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Third Conference on the Elementary Processes in Atomic Systems

31 Aug. - 2 Sept. 2005
University of Miskolc, Hungary

Book of Abstracts

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Foreword

It is the third opportunity that the CEPAS will be organized, now in Miskolc.

If you have a look for the rich program you can be convinced that the interest in the field does not decreased. On the contrary, one can see how high is the activity here. The spectrum of the topics as well as the number of the countries from where the participants arrived is very broad.

The conference was organized by the Physics Department of the Miskolc University but this work was supported by the Atomic Physics Section of the Institute of Physics of the Hungarian Academy of Sciences. Thus their experiences are unified in this respect and we can hope a really successful conference.

Dénes Berényi
Honorary chairmen

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INVITED LECTURES

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Photoionization and Auger decay in free atoms, molecules and small clusters

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Photoionization of atomic targets creates spectra with main and satellite line contributions. The main lines wich usually dominate the spectra are due to the single electron processes, the satellites instead are created by multielectron effects. In open-shell atoms the main lines display a multiplet structure, due to the coupling of the core hole with the electrons on partially filled outher shells. The multiplet structure of the spectrum is often distributed over a wide energy region and shows very different lifetime broadenings. Electron correlation plays an even stronger role than in case of closed shell atoms, giving rise to additional satellite contributions in the spectra.

A core hole state decays via an Auger transition, giving rice to the normal Auger electron spectrum. Each multiplet of a core hole state in an open-shell atom has a decay spectrum of its own. If the core ionization is accompanied by excitation/ionization of an other electron, Auger spectrum shows a rich satellite structure. Multielectron effects may also take place during the Auger, or in the final state of the Auger decay. Detailed fine structure of Auger spectra is a very sensitive tool to study the open-shell structure and the electron-electron correlation.

Core-hole states of small molecules display a domanant atomic character, with smaller contributions of molecular field effects. This does not hold any more for final states of Auger transitions with holes on outhermost molecular orbitals. Strenght of molecular effects depends on the character of the molecule, more covalent or ionic. Auger decay is a very sensitive method to test this character. Small atomic clusters can be considered to be small molecules, composed of the same atoms. Thus, photoionization and Auger studies of free atoms and molecules forms a starting point for the studies of small clusters. A short review of recent results will be presented.

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I-2

Positron Impact Ionization

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Differential studies provide detailed information on collision dynamics. In a previous study of the electron-capture-to-the-continuum (ECC), its occurrence by positron impact ionization of H_2 was studied at 50eV [1,2,3]. The possible origins of an observed energy shift between the experimental and theoretical distribution have now been investigated by considering two targets at the same final state energy. Molecular deuterium has been used to establish whether at this energy ionization is significantly accompanied by dissociation of the remnant ion. A helium target has also been employed to eliminate possible molecular excitation contributions. Both D_2 and He electron spectra have been found to be shifted as for the molecular hydrogen by ~ 1.6eV. In order to understand the energy discrepancy, the scattered positron projectiles have also been energy analysed. Unexpected asymmetries in the sharing of the residual kinetic energy between ejected electron and scattered positron are clearly shown from our results. Finally, the doubly differential ionization cross-section of water is also being measured. This is part of a general investigation of the interaction of positronic projectiles with water molecules. Results will be presented at the conference.

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I-3

Noble-Metal Nanostructures for Controlling Photons and Sensing Molecules

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The photon is clearly the fastest means to send information to and from the nanoscale. Noble-metal nanostructures are of particular interest to manipulate photons as they can support electromagnetic surface modes (surface plasmons) able to concentrate light field to a small fraction of wavelength and enhance the local field by several orders of magnitude.

In this report, we present our recent results in fabrication and characterization of ordered arrays of noble-metal nanoparticles and other regular nanostructured materials. Such nanostructures are highly desirable in several applications including optical energy and information transport, photonic crystals, near-field scanning optical microscopy, surface-enhanced spectroscopy, chemical and biological sensing. We currently employ noble-metal nanostructures for controlling photons propagation on the nanoscale and performing ultrasensitive optical detection of molecules [1, 2].

