^{(4)}$ (in au) for $n = 5$, $m = 0$, $\hbar\omega = 4|E_n|$, $F = 0.02$ au.

Parity	$\Delta E^{(2)}$	$\Delta E^{(4)}$	$\Delta E^{(2)} + \Delta E^{(4)}$
even	$(1.7728 - 0.0741i)10^{-2}$	$(1.3900 + 0.3680i)10^{-3}$	$(1.9118 - 0.0373i)10^{-2}$
odd	$(1.7617 - 0.1324i)10^{-2}$	$(8.149 + 2.440i)10^{-4}$	$(1.8432 - 0.1080i)10^{-2}$
even	$(1.5926 - 0.1206i)10^{-2}$	$(1.878 - 1.688i)10^{-4}$	$(1.6114 - 0.1374i)10^{-2}$
even	$(1.5522 - 0.0019i)10^{-2}$	$(-1.97 - 2.86i)10^{-6}$	$(1.5520 - 0.0022i)10^{-2}$
odd	$(1.5235 - 0.0178i)10^{-2}$	$(-2.095 - 0.809i)10^{-4}$	$(1.5025 - 0.0259i)10^{-2}$

Temperature dependencies of dissociative electron attachment to molecules of Gentisic acid, Hydroquinone and p-Benzoquinone

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The temperature dependencies of dissociative electron attachment (DA) by molecule of Gentisic acid (GA) which is one of the excellent matrix in MALDI (Matrix-Assisted Laser Desorption/Ionization) are investigated by means of Electron Capture Negative Ion Mass Spectrometry with purpose to light a problem of anions formation in MALDI. In according to our findings the negative ion mass spectrum of GA at low temperature consists of the next most intensive peaks $[M-H]^-$ (M/Z = 153, 100%), $[M-H_2]^-$ (M/Z = 152, 35%), $[M-COOH]^-$ (M/Z = 109, 14%) and $[M-CO_2-H_2]^-$ (M/Z = 108, 15%). Also there is a metastable anion due to a process $[M-H]^- \rightarrow [M-COOH]^-$ that means the dissociation lifetime of $[M-H]^-$ parent anion is about 10 μs. It is well seen on Fig.1[a] that there is a strong increasing of $[M-CO_2-H_2]^-$ anion yield as temperature of target molecule rising. Such a behavior of the threshold signal is not the condition of decomposition of the GA molecule at high temperature because there is still exists a $[M-H]^-$ anion signal at such temperature. Moreover molecules of Hydroquinone (HQ) and p-Benzoquinone (p-BQ) do not show such a threshold feature on the corresponding anions yield even at high temperatures (Fig.1[b, c]). Thus we suppose that threshold peak for $[M-CO_2-H_2]^-$ anion channel in GA is a pseudomolecular anion with a structure of p-BQ. Obtained experimental results are interpreted by means of quantum chemical calculations in terms of two-dimensional potential energy curves. This work is supported by INTAS grant #99-00647.

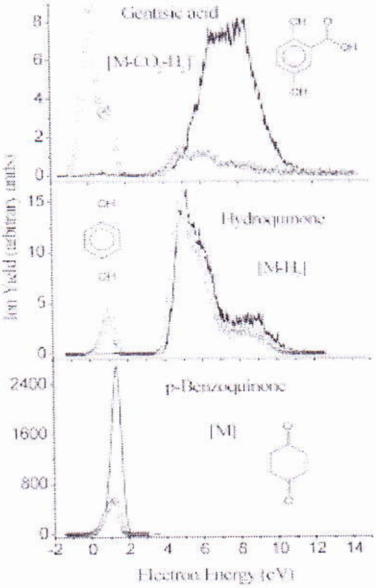

Fig.1. Anion yield for M/Z = 108, 80 °C (solid line), 300 °C (open circles)

B-23

SPIN ASYMMETRY IN (e, 2e) PROCESSES ON Li, Be$^+$, B^{+2} AND C^{+3} TARGETS BY TRANSVERSELY POLARISED ELECTRONS

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We present in this communication the results of our calculation of triple differential cross section and spin asymmetry in electron impact ionization cross section of lithium like ions (Li, Be$^+$, B^{+2} and C^{+3}) at an incident electron energy 49 eV above ionisation potential for equal as well as unequal energy sharing conditions. We have performed the calculation using distorted wave Born approximation (DWBA) formalism [1]. We also present our calculation of spin asymmetry for the same targets with energy sharing ratio and compare the spin asymmetry for Li atom with the available experimental data of Streun et al [2]. We discuss the role of exchange effect in producing spin asymmetry and the effect of Z on TDCS and spin asymmetry for lithium like ions.

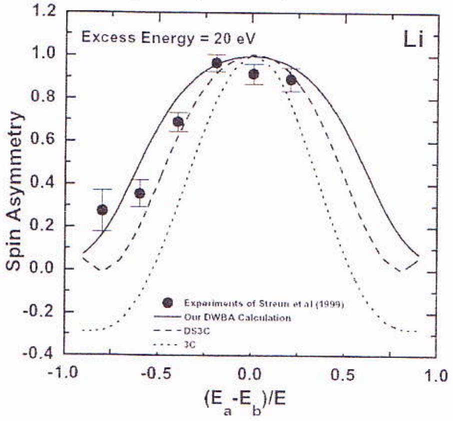

Figure: Spin asymmetry for the electron impact ionisation of Li as a function of the energy sharing ratio $(E_a-E_b)/E$, where E_a and E_b are the energies of the continuum electrons and $E=E_a+E_b=20$ eV, is the excess energy. Symbols (·): experimental data of Streun et al [2], (-----) DS3C, (·······) 3C and (——) our DWBA calculation.

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B-24

Ion-impact induced excitation and fragmentation of C_{60}

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We studied the multiple ionization, C_2 evaporation, fission, and multi-fragmentation of C_{60} in collisions with 50–300 keV H^+, He^+, Ne^+, and 6.5–300 keV·z Ar^{z+} (z =1-3) ions [1, 2]. The influence of projectile type and velocity on relative cross sections will be discussed. As an example Fig. 1 shows some results obtained in collisions with Ar-ions. At impact velocities $v \gtrsim 0.2$ a.u. the influence of the projectile velocity on the fragmentation pattern is comparatively small, whereas dramatic changes occur at smaller velocities [3]. This finding is comprehensible with recently published data for the energy loss of Ar-ions in collisions with C_{60} obtained with non-adiabatic quantum molecular dynamics calculations [4].

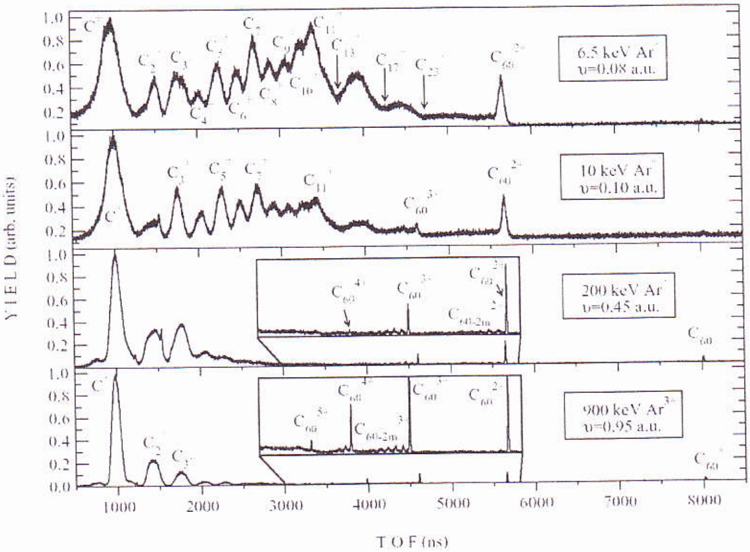

Figure 1: Time-of-flight (TOF) spectra of fragment ions produced in collisions of Ar^{z+} ions with C_{60}.

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B-25

SOME PROPOSALS FOR LASERS ON SELF-TERMINATING TRANSITIONS IN BLUE SPECTRAL RANGE

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In the combination with the Cu-vapor laser in green and Au-vapor laser in red an effective blue laser on self-terminating transition can be useful to elaborate the color projection systems with brightness amplifiers of images. But the Bi-vapor and Fe-vapor blue lasers tested till now do not satisfy the average power and efficiency requirements.