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I-4

YOUNG ELECTRON INTERFERENCE EFFECTS IN ATOMIC IONIZATION COLLISIONS

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Even though the concept of interference was already implicit in Newton´s 1688 explanation of the anomaly of the tides in the Gulf of Tongkin, it was Thomas Young in his Bakerian Lectures of 1801 who generalized this idea and applied it to a variety of situations. His celebrated double-slit experiment, first described in his *Course of Lectures on Natural Philosophy and the Mechanical Arts* of 1807, has been regarded as a prime demonstration of the wave-nature of light and, in its single electron interference version, was recently voted as the most beautiful experiments in Physics [1]. Since the foundational times of Modern Physics, the appearance of electron interference effects in different atomic processes has never failed to attract considerable attention. A recent wave of interest was triggered by the observation made by Stolterfoht et al. [2] of interference effects in the ionization of hydrogen molecules by energetic ion impact. Unlike electron diffraction experiments by matter, in ionization processes the electrons are not coming from a distant source, but from one of the two partners in the collision event. In this communication we review different interference mechanisms that occur in ionization collisions. In particular, by means of a Multiple-Scattering Theory we discuss the occurrence of re-scattering of the emitted electron by different centers. Finally, we propose a direct atomic realization of a Young interference experiment, where a single electron source and a two-center scatterer are prepared in each collision event [3].

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I-5

SPECTROSCOPY OF LASER EXCITED INDIUM, GALLIUM AND INDIUM-GALLIUM SYSTEMS

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The vapour composition of the group IIIA elements has a remarkable importance for the fabrication of various semiconductor devices. In spite of this, up to now there is a very limited experimental knowledge of the composition of In and Ga vapours or of their mixtures as the information on the electronic state structure of In_2, Ga_2 and InGa as well as of other cluster species of these elements is quite scarce.

A great step forward has been done by studying laser assisted collisions in dense resonantly (410.3 nm or 403.4 nm) laser excited In or Ga vapours. In this way Rydberg levels as well as autoionizing levels and products of recombination following collisional ionization have been evidenced for each element [1,2]. The fluorescence spectra have been recorded either from a vapour confined in quartz cells with or without buffer gas, or in stainless steel heat pipe ovens at temperatures ranging from 950 to 1100 °C. The analysis of the spectra has been done with a 1000 mm monochromator at 18 cm^{-1} resolution. The presence of a large density of excited atoms, favours the collision of an atom in the fundamental state and another one in the first excited state to give a molecule directly in an excited electronic state from which it radiates. In this way some In_2 molecular bands were found [3] and now evidence of other In_2 molecular structure has been obtained as shoulders of the In fundamental fluorescences, while some molecular bands appear in the fluorescence spectrum of the excited Ga vapour. We present also the spectroscopic study of the In-Ga system, obtained by laser exciting either one of the In or Ga fundamental transitions in a vapour mixture of In and Ga. The same regions of the spectrum were analysed following both excitations. Both spectra show the lines corresponding to the fundamental transitions of the non-directly excited element due to sensitized fluorescence. Fluorescences originating from the Rydberg levels of both In and Ga also appear to testify of the presence of homonuclear as well as heteronuclear laser assisted collisions. Both spectra show also In_2 molecular bands, already assigned in experiments with homonuclear vapours [3]. In addition, other features appear, as well as shoulders of the fundamental atomic fluorescences, that have not been detected in the corresponding homonuclear vapours. They are likely due to the In-Ga dimers or clusters. These results will be shown together with those obtained by the analyses of the spectra following the simultaneous excitation of both elements, which is performed at the moment.

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I-6

RESONANCES IN CORE-EXCITATION OF ALKALI ATOMS

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High intensity negative-ion resonances, which to a great extend determine dynamics of the near-threshold electron impact excitation of the lowest autoionizing states in alkali atoms, have been recently revealed experimentally [1-3] and considered theoretically [4-6]. In this report the experimental apparatus and methods for measuring the ejected-electron excitation functions of autoionizing states in metal vapours will be described. Recent experimental and theoretical results obtained for lithium, sodium and potassium atoms will be also presented.

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I-7

INTERFERENCE EFFECTS IN SINGLE IONIZATION OF H_2 OR D_2 MOLECULES BY FAST CHARGED-PARTICLE IMPACT

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Studies of particle-induced ionization have focused particular attention to the molecular target H_2 (or D_2), which is the simplest molecule composed of two atoms. This review deals with phenomena associated with the indistinguishibility of the atomic H centers, in particular, coherent emission from the two centers leading to interference effects in the ejected electron spectra.

In the past decades, efforts have been devoted to reveal these interference effects in atomic collisions with H_2. Early studies of collisionally induced interferences from H_2 centered on the processes of electron capture and photoionization. Recently, experimental evidence for interference effects was found in H_2 electron emission spectra induced by very fast charged particles (60-MeV/u Kr^{34+}) [1], with the electron spectra exhibiting an oscillatory structure as a function of electron energy in good agreement with model calculations.

This observation [1] prompted several new experimental investigations [2-7], and motivated various theoretical studies [8-12] that reveal detailed properties of the interference effects. It was recognized that dipole transitions and binary-encounter processes play different roles in the ionization process leading to interference [1,8]. Moreover, the interference effects were predicted to depend on the electron emission angle [9,11]. Later experiments [2-5,7] confirmed the general predictions of the theories. In the case of electron impact at 2.4 keV, comparison with theory shows that, in addition to the interferences associated with electron emission following soft collisions, interference effects appear for ejected electron energies corresponding to the binary encounters [7].

Measurements with 68-MeV/u Kr^{33+} projectiles [2] revealed higher frequency oscillations superimposed on the primary interference structures [3], indicating the presence of second-order interferences. Similar observation has been made for 1-5 MeV H^+ impact [13]. While the primary oscillatory structures are analogous to Young-type interferences, the secondary oscillations have been attributed to additional scattering within the molecule [3].

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I-8

DOPPLER TOMOGRAPHY OF EXCITED SPUTTERED ATOMS

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The report contains new results on the development of the Doppler Tomography method [1] and its usage for investigation of three-dimensional velocity distributions $F_i(\mathbf{v})$ of atoms sputtered in one or another excited state "i" from the surface of metals and alkali halide crystals.

In Doppler Tomography $F_i(\mathbf{v})$ distribution is measured in two steps. First by means of Doppler method one obtain distribution of excited atoms $f_i(v_\mathbf{l})$ on their velocity projections on the set of chosen space directions $\mathbf{l}$. Then the obtained set $\{f_i\}$ of $f_i(v_\mathbf{l})$ functions which correspond to different $\mathbf{l}$, by means of Computer Tomography is converted into three-dimensional distribution $F_i(\mathbf{v})$. During these steps one solves so called incorrect mathematical problems [2]. To solve these problems one must use available a priori information on $f_i(v_\mathbf{l})$ and $F_i(\mathbf{v})$ functions. We elaborated such algorithms of DT, which take into account all available a priori information on these distributions. By this we ensure the maximal accuracy of reconstruction of $f_i(v_\mathbf{l})$ and $F_i(\mathbf{v})$ distributions from the initial experimental data.

With help of DT we investigated rather completely differential characteristics of emission of excited atoms from the surface of simple metals. Owing to this the significant progress in understanding of mechanisms of this phenomenon was achieved. In particular, basing on the obtained $F_i(\mathbf{v})$ distributions, for the first time the velocity dependence of the excitation probability of secondary atoms of metals was obtained. This allowed to test successfully the quantum mechanical model of phenomenon.

Now the similar program of investigation of emission of excited atoms from the surfaces of alkali halide crystals and other insulators with sufficiently simple electron structure is being realized.

Applied side of Doppler Tomography is presented by optical method of surface diagnostics, which was recently elaborated by us. It not only opens possibility of standard free element analysis of surface and bulk of different materials by ion beams but by its concentration sensitivity significantly (by orders) it surpasses all known methods.

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I-9

Ionization Studies using Positron and Electron Beams

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Lepton impact ionization of atoms has long been used to provide information and test theoretical predictions relating to atomic structure, energy deposition in matter, and interaction dynamics. Measurements performed using both electron and positron impact are particularly useful since they can be used to isolate and probe contributions from specific channels, to identify charge sensitive effects in the interaction dynamics and target polarization, or to test theoretical approximations in greater detail. For example, influences from the electron exchange channel which are present for electron impact can be deduced via comparisons with positron impact data, where it is absent. Or, comparisons of electron and positron impact data yield information about target polarization and interaction dynamics since changing the sign of the charge influences the target polarization as well as the impact parameter during the collision. Single and double ionization cross sections for electron and positron impact are useful in testing theoretical models since the single ionization cross sections are nearly identical whereas the double ionization cross sections differ by roughly a factor of two. Another example are e-2e type studies performed using positron impact since the ejected target electron and the scattered projectile can be identified; thus expanding the range of energy losses that can be investigated and facilitating comparison with theory.