An indium atom has an appropriate energy level structure with self-terminating transition 451.1 nm that origin from an isolated resonance $6^2S_{1/2}$ level to the $5^2P_{3/2}$ metastable level. The quantum efficiency of this transition is more than 90%. But a small energy distance between the ground and metastable levels (0.274 eV) makes it impossible to use pure indium metal probe as a lasant.

In our investigations aimed to search for the laser action on indium atom an InI salt was used. The time integrated emission spectra of discharge excited by high voltage discharge (Fig.1) demonstrate the main feature – dominating intensity of indium atom emissions. A →X and B →X molecular emissions of InI have also been observed. In the absorption spectra the X – A, X – B and X – C bands are observed. The resonance indium line 410.2 nm lies in the region of X – A transition absorption band.

Unfortunately, no laser action was obtained in spite of a great variety of experimental conditions used. Especially the pulse frequency was established in three different regimes: 100 Hz, 3-10 kHz and pulse sequences (series of 10-20 pulses with interpulse distance 100 μs repeated with 10 Hz).

The largest intensity of indium lines was observed at 300 °C tube temperature. The additional efforts might be undertaken to use another indium chemical compound ($InBr_3$) with lower working temperature (not more than 200 °C) and to shortening the pumping pulse duration.

Another element is also proposed for the same purpose having some self-terminating transitions in blue, especially 431.5, 472.3 and 471.0 nm - the titanium one. Experiments with laser vaporization of Ti metal and subsequent excitation by discharge are prepared.

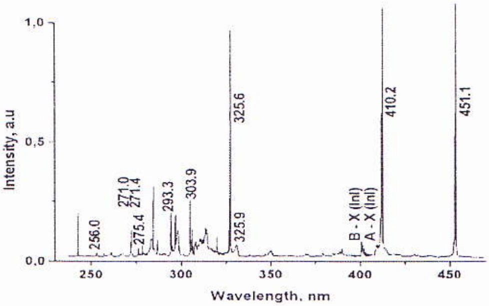

Fig. 1. The emission spectrum of the InI - Ne discharge (p_{Ne} = 2 mm Hg, f = 4.7 kHz, t = 370 °C).

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B-26

CLUSTER EXPLOSION IN AN INTENSE LASER PULSE

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Due to collective many-body effects the laser interaction with the atomic clusters differs substantially from that of simple atomic and molecular systems. For instance, recent experiments on clusters irradiated by the intense laser pulses have revealed several extremely high energetic phenomena not encountered in previous experiments restricted to atoms and small molecules: efficient generation of highly-charged atomic ions, generation of electrons and ions with MeV kinetic energies, and emission of intense X-rays [1]. In this paper, the dynamics of small rare-gas atomic clusters ionized by a high-intensity femtosecond laser pulse is studied qualitatively using a three-dimensional refinement [3] of the time-dependent Thomas-Fermi model [2]. It is confirmed that the explosion is neither instantaneous nor uniform. It exhibits a layer-like structure in which shells of cluster ions are expelled sequentially. It seems that the inner shells of the cluster start to expand first and "push" the outer shells. Stepwise character of the explosion is seen also in the kinetic energy of the outgoing atomic ion fragments: the ions leaving first were far more energetic than those leaving later. The role of hot electron dynamics in the cluster explosion at the initial stages is also investigated. It turna out that ions coming from the outer shells of the cluster are indeed a little bit accelerated by thermal expansion of the electron gas. On the other hand the thermal expansion of the electron gas causes the electrons to leave rapidly the innards of the cluster. This slows down the rate of the space-charge ionization inside the cluster and thus the Coulomb explosion of the inner shells is decelerated. Contrary to the previous believes it seems that the hydrodynamic explosion scenario is important for most energetic ions only. The expansion of slower ions from inner shells is governed mainly by the Coulomb forces. The model used was also checked to give correct quantitative predictions in the case of small argon clusters.
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B-27

ATTOSECOND PHASE CONTROL OF MOLECULAR WAVE PACKETS

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The temporal coherent control using a pair of femtosecond (fs) laser pulses is employed to manipulate molecular wave packets (WPs) created on the *A* state of HgAr molecules [1]. The laser pulse (center wavelength 254.4 nm, time duration 300fs) induces the $(A\,^30^+,\ v) \leftarrow (X\,^10^+,\ v=0)$ transition and a WP is generated on the *A* state. The WP is a superposition of the vibrational eigenfunctions (v=3, 4 and 5), oscillates with a period $T_{VIB} \approx 1$ps. The two WPs, generated by the pulse pair, interact constructively or destructively depending on the phase difference given by the inter-pulse-delay τ. The WP interaction results in a modulation of the *A* state population. We have achieved 5attoseconds (as) or higher resolution in tuning τ and observed almost 100% modulation depth of the individual vibrational populations. The modulations appear in harmony with the laser field oscillation cycle $(2\pi/\omega_L) \approx$ 848as.

Figure 1 is obtained by numerical integration of the time-dependent Schrodinger equation for the HgAr in the field of the double-pulse laser. The modulation in the probability density with the delay time tuning is shown for the vibrational levels v=3, 4 and 5 in regions $\tau \approx 1.5\,T_{VIB}$ and $\tau \approx 2\,T_{VIB}$. The modulation curves are quite different between the two regions of τ. For $\tau \approx 1.5\,T_{VIB}$, two WPs crosses with relatively weak interaction each other. In this case, phase of the modulation for v=3 differs by π from the one for v=4. This suggests a possibility of the rotational quantum operation by means of the double-pulse phase control. For the delays $\tau \approx 2\,T_{VIB}$, two WPs overlaps well and interfere significantly each other to results in asymmetric Beutlar-Fano type modulation profiles. This is a time-domain version of inter-channel interaction.

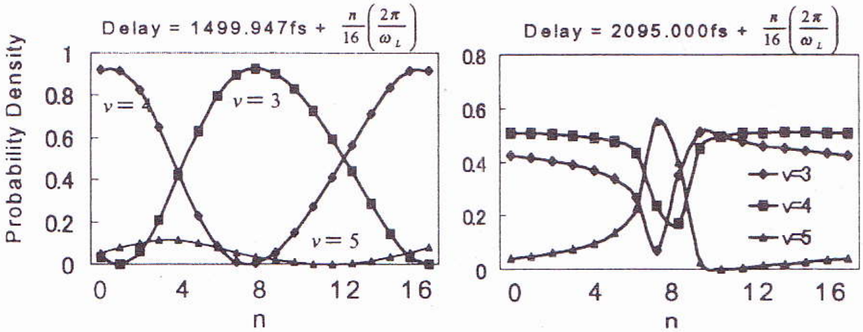

Fig. 1 Delay time dependence of the probability density of the *A*-state vibrational levels.

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B-28

HIGH RESOLUTION STUDY OF DISSOCIATIVE ELECTRON ATTACHMENT TO CH_2Br_2 AND CCl_3Br

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Using two different experimental setups with mass spectrometric ion detection, we have investigated dissociative electron attachment $e^-(E) + XY \rightarrow X + Y^-$ (DA, short notation Y^-/XY) to the two dipolar molecules CH_2Br_2 and CCl_3Br. Relative DA cross sections from 0 eV to about 2 eV were measured with a magnetically-guided electron beam (energy width around 70 meV) and, using the laser photoelectron attachment (LPA) method [1,2], with very high resolution (energy width ≤ 1 meV) over the electron energy range $0.2 \leq E/\text{meV} \leq 172$. With reference to thermal attachment rate coefficients [3,4] absolute DA cross sections $\sigma_e(E)$ have been derived from the combined experimental data for the processes Br^-/CH_2Br_2, Br^-/CCl_3Br and Cl^-/CCl_3Br. At thresholds for vibrational excitation of the CH_2Br_2 molecule, the DA cross section exhibits pronounced structure due to coupling of the attachment process with scattering channels; below the $\nu_3 = 1$ onset for the CBr stretch vibration, a clear vibrational Feshbach resonance is observed. At low energies, the cross sections $\sigma_e(E)$ show an energy dependence between $E^{-1/2}$ and E^{-1}, in essential agreement with predictions of an extended Vogt-Wannier (EVW) capture model [5] which includes the long-range electron-dipole interaction in addition to the polarization force. The measured absolute values are, however, substantially smaller than those predicted by the EVW model. Comparisons are made with cross sections and rate coefficients obtained in previous photoelectron attachment work and in electron beam and swarm experiments. Based on our joint experimental results for $\sigma_e(E)$, we calculate and report the electron temperature dependence of the rate coefficients $k_e(T_e)$ for free electron attachment involving a Maxwellian electron ensemble and a gas at room temperature ($T_G = 300$ K).