Thus, since the advent of modern atomic physics, electron and positron impact ionization has been studied and compared. For electron impact, very sophisticated data ranging from total to highly differential measurements have been available for decades. In contrast, for positron impact experimental difficulties have limited the vast majority of the studies to total cross section measurements. However, in the past decade several doubly differential ionization measurements have been made for positron impact. In our lab we have recently taken the next major step by initiating triply differential measurements. From coincidence measurements between the scattered positron, the ionized electron, and the recoil ion we are able to study single and multiple ionization precesses where the interaction dynamics are totally defined for single ionization and e-(3e-1) data are obtained for double ionization.

This talk will present examples and review what has been learned from total and differential measurements to date, plus present ideas for how positrons might be used in future studies to explore unique situations or enhance our understanding of the physics. Concentration will be on intermediate energy collisions, i.e., between roughly 100 and 1000 eV. Experimental problems and techniques associated with positron impact studies will also be discussed.

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I-10

Interaction of Highly Charged Ions with the Surface of Insulators

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The interaction of highly charged ions (HCIs) with surfaces has been the subject of intense scientific research in the last years. Special attention was paid to the interaction with the surface of metals, where the formation of hollow atoms and their relaxation dynamics has been studied in detail [1]. From theses studies the interaction scenario for metal surfaces has been revealed and found to be consistent with the classical-over-barrier-model [2]. In contrast, the study of the interaction of HCIs with insulating surfaces is not as complete and still lacks some understanding [3].

The main differences between metals and insulators can be found in the higher work function, the lower density of electrons in the conduction band, and the much lower conductivity. Therefore, the microscopic and macroscopic charging of insulating surfaces, which constitutes an important part of the interaction mechanisms, makes these studies difficult. Different methods can be used to overcome this difficulty. Using thin layers of a deposited material is one of the possibilities and will be presented here for the interaction of highly charged Ne ions with the SiO_2 surface. Secondary electron emission from these layers and the calorimetric determination of the potential energy retention in these layers will be compared to results on Au surfaces.

In addition, the main aspects of the interaction of HCIs with insulating surfaces will be reviewed briefly. By means of the emission of x-rays and secondary electrons the formation and relaxation of hollow atoms above insulating surfaces will be discussed. Furthermore, the more applicative aspects of the interaction of HCIs with insulators like potential sputtering and single ion induced surface tracks and modifications will be covered.

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I-11

CO AND CO_2 INNER-SHELL IONISATION AND EXCITATION BY ELECTRON IMPACT

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Auger electron spectroscopy is a very useful tool to investigate the decay dynamics of inner shell excited/ionized systems. The aim of this work was to i) obtain high quality C and O Auger spectra of CO and CO_2 molecules in order to investigate the high binding energy part of the spectra where the theoretically predicted effects of nuclear dynamics [1] of the decaying states are observable; ii) unravel the resonant Auger spectrum due to the excitation of the optically forbidden $CO(1s\sigma_c)^{-1}(2p\pi)\ ^3\Pi$ transition.

The Auger spectra were studied by electron impact at different electron energies ranging from 0.5 to 3 keV. The multicoincidence electron spectrometer at Elettra and electron spectrometer at CNR-IMIP (Rome) were used in this experiment [2,3].

The experiments have been compared with the theoretical calculations of the Auger spectra of CO and CO_2 molecules by Green s function algebraic diagrammatic construction methods [1]. It is the first time that such a calculation has been performed for CO_2.

The main feature in the CO spectrum in the region of interest is a broad peak at a binding energy of about 98.6 eV in the C Auger spectrum and at 94.5 eV in the O one. The energy difference between the two peaks is about 4 eV. The main configuration of this structure is the $3\sigma^{-2}$ one. According to theory, all the lines in the 90-100 eV range are shifted towards higher energy by about 3 eV in the C spectrum and towards lower energy by about 1 eV in the O spectrum. This is in very good agreement with the experimental observation.

To study the resonant Auger spectrum of the optical forbidden transition we have measured several energy loss spectra at large momentum transfer and several resonant Auger spectra at the same incident energies between 400 and 1500 eV. In the energy loss spectra and in the resonant Auger spectra at the lowest incident energies (400-600 eV) the spin-forbidden process leading to the population of the $(1s\sigma_c)^{-1}(2p\pi)\ ^3\Pi$ state is clearly observed.