This work has been supported by the *Deutsche Forschungsgemeinschaft* and by the *Zentrum für Lasermesstechnik und Diagnostik (Universität Kaiserslautern)*.

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B-29

EFFECTIVE ELECTRON SCATTERING CROSS SECTIONS FOR ZINC ATOMS

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Collisions of electrons with Zn atoms have been studied in many experimental and theoretical papers. Nevertheless, no data are available up to date on the effective elastic electron scattering cross sections, and excitation cross sections for lower (including metastable) levels. This is due to a number of reasons, one of which being the problem of absolute calibration of measured relative scattering cross sections.

Here we report on the absolute elastic electron scattering cross sections and excitation cross sections for the 4^3P_{012} - and 4^1P_1 - levels in Zn atom as well as their energy dependences within the 0-10 eV energy range.

The experiments were carried out by a crossed electron and atomic beams technique with the use of a hypocycloidal electron spectrometer (HEM) and a multichannel effusion atomic beam source. A detailed description of HEM design is given elsewhere[1]. It comprises two serially mounted hypocycloidal energy analyzers, first being an electron monochromator and the second – an inelastically scattered electron analyzer. The elastically scattered electrons were detected by the walls of the collision chamber, on entrance and exit of which the diaphragms were placed with the applied potential close to that of cathode providing a barrier for inelastically scattered electrons as well as for the electrons scattered elastically at the angles exceeding a certain minimal one.

Besides the measurements of elastic and inelastic electron scattering we have studied the ionization function for Zn atom close to the threshold. The ions produced were detected by an electrode mounted normally to the atomic beam direction. A special attention was given to the selection of the potentials at this electrode in order to minimize its influence on the electron motion in the collision region. A constant geometry of experiment and the constant sensitivity of the detection unit have allowed the total electron scattering cross sections and excitation functions for lower levels to be normalized to the absolute values of the single-ionization cross section for Zn atom[2]. A typical electron energy spread was 0.15 eV at the incident electron beam current of 10^{-8}A.

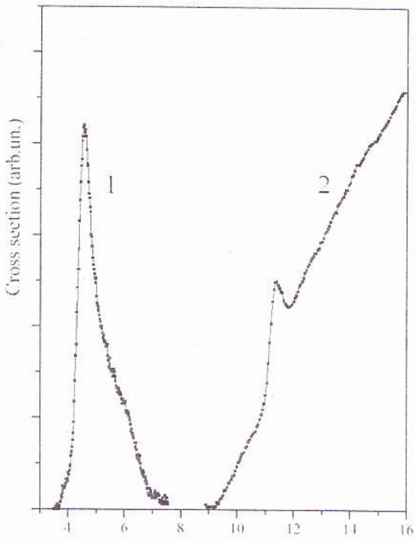

Figure 1. The relative excitation cross section for the 4^3P_{012}-level of the Zn atom (curve 1) and the ionization efficiency (curve 2).

Figure 1 shows the energy dependence of the relative electron excitation cross section for the $4^3P_{0,1,2}$-level of the Zn atom (curve 1) and the ionization efficiency (curve 2). The energy dependences of the elastic cross section and the excitation cross section of the 4^1P_1 state of Zn will be presented at the conference.

The research described in this publication was made in part under Award No UP2-2118 of the CRDF.

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B-30

ELECTRON EXCITATION OF MERCURY ATOM SPECTRAL LINES AT meV RESOLUTION

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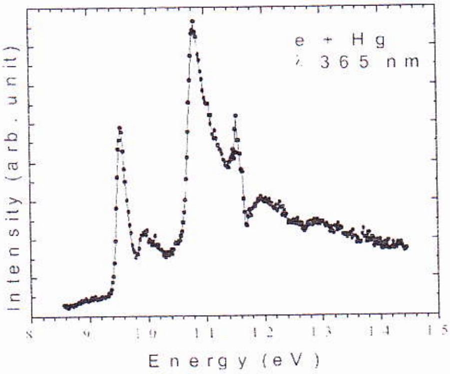
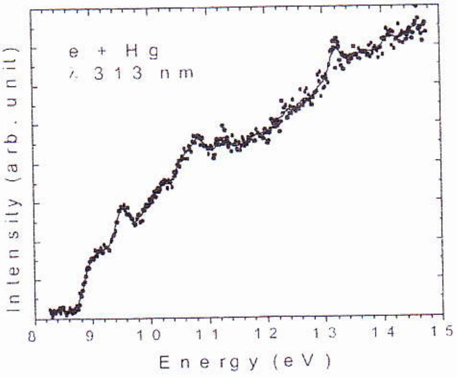
Up to date, rather large number of works devoted to the electron-impact excitation of Hg atoms is available [1], the energy resolution of incident electrons being ≥ 100 meV. We have modified a hypocycloidal electron monochromator (HEM) [2] to produce an electron beam of ~(10-70) meV energy spread. The experimental apparatus developed on the basis of HEM is automated by means on an IBM PC. HEM is connected to the collision cell filled with Hg vapors. Optical emission was detected by a photomultiplier operating in the photoelectron counting mode. Experiment controlling program allows all the HEM mode to be studied, as well as the photoelectron signal, electron beam parameters to be detected and results to be primarily processed.

Figures illustrate the measured total excitation functions (EFs) for Hg atom spectral lines - the unseparated $6^3D_{3,2}$ - 6^3P_2 ($\lambda \approx 365$ nm) and ($6^3D_{2,1}$ - 6^3P_1)+(6^1D_2 - 6^3P_1) ($\lambda \approx 313$ nm) transitions. Electron energy spread was 40 and 60 meV, respectively, and the energy step was 20 meV.

The analysis of the results of measurements has shown a good agreement between our EFs for the $6^3D_{3,2}$ - 6^3P_2 transitions (revealing more reach structure) with those of one of the authors [3] obtained at the ~100 meV energy resolution. Of special interest is the fact that our EFs measured for the same initial levels have completely different character. Worthy of notice is good coincidence of the energy positions of 12 features in the measured EFs. The origin of the above features will be discussed at the conference.





This investigation was supported by the CRDF grant UP2-2118/6435.

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B-31

The polarization model for valence-core correlation in molecules

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The valence-core correlation is difficult to calculate because of roughly equal contributions made by a very large number of virtual core excitations [1]. Nevertheless, the dependence of the valence-other-core correlation on internuclear separation can be critically important to the shape of molecular potential surfaces, particularly when heavy atoms are involved. We propose an extension to polyatomic molecules of the simple polarization model used successfully in electron-atom calculations [2].

The valence-self core correlation is given by term

$$-\frac{1}{2}\alpha_c < \varphi_c|\mathbf{E}_c|\varphi_c >,$$

where α_c is the dipole polarizability of the atom c, φ_a is the n_c-electron wavefunction and $\mathbf{E}_c$ is the electric field due to all valence electrons and other charged cores, appropriately averaged over the distribution of c. The above term is independent on the internuclear separation, so it could be accounted for adjusting of asymptotic energies. In atomic units the electric field at c can be written as

$$\mathbf{E}_c = \sum_n \frac{\mathbf{r}_n}{r_n^3} \mathrm{X}(r_n),$$

where $\mathrm{X}(r)$ is the cut-off function. A simple way to extract model polarization parameters is to average the energy adjustment of a given triple state with that of corresponding singlet

$$\frac{1}{2}[< \varphi_c^{(+)}|v + w|\varphi_c^{(+)} > + < \varphi_c^{(-)}|v + w|\varphi_c^{(-)} >] = \sum_n < \psi_n|v_1|\psi_n >,$$

in which $\varphi_c^{(+)}$ and $\varphi_c^{(-)}$ are the singlet and triplet wavefunctions, respectively, v and w are one- and two-electron (dielectric) terms of the valence-self core interaction ($-\frac{1}{2}\alpha_c\mathbf{E}_c^2 \equiv v + w$), ψ_n is the one electron atomic orbital centered on c. The one-electron term can be written as

$$v = \sum_n v_n = -\frac{1}{2}\alpha_c \sum_n r_n^{-4}\mathrm{X}^2(r_n).$$

The emphasis here is on practical techniques which allow application of the model as a first-order perturbation in the final stage of a CI computation with gaussian-type orbitals. The model is being applied to the diatomic molecules.