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ALIGNMENT AND POLARIZATION EFFECTS IN RELATIVISTIC ION–ATOM COLLISIONS

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During the last decade, *relativistic* collisions of highly–charged ions with different target materials have been studied intensively at the GSI storage ring and elsewhere. In such collisions, one of the major processes is due to the capture of a free or quasi–free electron into a bound state of the ion, accompanied by the simultaneous emission of one or several photons. Apart from the capture into the $K-$shell of bare ions, much of the recent interest was focused on the alignment of excited states, the angular distribution and polarization of the subsequently emitted radiation, or even the recombination of high–Z, few–electron ions.

To facilitate the set–up and interpretation of the experiments at storage rings, a number of theoretical studies have been carried out within the framework of the density matrix approach to explore such capture processes in detail. These studies demonstrate that the polarization properties of the incident ions (and electrons) are quite uniquely *transfered* to the properties of the emitted radiation. In particular, it was shown that a *rotation* of the polarization vector occurs if spin–polarized particles are involved in the collisions [1–3]. For high–Z ions, therefore, the polarization of the emitted x–ray radiation may serve as a *signature* and a quantitative measure on the polarization of the incident particles, when compared with proper theoretical predictions.

In this contribution, we review the recent work on the (correlated) capture and decay processes of high–Z ions. Using the density matrix approach, we discuss (i) the angular distribution and polarization [1–3] of the recombination and subsequent photons, (ii) the differential alignment of the (excited) levels as well as (iii) *interferences* due to higher multipoles [4]. Although most examples concern the capture into bare, high–Z ions, we also show how the theory can be applied to the radiative recombination of few–electron ions [5].

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I-13

COMPLETE EXPERIMENTS IN PHOTOIONIZATION WITH EXCITATION AND RESONANT AUGER DECAY

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Quantum reactions are completely characterized by the absolute magnitudes and phase differences of the complex amplitudes for transitions between the initial state and each of the degenerate final states (channels). A complete set of experimental data is defined as a set, from which all these amplitudes can be extracted, within a certain theoretical model. From this information any observable can be predicted, thereby providing data for the most comprehensive test of theory. In photoionization with excitation (PIE), the absorption of a single photon leads to one electron being ionized and the second electron being excited. The occurrence of PIE, therefore, is a consequence of electron-electron correlations. Studying PIE by means of a complete experiment can provide very detailed information on such correlations and the mechanisms of PIE itself. A complete experiment for PIE was already realized for the resonant regime, i.e., through photoexcitation of an intermediate resonance state with subsequent Auger decay into an excited residual photoion (resonant Auger process). From the viewpoint of general theory, there is no difference between approaches to the complete experiment for resonant Auger decay and the direct PIE process.

Generally, a complete set of data, as defined above, cannot be obtained solely from the properties of the photo/Auger electrons. Instead, a combination of different experimental techniques is required to provide the complete information on the process. A natural way to obtain additional independent parameters for the PIE and/or resonant Auger decay to the excited ionic state is to study the polarization of the final ionic state by detecting the angular distribution or the polarization of the fluorescence radiation (for discrete final ionic states) or the ejected electrons (for autoionizing/Auger final ionic states). We concentrate on radiatively decaying discrete ionic states and fluorescence polarimetry as a method to complete the experiment. A resonant Auger decay, induced by photoexcitation of the ground Xe $5p^6$ atomic state into the Xe* $4d_{5/2}^{-1}6p$ (J=1) resonance, with subsequent Auger decay to the excited Xe II $5p^4 6p$ ionic states is considered [1,2] to illustrate the principal ideas and realization of a complete experiment for PIE and the resonance Auger decay.

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TESTING CPT INVARIANCE WITH ANTIPROTONIC ATOMS

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Abstract

The structure of matter is related to symmetries on every level of study. CPT symmetry is one of the most important laws of field theory: it states the invariance of physical properties when the signs of the charge and of the spatial and time coordinates of particles are simultaneously changed. This implies, e.g., that an antiparticle can be described as a particle going *backward* in space and time. Although in general opinion CPT symmetry cannot be violated in Nature, there are theoretical attempts to develope CPT-violating models [1].

The Antiproton Decelerator [2] at CERN was built to test CPT invariance by comparing the properties of the proton and the antiproton. Two of its experiments, ATHENA [3] and ATRAP [4] have produced and studied antihydrogen atoms, antiproton-positron bound systems, with the long-term aim to measure its 2S-1S transition in comparison with that of ordinary hydrogen. The third experiment, ASACUSA [5] uses laser spectroscopy to measure transition energies and state populations in antiprotonic helium atoms deducing the mass, charge and magnetic moment of antiprotons. No deviation was found from the CPT invariance.

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I-15

HIGH RESOLUTION STUDIES OF ELECTRON SCATTERING RESONANCES

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Electron scattering resonances, i.e. temporary compound states of the electron-target system, have a substantial influence on low-energy electron collisions with atoms [1], molecules [2,3], and clusters [3]. Exhibiting lifetimes comparable to or even larger than vibrational periods, resonances strongly enhance cross sections for vibrational excitation, and they are essential for anion formation through dissociative electron attachment. In this lecture we concentrate on progress recently made in studies of narrow resonances observed in electron collisions with atoms and molecules. Both electronic Feshbach resonances and vibrational Feshbach resonances (VFRs) will be addressed. Recently, VFRs have also caught substantial attention with regard to their ability to dramatically enhance positron annihilation in low-energy positron collisions with hydrocarbon molecules [4].

Experimentally, systematic improvements of conventional electron scattering spectrometers have allowed studies of gaseous targets with high sensitivity and a resolution down to about 7 meV [5] and over the full angular range [6,7]. Laser photoelectron sources have enabled investigations of angle-differential scattering studies at currents around 80 pA and energy widths down to 4 meV [8]. The use of energy-variable laser photoelectrons has allowed to elucidate the threshold behaviour of (dissociative) electron attachment to molecules and molecular clusters at (sub) meV resolution and to observe very narrow VFRs (width down to about 2 meV) in the attachment spectra [3]. Low-energy positron beams, based on positron accumulation and thermalization in Penning traps, have enabled the first measurements of vibrational excitation and of positron annihilation in positron-molecule collisions at energy width of about 30 meV [4]. The lecture will highlight some of these recent experimental observations and compare them with theoretical results.

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I-16

RELATIVISTIC CALCULATIONS FOR HIGHLY CORRELATED ATOMIC SYSTEMS INCLUDING HIGHLY CHARGED IONS

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In recent years, the spectroscopic measurement became to give us quite a sophisticated set of data that requires a proper theoretical treatment. To obtain the theoretical values with reasonable precision, we sometimes find that a fully relativistic treatment for the problem is indispensable. And an inclusion of the correlations between various many electronic configurations is also found to be quite important. In this report, we discuss an extension of the variational methods for calculations of the many electron atomic system. Firstly, we give a brief review of the methods for relativistic calculation of atomic structures and dynamics. Secondly, we give a brief review of the relativistic effects or processes in atoms or ions. And furtheron the electron correlations in highly excited atomic or ionic states including the deep inner shell excitations and/or multiple excitations will be reviewed.

If we want to evaluate the energies of many electron atomic ions with large atomic numbers within an accuracy of one electron volt or less, a relativistic Hamiltonian must be employed for variational calculations, because the single-electron orbitals themselves are to be modified by the relativistic effects. It does not constitute any plausible methods to split the relativistic effects into various terms such as spin-orbit interactions or others. We may use the family of codes which are based on the multi-configuration Dirac-Fock method and their extensions [1, 2, 3].

In atomic ions with 4d-open valence-shells, there are quite strong mixings among the principal quantum number n=4 electron excited configurations, which was pointed out firstly by O Sullivan and Faukner [4] for 4d-4f optical emissions in tin ions. By a series of elaborate calculations we reveal that this type of configuration mixing is quite common to the atomic species with the atomic numbers Z = 48 56.

In atoms with multiple excitations of core orbitals, there are quite serious modifications of inner-shell orbitals due to their contractions [5, 6], which constitutes one of the characteristic features of the hollow atom excitations. We illustrate these effects for a couple examples based on a series of precision calculations for lithium, beryllium, and neon atoms.

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I-17

ION IMPACT-PARAMETER FORMULAS FOR MULTIPLE IONIZATION

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I-18

Interaction of slow multicharged ions with surfaces: Status of theoretical and experimental understanding

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The investigation of slow highly charged projectiles interacting with solid surfaces has changed its character over the past few years from purely academic interest to applied research e.g. in the field of nanofabrication. Refined experimental techniques allow to investigate interaction processes for projectiles with well-defined trajectories monitoring in coincidence two or more observables (emitted secondary particles, energy loss of the projectile, scattering of the projectile at the surface, ...).