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B-32

Critical minima in elastic scattering of electrons from Ar and Zn

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Ab initio relativistic calculations have been carried out to search for minima in the angle and energy differential cross sections for the elastic scattering of electrons from argon [1] and zinc [2] (fig. 1). Comparison is made with the recent experiments [3] and previous computations.

The position of the minima depends very sensitively on the theoretical method which is used for description. A proper treatment of the exchange potential of the incident electron with the bound-state density and a rather careful choice of the target polarization potential is required. A precise knowledge of the *critical* minima is also important to the region with the highest degree of spin polarization of the scattered electrons. Our relativistic approach allows both to compute the minima of the angle and energy differential cross sections as well as the degree of spin polarization. The precise measurement of the minimum position is difficult since it requires a very good angular and energetic resolution. We hope that our results will be attractive from an experimental point of view since they allow to focus further experimental effort on certain local areas.

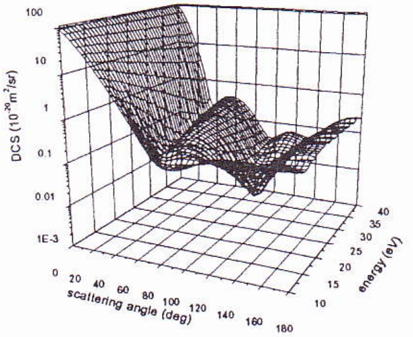

Figure 1: Three-dimensional plot of the differential cross section for elastic electron scattering from zinc.

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B-33

EXCITATION CROSS SECTIONS FOR SrII SPECTRAL LINES EXCITED FROM ATOMIC METASTABLE STATES BY ELECTRON IMPACT

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Here we report on the experimental data on electron interaction with metastable strontium atoms providing absolute excitation functions for low-lying spectral lines of single-charged ion. Experiments were carried out by an optical method with the use of crossed beams of the metastable Sr atoms (with the $\sim 5 \cdot 10^9$ cm^{-3} concentration) and monoenergetic electrons. The absolute cross section determination accuracy was 60%. The experimental technique and method are described in detail elsewhere [1].

Table shows the absolute cross sections for the four spectral transitions in SrII (at the 15 eV electron energy) normalized to that for the $\lambda = 481.1$ nm line excited from the metastable state measured by us experimentally (a) and calculated theoretically [2] (b), as well as to the excitation cross sections for the same transitions excited from the ground atomic states measured in [3] (c) and [4] (d).

Transition,	λ (nm)	Q_{15}, 10^{-17}, cm^2			
$5^2S_{1/2} - 5^2P_{3/2}$	407.6	10^{a}	42^{b}	20^{c}	26^{d}
$5^2S_{1/2} - 5^2P_{1/2}$	421.5	4^{a}	17^{b}	9^{c}	13.5^{d}
$5^2P_{3/2} - 6^2S_{1/2}$	430.5	1.4^{a}	6^{b}	4.5^{c}	—
$5^2P_{1/2} - 6^2S_{1/2}$	416.1	0.6^{a}	2.5^{b}	1.3^{c}	—

It is seen that the cross sections differ by several times and this is rather difficult to be explained at the moment. Nevertheless, note the following. The ionization cross section out of the metastable states for Sr atom at 15 eV is $\sim 2 \cdot 10^{-15}$ cm^2 [5]. The sum of the excitation cross sections for lower ionic spectral lines measured by us is $\sim 2 \cdot 10^{-16}$ cm^2, and this corresponds to ~ 10% of total ionization cross section, while for Mg atom that value reaches 30% [1]. However, this is quite consistent, since the strontium ion has the metastable ^{2}D-state lying below those studied by us, and, therefore, the part of ions is produced just in these states, the decay of which via the optical channel is forbidden (in magnesium ion the similar state lies above the resonance levels).

If one takes the cross sections obtained by other authors as the reference ones, the above contribution reaches 25–35% (see table), that, in our opinion, is less probable for the Sr$^+$ ion (in accordance with mentioned above). The behavior of the energy dependences of excitation cross sections will be discussed at the conference.

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B-34

MASS-SPECTROMETRIC STUDIES OF C_3D_7NO MOLECULE IONIZATION BY ELECTRON IMPACT

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Present paper is a continuation of a series of our previous studies on the production of ionized fragments resulted from electron-impact ionization and dissociative ionization of complex molecules containing isotope-differing species. Recently we have measured the energy dependences of ionization cross sections for benzene (C_6H_6, C_6HD_5) and pyridine (C_5H_5N, C_5D_5N) molecules with a special emphasis having been given to determination of appearance energies of dissociative ionization products [1,2].

Experiments were carried out by using a set-up with a quadrupole mass analyzer providing the ±1 a.m.u. mass and ±500 meV energy resolution. The beam of molecules under study was produced by a multichannel effusion source operating in high-vacuum ($\sim 10^{-7}$ Torr) conditions. The electron energy was scanned in a stepwise mode with the 0.13–1.26 eV step. The final energy dependences of ionization and dissociative ionization cross sections were processed by using the SIGMAPLOT software package allowing the initial areas of ionization curves to be fitted using the least-square method. Electron energy scale was calibrated against known ionization threshold for reference Ar and Kr atoms providing the calibration accuracy not worse than ±500 meV.

Fig. 1 shows the mass spectrum of the C_3D_7NO molecule fragments, while fig. 2 presents the ionization cross section for the parent C_3D_7NO molecule vs the incident electron energy. The lack of the data in literature, unfortunately, makes impossible direct comparison of our results with any available data obtained by other authors. The discussion of the results will be presented at the Conference.

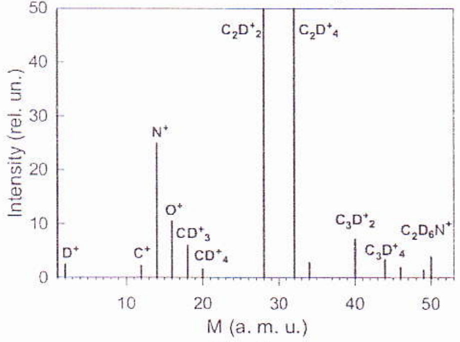

Fig. 1

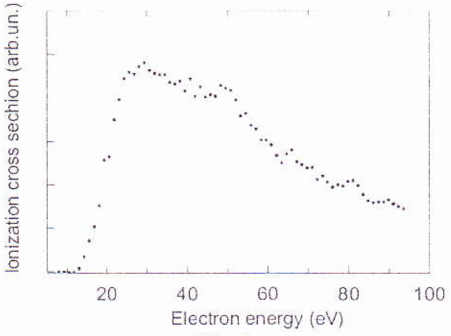

Fig.2

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B-35

LONGITUDINAL SPIN ASYMMETRY IN (e, 2e) PROCESSES ON ATOMS BY RELATIVISTIC ELECTRONS

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The investigation of (e, 2e) processes on atoms by spin-polarized electrons offers a sensitive tool for stringent test of theories by probing different physical mechanisms like exchange scattering, spin-orbit coupling of both bound and continuum state, orbital orientation and alignment etc. as well as their interplay. In recent years extensive theoretical and experimental investigations of the (e, 2e) processes on atoms by transversely polarized relativistic electron beam have been performed [1]. Bhullar and Sud [2] have computed and demonstrated longitudinal spin asymmetry in triple differential K-shell ionization of atoms by longitudinally polarized relativistic electrons. In this talk we will present the results of longitudinal spin asymmetry in (e, 2e) process on atoms computed in one photon exchange approximation. We will also discuss the dependence of the longitudinal spin asymmetry on atomic number of the target and incident electron energy. Finally we will discuss the role of interplay of longitudinal and transverse interaction between the two active electrons on the asymmetry in (e, 2e) processes by transverse as well as longitudinally polarized relativistic electrons.