Charge transfer processes involved in the interaction can be understood on the basis of the classical over-the-barrier model developed by Burgdörfer and coworkers in 1991 [1]. We have used extensions of this model in combination with techniques to describe excitation processes in the target material to model the history of slow HCI interacting with metal and insulating surfaces.

In my talk I will give a short review on current experiments (HCI on single crystal surfaces, magnetized materials, transmitted through insulating nanocapillaries), describe methods to simulate the relevant interaction processes, and present simulation results for recent experimental data.

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I-19

ELECTRON COLLISIONS BY METAL ATOM VAPOURS

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A systematic study of low and medium energy electron interactions with metal atom vapours has been performed exploiting crossed beam technique. A monochromatic electron beam of energies from 10 to 100 eV has been elastically and inelastically scattered by effusive beam of metal vapours of II A (Mg and Ca) [1] and II B (Zn, Cd, Hg) [2] group atoms as well as other metal atoms such as Yb [3] and Pb. Differential cross sections (DCS) were put on absolute scale by normalization trough optical oscillator strengths of the resonant transitions. After obtaining the transmission of the electron spectrometer, relative intensities between resonant transition and other features in energy loss spectra were determined for each impact energy. DCS were obtained in the angular range from 0° for the excitations and 10° for elastic scattering to 150° with the angular resolution of typically 1.5°. DCSs were extrapolated to 0° and 180° and numerically integrated to yield integral, momentum transfer and viscosity cross sections. Results are compared with available calculated values and other experimental data. Experimental DCS data serve as a stringent test for different theoretical approaches that intend to reproduce angular distribution curve in the whole domain of scattering angles and a wide range of energies.

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I-20

Atomic and Molecular Processes in Atmospheric and Environmental Science

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Environmental science will be one of the most important and active areas of 21st scientific research. The effects of global warming, ozone depletion, air pollution, desertification, land use etc all have political and socio-economic consequences that will require major changes in industrial, social and political policies. However in order to convince governments, industry and the public of the need for action there must be a solid scientific base upon which any plan of action may be developed. Key scientific questions remain such as;

- To what extent is global warming due to natural cycles in the Earth s climate and how are these being altered by human industrial development ?
- What is the role of the terrestrial biosphere on the Earth s atmospheric processes ?
- Have we taken sufficient measures such that the ozone hole will now be closed ?
- What is the long term effect of air pollution ? and how might such pollution be reduced ?

Atomic and molecular physics pervades many areas of modern atmospheric and environmental physics. For example many of the physical and chemical processes in our atmosphere are studied remotely through a knowledge of the spectroscopy of chemical species; photolysis underpins many of the chemical processes in the stratosphere (e.g. ozone chemistry) and is largely responsible for the photochemical processes leading to urban air pollution, while in the upper atmosphere photo-ionization plays a key role in ionospheric processes. Infrared radiation and its interaction with trace gases, water droplets and dust in the terrestrial atmosphere underpins our understanding of heat exchange in the atmosphere and hence the potential for global warming.

In this talk I will give several examples of how current research in atomic and molecular physics is being used to study atmospheric processes and thence provide scientific evidence for several of the major environmental issues being discussed today. The role of synchrotron radiation as a mimic of solar radiation will be demonstrated and the importance of photon and electron induced chemistry on surfaces discussed. I will also present those areas for which more research is required and discuss how the atomic and molecular community may provide vital data.

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I-21

MEASUREMENTS OF DIFFERENTIAL CROSS SECTIONS IN THE BACKSCATTERING REGION

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In the past ten years progress has been made in the experimental studies of electron scattering from atoms and molecules in the range of large scattering angles. With the development of new experimental techniques [1-3] it became possible to detect electrons scattered in elastic and inelastic processes at the angles above 130^0 up to 180^0. Knowledge of differential cross sections for scattering in the backward directions is vital in the studies of electron-target interactions. It is expected that short-range interactions, such as polarization-correlation and exchange, play important role in the backward scattering especially at low and intermediate electron energies.