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B-36

Theory for coherent control of quantum system dynamics

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We have developed a general coherent control theory for manipulating quantum system dynamics. For designing the external control field, we introduce the performance index defined as $y(t) = y(\langle\hat{O}_1(t)\rangle, \langle\hat{O}_2(t)\rangle, \cdots, \langle\hat{O}_N(t)\rangle)$ where $\langle\hat{O}_i(t)\rangle (i = 1, 2, \cdots, N)$ denotes the expectation value of the i-th observable. Here, $y(t)$ indicates how well the current state satisfies the desired physical property. By differentiating $y(t)$ with respect to t, and considering the the Schrödinger equation we formally obtain $\dot{y}(t)$ as

$$\frac{dy(t)}{dt} = \sum_{i}^{N} \frac{\partial y(t)}{\partial \langle O_i(t)\rangle} \left(\left\langle \frac{d\hat{O}_i(t)}{dt} - i[\hat{O}_i(t), H_0] \right\rangle + 2\mathrm{Im}\langle \hat{O}_i(t)\hat{V}\rangle\, u(t) \right), \qquad (1)$$

where $\hat{H}_0$ and $\hat{V}$ denote the system Hamiltonian and the system-field interaction operator. Here, we enforce the operator $\hat{O}_i(t)$ to obey the equation of motion, $\frac{d\hat{O}_i(t)}{dt} = i[\hat{O}_i(t), H_0]$. One can realize the monotonous increasing condition of $y(t)$, i.e., $y(t) \geq 0$, by simply setting the external field as $u(t) = A_0 \sum_i^N \left(\partial y(t)/\partial\langle\hat{O}_i(t)\rangle\right) \mathrm{Im}\langle\hat{O}_i(t)\hat{V}\rangle$ with the positive amplitude parameter A_0.

We applied the present theory for the population dynamics control of the vibrational states of Hydrogen Fluoride molecule. We aim to realize eq-distributed state over lowest five vibrational eigenstates $\{|0\rangle, |1\rangle, \cdots, |4\rangle\}$, whereas the initial state is taken to be the ground state. Shown in Fig. 1(a) and (b) are the obtained control field and the population dynamics under the field. It is seen that the desired eq-distributed state is neatly generated by the designed control field.

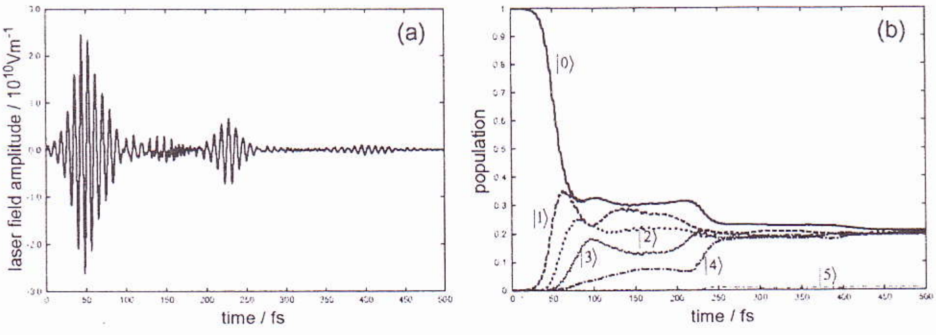

Figure 1: (a) Time-dependence of the control field, (b) Population dynamics.

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B-37

Electron capture processes in a static electromagnetic field

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Electron capture processes in atomic collisions in the presense of a strong electromagnetic field are of importance in relation to high density plasmas, high intensity lasers, and astrophysics. In this study, we have calculated the electron capture cross sections for $(O^{5+}+C^{6+})$ collision system in the static electromagnetic field. We used a close-coupling method with molecular state expansion with the field effect being included up to the first order terms [1,2]. Twenty-six channels were included in this calcutation: $O^{5+}(1s^2 2s) + C^{6+}$ (initial state), $O^{5+}(1s^2 2p,\ 1s^2 3l) + C^{6+}$ (excited states), and $O^{6+}(1s^2) + C^{5+}(2l,\ 3l)$ (electron-captured states).

Table 1. shows the field effects of the reduced-differential cross sections for electron capture in the field directions. The electric field effect is much larger than the magnetic field effect when both of the field strength are 0.05 a.u.

	E=0	**E//b**	**-E//b**	**E//v**	**-E//v**	**E//y**	**-E//y**
B=0	0.0	-27.8	+85.1	+22.7	+11.7	+0.9	+0.9
B//b	+0.1	-27.6	+85.4	+24.2	+13.6	+1.0	+2.8
-B//b	+0.1	-27.6	+85.4	+24.2	+13.6	+2.8	+1.0
B//v	-0.0	-28.3	+83.0	+23.2	+12.4	+0.5	+3.4
-B//v	-0.0	-28.3	+83.0	+23.2	+12.4	+3.4	+0.5
B//y	-0.1	-30.2	+86.7	+25.5	+10.5	+1.2	+1.2
-B//y	+0.2	-25.9	+82.0	+23.0	+17.5	+1.0	+1.0

Table 1. The rate of increase (%) of the cross sections for electron capture into n=2 states of carbon ion at several field directions. The collision energy, the electric field strength, and the magnetic field strength are 1keV/amu, 0.05a.u. (25.7GV/m), and 0.05a.u. (11.8kT), respectively. The cross section is 4×10^{-17} cm^2 at the field free case. The vectors **b**, **v**, and **y** are the impact parameter vector, incident velocity, and **bxv** / |**bxv**|, respectively.

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B-38

RELATIVISTIC MULTICONFIGURATION METHOD IN LOW-ENERGY SCATTERING OF ELECTRONS FROM XENON ATOMS

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The elastic scattering of slow electrons from Xenon atoms is calculated in a relativistic multiconfiguration method [1], [2]. The correlation effects responsible for target polarization are treated in a relativistic configuration-interaction scheme that allows for dynamics effects. Calculations of the spin polarization and differential cross sections are discussed and compared with experimental and other theoretical data.

We define the $(N+1)$-electron scattering-state wave function as the coupled state of an N-electron atomic wave function and a scattering-electron wave function. The atomic state wave functions are calculated by the relativistic multiconfiguration computer code GRASP92 [3]. The transverse Breit interaction is included in these calculations, as well as radiative corrections. The continuum orbitals are solutions of the Dirac-Hartree-Fock equations and are calculated using the modified COWF code [4], and then coupled with atomic state. The original COWF code [5] has been rewritten and adapted to run on multiprocessor computers by using MPI parallelization. Relativistic phase shifts are calculated by comparing the numerical solutions of the Dirac-Hartree-Fock equations to the analytical formula at large r.

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B-39

IONIZATION INDUCED BY POSITRON IMPACT

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In the scattering of positrons off atoms at low and intermediate energies, the inelastic processes that may result in target ionization are positronium (Ps) formation, direct ionization and annihilation. The latter is particularly topical at present since the first evidence of vibrational enhancement of positron annihilation in molecules has been reported [1]. There are also debates in the literature on annihilation mechanisms [2] and its importance in the vicinity of inelastic thresholds [3,4]. There is generally good agreement among recent measurements for the energy dependence of the single ionization cross-sections by positron impact in the noble gases [5]. However, there are significant discrepancies for Ps formation cross-sections for these targets among various experimental and theoretical data.

Ps formation cross-sections in the noble gases have been a subject of recent study in our group [6]. The lower and upper limits to the contribution of excited state positronium (Ps*) formation have been obtained and the estimates suggest that the Ps* formation may occur more copiously than previously thought [7]. The evaluation of the upper limits follows our recent finding that plots of $Q_{Ps}/(Q_{Ps})_{max}$ vs. E/E_{Ps} broadly yield a common curve for a variety of targets ($(Q_{Ps})_{max}$ being the peak value of the cross-section and E_{Ps} is the Ps formation threshold). It is anticipated that these results will be presented at the conference.

Prompted by the results of [8], annihilation below the Ps formation threshold for Ne, Xe and O_2 has been studied. The experimental approach relies on the detection of ions produced by a monoenergetic positron beam in coincidence with annihilation photons. Details of the experimental method as well as the results obtained will be presented at the meeting.

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B-40

MEASUREMENTS OF ABSOLUTE TOTAL CROSS SECTIONS FOR ELECTRON SCATTERING FROM TRIATOMIC MOLECULES

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The absolute total cross sections for electron scattering from triatomic polar molecules, H_2S, NO_2 and SO_2, were determined from the attenuation of intensities of energy-selected electron-beam transmitted through the target volume. The electron beam was formed by an electron-optical system (figure 1) composed of a number of electrostatic elements: an electron gun with a thermionic electron source, a 127^o cylindrical monochromator and a system of electron lenses. Electrons of desired energy E were directed into a collision cell filled with the gas-target. Finally, those electrons which passed through the exit of the reaction volume were energetically discriminated with a retarding field element and collected in a Faraday cup. The absolute total cross section $Q(E)$ was derived from the Bouguer-de Beer-Lambert attenuation law, where all required quantities (the intensity of electron beam, the effective path-length of electrons in the target volume, target temperature and its pressure) were measured absolutely. The results will be presented at the Conference.

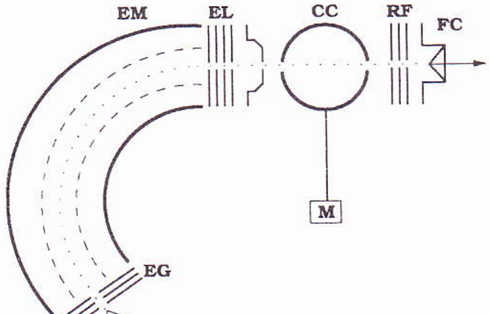

Figure 1: Schematic of the experimental setup: EG, electron gun; EM, electrostatic electron monochromator; EL, electron lenses; CC, collision chamber, and M, manometer head; RF, retarding field analyzer, and FC, electron collector.

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B-41

THE DIRAC–COULOMB STURMIAN FUNCTIONS: A TOOL FOR RELATIVISTIC ATOMIC PHYSICS

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The Schrödinger–Coulomb Sturmian functions, popularized by Rotenberg [1], have been proved to be a valuable tool for solving various problems in non-relativistic atomic physics. Their relativistic counterparts are the first-order Dirac–Coulomb Sturmian basis sets, constructed recently by the author [2, 3, 4, 5].

The radial Dirac–Coulomb Sturmian functions are non-trivial solutions of a Sturm–Liouville problem constituted by two coupled first-order radial Dirac–Coulomb equations augmented by appropriate boundary conditions at zero and infinity. Two kinds of the Sturmian functions are found depending on the way in which an eigenvalue parameter is chosen. For $|E| < mc^2$ the Sturmians form discrete functional sets which are complete in the space of two-component spinor functions. The Sturmians of either kind obey two orthogonality and two closure relations. They are ideally suited for constructing a discrete expansion of the Dirac–Coulomb Green function [2, 3, 4].

The Dirac–Coulomb Sturmians may find wide applications in relativistic atomic physics and in QED. For instance, the Sturmian expansion of the Dirac–Coulomb Green function may be used in calculations based on the perturbation theory. We have illustrated this by evaluating analytically static [2] and dynamic [6] electric dipole polarizabilities and a static magnetizability [7] of the relativistic hydrogen-like atom in the ground state. Other examples of applications of the Dirac–Coulomb Sturmian functions in relativistic atomic physics will be presented at the Conference.

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B-42

Study on Multi-Charged Xe Ions Formed Through 3d Hole States Using a Coincidence Technique

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Multiply charged Xe ions produced through photoionization of a 3d electron have been measured using the coincidence technique. The coincidence measurement between the energy selected Auger electron and ions specifies the individual Auger decay channels for the various multiply charged ions [1].

The non-coincidence time of flight spectrum (Total TOF) and Auger electron photoion coincidence TOF spectra observed at the photon energy of 709 eV are shown in Fig.1. The selected Auger electron energy is indicated at the right end of each panel in order of the kinetic energy of the Auger electron.

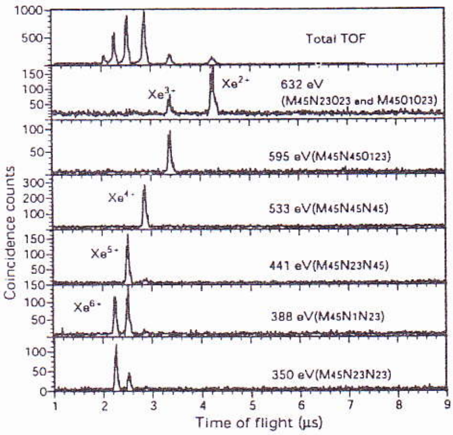

Fig.1. Coincidence TOF mass spectra of multi-charged Xe ions.

These spectra consisting of several charge-state ions indicate that the number of the charge in Xe ions increases with the decrease in the Auger electron energy. In other words, the charge number does increase with the increase in the Auger final state energy. The electron kinetic energy selected with the electron spectrometer was 632 eV in the second top panel, where the $M_{45}O_{23}O_{23}$ and $M_{45}O_1O_{23}$ decay takes place, yielding Xe^{2+} and Xe^{3+}. Only triply or quadruple-charged ions are formed through the Auger decays of $M_{45}N_{45}O_{123}$, and $M_{45}N_{45}N_{45}$, respectively. The $M_{45}N_{23}N_{45}$ Auger decays yield Xe^{5+} dominantly.

These findings indicate that most Xe ions produced through the initial M_{45} Auger transitions turn into the highest charge state among energetically accessible states through subsequent successive Auger decays. However in the $M_{45}N_1N_{45}$ and $M_{45}N_{23}N_{23}$ decays the intensity ratio of Xe^{5+} with Xe^{6+} depends on the energy level of the Auger final states.

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B-43

Nonlocal Effects in Associative Electron Detachment for Low-Energy H+X$^-$ Collisions (X= Cl and Br)

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A recent theoretical treatment [1] of associative electron detachment in low-energy collisions, H + $X^-(E_{\rm rel}) \longrightarrow \mathrm{H}X(v,J) + e^-(\varepsilon)$ (where $E_{\rm rel}$ is the center-of-mass collision energy and ε the energy of the departing electron), concluded that the use of the nonlocal resonance theory is essential for describing these processes for X=F, Cl and Br. It leads to a prediction of the distribution of the final states (v, J) differing qualitatively from that of the simpler local complex potential theory.

The nonlocal theory predicts two kinds of features to occur in the energy spectra of the departing electrons: step-like structures associated with rovibrational onsets and steep rises which are associated with interchannel coupling and which are not present in the local complex potential theory. Our experimental spectra [2] confirm the presence of both types of structure and, thus, the necessity of including nonlocal effects to properly describe the associative electron detachment.

Figure 1 shows an experimental energy spectrum of electrons detached in H + Br$^-$ collisions compared to the nonlocal theoretical prediction (smooth line). The rotational onsets are marked by vertical bars and the corresponding values of v. In addition, the cross section for $v = 0$ rises at a given J as a consequence of the closure of the $v = 1$ vibrational channel and this 'nonlocal step' is marked with S$_0$. In Figure 2 the resulting spectrum from H + Cl$^-$ collisions is depicted. In this case the highest accessible vibrational level is $v = 2$ and the nonlocal steps can be found both in the $v = 0$ and $v = 1$ channel. Both experiments clearly confirm the nonlocal steps S$_0$ and S$_1$ which are missing in a local complex potential model calculation.

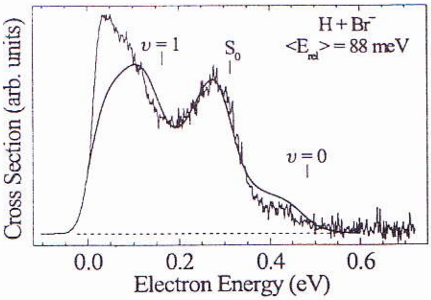

Figure 1: H+Br$^-$ collisions

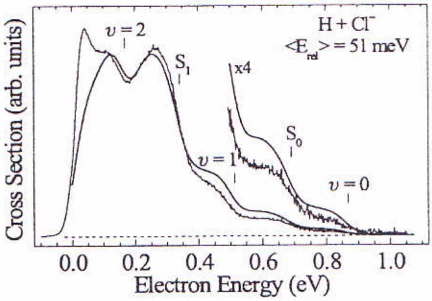

Figure 2: H+Cl$^-$ collisions

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B-44

Theoretical investigation of the autoionization process in the molecular collision complex Ar$^*(4s\ ^3P_{2,0})$+H

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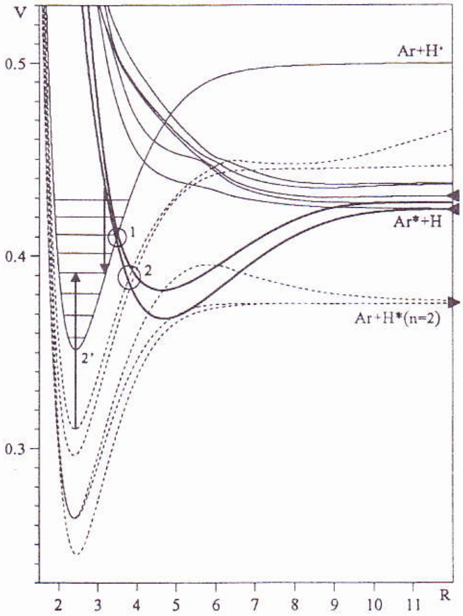
Penning systems like the basic collision system He$^*(2^3S)$+H, in which only relatively fast electrons occur, can be well described by the local complex potential theory within the Born-Oppenheimer approximation [1]. In thermal energy collisions of metastable Ar* with H, ionization is only possible through ArH$^+$ formation (associative ionization, AI) resulting in slow and threshold electrons [2].

Two mechanisms are discussed to describe the AI process:

(1) a direct ionization mechanism where the collision system propagates along a diabatic potential energy curve which crosses at short internuclear distances into the electronic continuum and ionization can take place by electronic coupling,

(2),(2') a two-step ionization mechanism where Rydberg states are populated first which then can autoionize by vibrational or rotational coupling.

We have calculated diabatic potential energy curves for the resonance state Ar*H and the low-lying Rydberg states including spin-orbit coupling in the Ar$^+$ core. The figure shows the obtained potential curves of ArH for $\Omega = 1/2$. The dashed potentials correspond to Rydberg states, the thick lines indicate the two potentials responsible for the AI process and the thin lines are the repulsive potentials belonging to the Ar*H asymptote. For the direct ionization mechanism, we have calculated electron energy spectra using a local complex potential obtained by Feshbach projection.



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B-45

DISSOCIATION ENERGIES OF PROTONATED WATER CLUSTERS

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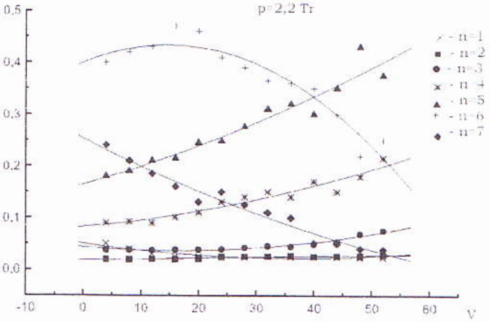
Hydrated ions and ionic water clusters are the subject of increasing interest, both experimental and theoretical (see [1] for references). Protonated water clusters constitute the most abundand ionic species in the low stratosphere; water ions are important in atmospheric nucleation and chemical reactions. In spite of numerous research the very existence of certain protonated water oligomers in the atmospheric conditions and in particular their dissociation energies are uncertain.

We note two conceptually opposite practical approaches for generating water clusters: from a macroscopic liquid phase by dispersion, for example in electrospray method and by aggregation, for example in supersonic beams. In the present work we present a different approach, allowing to select "smoothly" protonated water clusters $H^+(H_2O)_n$ with n=1-7. Clusters are formed in electrical HF or DC discharge in pure water vapour at room temperature and at pressure in a few hPa range. These clusters and/or water ions enter the drift region, with a constant electric field, where they undergo multiple collisions with neutral water molecules, reaching at a given pressure and field intensity a statistical equilibrium between clusters with different n, see fig.1.



This statistical equilibrium is determined by the kinetic energy gain from the field, by the cross section for interaction between ionized clusters and neutral water molecules and by dissociation energies of clusters. Normalizing the population curves to the same values of the reduced electrical field, dissociation energies in a good agreement with recent experiments [2] and theories [3] can be obtained.

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B-46

EXPERIMENTAL APPARATUS FOR STUDYING THE VI GROUP ATOMS IONIZATION BY ELECTRON IMPACT

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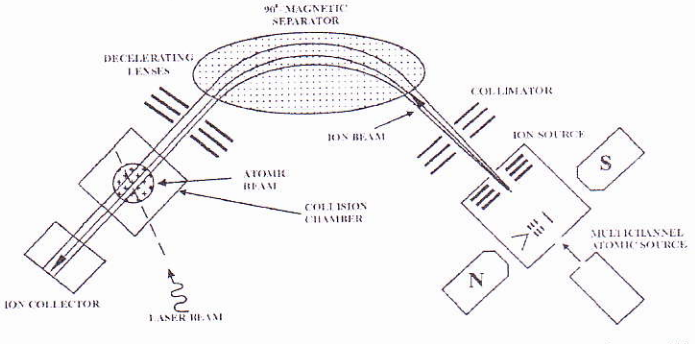
During last decade our group has been working on the studies of electron-impact ionization of atoms and molecules with the use of a quadrupole mass-spectrometer. Despite the high quality of this device, its use for studying the ionization of certain metal atoms and their compounds producing under condensation the dielectric layers at the mass-analyzer electrodes is quite complicated problem. Nevertheless, in a number of practical applications we deal with a necessity to obtain reliable data on the ionization of just such atomic systems, in particular, the VI group elements (S, Se, Te), the data on atomic constants for which are rather scarce. The above elements are being widely used as basic components of complex semiconductor compounds, including crystalline ones.

To study the processes of single and multiple ionization we have developed an experimental apparatus with magnetic ion separation. The schematic layout of the apparatus is shown in the figure. It consists of an ion source, a magnetic mass-analyzer, a power supply system and an ion detector. To produce the ion beam we have designed an ion source with a V-shaped tungsten filament cathode, three electrodes with relevant apertures and an electron detector. The longitudinal magnetic field is produced along the electron beam axis allowing the electron beam geometry to be kept within a wide energy range. Thus, at certain electron energies the effective ionization cross sections could be studied. In future, the electron gun would be replaced by a hypocycloidal electron monochromator to provide the improved electron beam energy resolution.



The introduction of an atomic beam and laser radiation into the collision region (see figure) would allow the ion-atom collision processes to be studied in the strong laser fields. One more specific feature of the ion source is that the neutral atoms are directed to the electron beam intersection region by a multichannel effusion source allowing the working medium consumption to be reduced considerably. At the moment the basic units of the apparatus have been mounted and the test experiments with gaseous targets have been carried out providing good operating stability and reliability.

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B-47

A NOVEL SET-UP FOR POSITRON SCATTERING IN GASES

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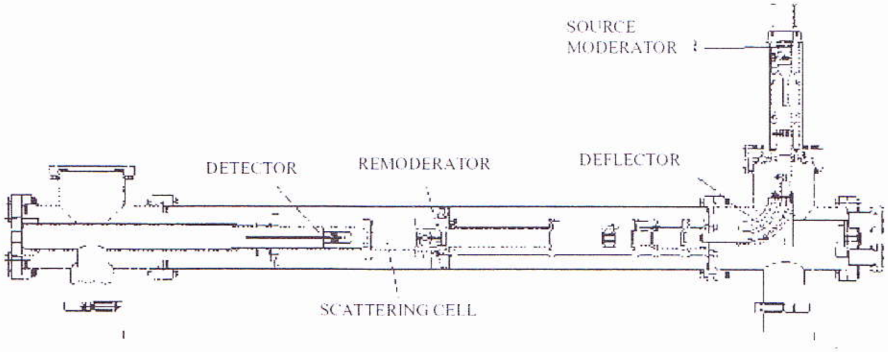
A novel set-up for measurements of total cross sections for positron (and electron) scattering at low energies (1-10 eV) has been developed. Sodium Na^{22} isotope and 1 micrometer thick tungsten monocrystal are used as a source for slow positrons (and secondary electrons). The optical system consists of a first stage, wide-angle electrostatic optics, a 90° electrostatic spherical deflector [1], a remoderator stage [2] and a simple injection optics formed by three aperture electrodes. The injecton optics is projected to work in a time-of-flight regime.

A weak longitudinal magnetic field, used in focusing conditions [3], guides positrons though 10 cm long scattering cell. The detector (channeltron) is movable, in order to allow measurements of both total and partial (vibrational-excitation) cross sections. An about 75% transmission efficiency has been obtained for slow positrons through the second stage of optics and about 10% remoderation efficiency. The preliminary estimate of the energy resolution of the apparatus, without time-of-flight stage applied is about 130 meV.



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B-48

EXCITATION OF THE $^1\Delta_u(V^1B_2)$ STATE OF CARBON DISULFIDE BY ELECTRON IMPACT

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Excitation of the valence $(2\pi_g)^3(3\pi_u)$ $^1\Delta_u(V^1B_2)$ state of carbon disulfide (CS_2) has been studied by electron impact optical method. The measurements have been carried out using an electron trochoidal spectrometer described previously [1]. The energy selected electron beam with the energy spread of 120 meV and beam intensity of about 250 nA is accelerated into the collision region filled with vapour of carbon disulfide. Molecular optical emission from the collision region in the 300-600 nm wavelength range is analysed by the 0.25 m Ebert monochromator equipped with a grating blazed at 300 nm and is detected by a cooled 9813QB photomultiplier.

Figure 1 presents excitation cross section of the $^1\Delta_u(V^1B_2)$ state obtained in the electron energy range from 3 eV to 12 eV from measurements of emission excitation functions taken at fixed wavelengths. Three pronounced maxima at 5.9 eV, 8.2 eV and 10.1 eV and a weaker structure at 4.8 eV are seen in the energy dependence of the cross section which excitation threshold has been determined to be at about 3.6 eV. Dressler et al [2], in their electron scattering experiment observed two overlapping peaks below 7.5 eV which correspond well to the present observations. The structures in the excitation cross section of the $^1\Delta_u(V^1B_2)$ state result from decay of core-excited shape resonances which most likely electronic configurations are $(2\pi_g)^3(3\pi_u)^2$ and $(2\pi_g)^3(3\pi_u)(7\sigma_g$ or $6\sigma_u)$.

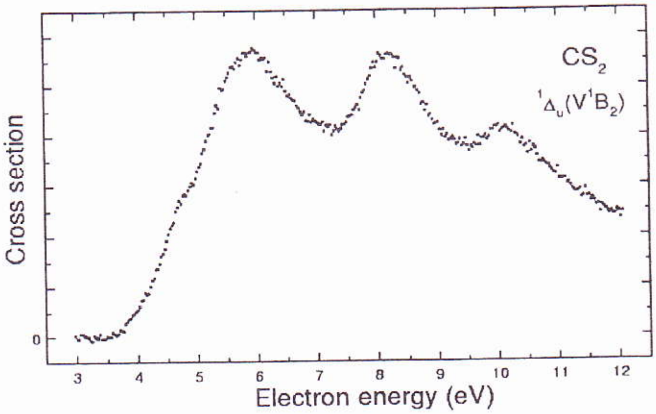

Figure 1: Cross section (in arbitrary units) for excitation of the $^1\Delta_u(V^1B_2)$ state of carbon disulfide.

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Second Conference on the

ELEMENTARY PROCESSES IN ATOMIC SYSTEMS

Gdańsk, Poland, 2–6 September 2002
Gdańsk University of Technology

POST-DEADLINE ABSTRACTS

PD-1

PARTICLE-IN-CELL MONTE CARLO (PIC-MC) SIMULATIONS OF PLASMA-WALL INTERACTIONS

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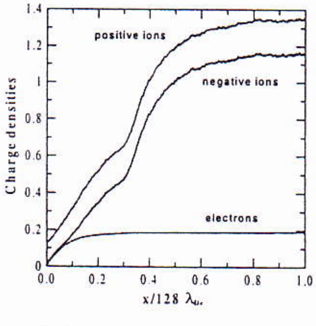
The plasma-wall interactions are of great importance when studying a problem of a floating wall, an anode zone in gas discharge or a diagnostic probe embedded in plasma. Its relative importance increases when bulk plasma dimensions or species concentration decreases, i.e. when the frequency of bulk processes become comparable with rates of specie-wall interaction.

There are various approaches to investigate plasma-wall interactions. Generally, they are based on solution of Boltzmann (or its moments i.e. continuity, momentum and energy conservation-equations) and Poisson's equation. In Monte Carlo based models, the solution of Boltzman equation is substituted by numerical integration along the particle trajectories using probability laws and related cross sections. **Particle-in-cell Monte Carlo** models solve Poisson's equation using density of charged "quasi-particles" in grid points determined by MC trajectories. Each "quasi-particle" represents large number ($\sim 10^5$-10^{10}) of electrons, positive and negative ions moving in the electric field determined by solution of Poisson's equation. A simulation box is divided by computational grid, with spacing ¼ λ_D often assumed. The number of grids points considered vary between few hundreds and thousands. The particle close to the simulation box boundary are removed (or specular-reflected) while particle injected at the boundaries are added to the simulations. The collisions in MC trajectories are treated as instantaneous processes govern by probability law related to the measured cross sections. The various approximations are applied in order to make problem computationally treatable.



In this work, the results of **planar 1 – dimensional (1D) PIC-MC model** [1,2] and the **1d3v PIC-MC model [3]** are briefly presented and discussed.

Figure 1 presents the charged particle densities and the profile of electric field-potential as calculated using the 1D planar model [1,2]. In that model, a Boltzmann density profile is assumed for electrons. The plasma potential may be significantly disturbed even at the distance larger than 20 λ_D, while sheath lengths was in the order of ~ $7\lambda_D$.

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PD-2

Photoelectron angular distributions of rotationally resolved states in para- H_2^+ : A closer look at the dynamics of molecular photoionisation.

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Molecular hydrogen is both the simplest and most abundant molecule in the universe. The interaction of this molecule with a photon of sufficient energy can lead to various processes, such as direct and indirect ionisation, dissociation and fluorescence. In spite of the molecule's simplicity, the photoionisation spectrum of H_2 presents a wealth of rich structure above the first ionisation threshold due to the presence of autoionising states [1]. This structure dominates the weak continuum of direct ionisation. These autoionising states decay by the transfer of energy and angular momentum from the molecular core to the excited electron in a process known as rovibrational autoionisation [2]. In a recent experimental study, at the GASPHASE beamline, we have measured photoelectron angular distributions for ionisation into the four lowest vibrational levels of H_2^+, over the photon energy range that includes the dominant autoionising resonances. For the first time we have been able to measure angular distributions of photoelectrons produced in individual rotational transitions.

Para-H_2 has been used to facilitate the isolation of individual rotational levels. The para-H_2 was produced at the beamline using a conversion technique based on the use of a paramagnetic catalyst, granulated nickel sulphate ($NiSO_4$), maintained at low temperature (~20K) [3]. In order to study the angular distributions of the photoelectrons with the necessary energy resolution a photoelectron spectrometer of mean radius 165 mm was employed. The spectrometer featured a magnetic angle changer device [4] that allowed angular distribution measurements to be obtained without physically moving the analyser.

The angular distribution measurements in para-H_2 have allowed us to determine variations in the asymmetry parameter (β) of photoelectrons produced in different rotational transitions as a function of photon energy. Preliminary analysis of the data shows sharp variations of the β-parameter across the resonance energy region. This behaviour is indicative of the complex angular momentum exchanges between the core and the autoionising electrons. We hope that these first observations at the individual rotational level will stimulate further theoretical calculations of these β-parameter variations [5]. Theories that have been successful in the prediction of total photoionisation features, are more challenged in their ability to predict differential cross sections. State selected measurements, such as those obtained in the present work present an ideal test bench for these theories.

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PD-3

EQUILIBRIUM ELECTRIC CHARGES OF HEAVY IONS WITH Z = 89 ÷ 116 TRAVERSING DILUTE HYDROGEN

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Using the Dubna gas-filled recoil separator we measured the mean charge states of heavy atoms with $Z = 89$ through 116, traversing hydrogen at 1 Torr in the velocity range of 1 to 2.6 v/v_0, where v_0 is the Bohr velocity. In the first approximation, the average charges follow an empirical linear dependence on the velocity (see Figure 1), in agreement with Bohr's theory [1].

The atoms under study were obtained as evaporation residues (EVRs) of compound nuclei produced in complete-fusion nuclear reactions between beams of accelerated heavy ions and heavy target atoms. The projectile particles were delivered by the U400 cyclotron of the Flerov Laboratory of Nuclear Reactions in Dubna.

After emerging from the target layer, the heavy atoms retain a relatively low number of electrons and thus have a correspondingly large electric charge. Furthermore, the distribution of the ionic charge states is quite broad. Due to charge exchange in consecutive collisions with the gas atoms, the distribution of the electric charges rapidly becomes narrower and the mean charge decreases to the equilibrium value $<q>$.

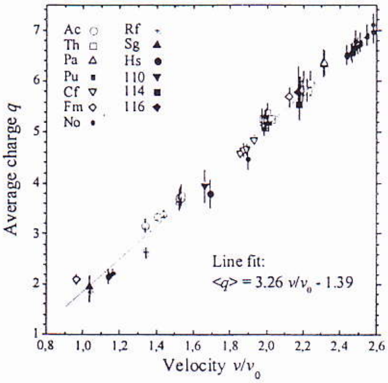

Figure 1. Systematics of the equilibrium charge states of heavy atoms in dilute hydrogen *vs* v/v_0.

The average charge states of the EVRs were measured in the experiments aimed at the synthesis of isotopes of heavy and superheavy elements [2,3] and in the reactions used for calibration of the detection system and the separator.

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