In the present contribution experimental techniques used to observe electron backscattering will be presented. A comparison of recent results of extensively studied both experimentally and theoretically rare gases (Ar, Kr) [4-8] and simple molecules (N_2, O_2, H_2O) [9-11] in electron backscattering will be also given.

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I-22

EVOLUTION OF SATELLITE LINES ACCOMPANYING PHOTOIONIZATION

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When inner-shell photoionization takes place, it is well known that other electrons in the same atom have a small, but definite probability to be excited into unoccupied bound states or ionized to the continuum [1]. Experimentally such multi-vacancy states can be observed as satellite lines in x-ray emission spectra and Auger spectra.

For low-energy incident photons, the velocity of the photoelectron is low and the change in the atomic potential due to the inner-shell vacancy is so slow that atomic orbitals can relax adiabatically. The electron transition probability should be treated in the time-dependent perturbation theory and the problem can be solved only under some simplifying assumptions. Up till now there have been developed three models for the electron transition in the adiabatic approximation.

Thomas [2] assumed that the time dependence of the Hamiltonian due to the presence of the photoelectron is written by the error function. Vatai [3] retained only the monopole term in multipole expansion of the Coulomb interaction and adopted the classical straight-line trajectory for the ejected photoelectron. In the recent model of Roy *et al.* [4], the time-dependent part of the Hamiltonian is assumed to be the exponential function and the final-state electron is in the continuum state.

The Thomas model has been often applied to analyze the experimental results on evolution of x-ray satellites, but other two models have been scarcely used. Furthermore, no comparison of these three models has been performed so far. In the present work, we modified the model of Roy *et al.* and obtained an additional model. The experimental evolution curves for x-ray and Auger satellite lines accompanying photoionization were fitted to these four theoretical models and comparison between them is made.

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I-23

INTERFERENCE EFFECTS IN THE IONIZATION OF MOLECULES

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Interference effects occurring in the ionization of H_2 by fast charged projectiles and photons have been widely studied experimentally [1, 2] and theoretically [3, 4, 5, 6, 7] in the last few years. Because of the two-center character of the target, the waves associated to the ejected electron may add up in constructive or destructive interference, depending on the ejection velocity and angle. Very recently interference effects have been observed during high-order harmonic generation from aligned CO_2 molecules using ultrashort laser pulses [8].

We have studied the interference effects in the ionization of H_2 by charged particle [3] and photon [7] impact. In case of charged particles we have predicted the dependence of the period of the oscillations in the cross section on the ejection angles, dependence confirmed experimentally [2]. Interesting features may be observed when the $\sigma_{H_2}(\mathbf{k})/2d\sigma_H(\mathbf{k})$ ratio is represented as a function of ejected electron momentum and angle (see Fig. 1). The dependence of the cross sections on the molecular orientation have been also studied.

In case of the photoionization the basic cause of the interference is the same, but the interference features are different in detail. In this case the angular dependence of the period of the oscillations on the ejection angle is much weaker.

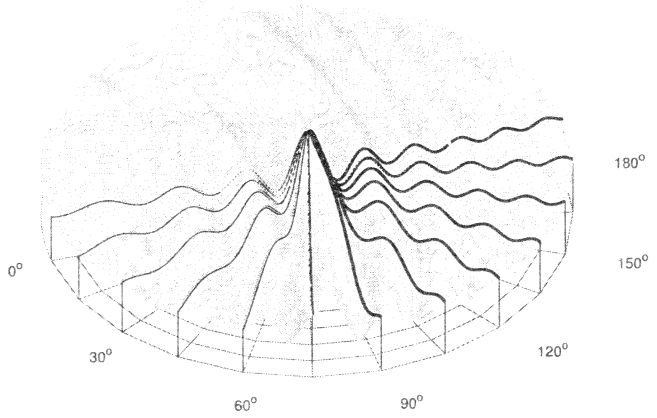

Fig. 1. Polar representation of the $d\sigma_{H_2}(\mathbf{k})/d\sigma_H(\mathbf{k})$ ionization cross section ratios (for 60 MeV Kr^{34+} projectile) as a function of the ejection angle and velocity of the electrons. The maximum value of electron velocity is 20 au.

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Study of nonradiative decay properties following resonant double excitation to the $[1s2p](^{3,1}P)3p^2$ states of Ne atom using soft x-ray undulator radiation

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We have been carrying out spectroscopic studies on the $[1s2p]nln\,l$ doubly excited states of Ne atom, where square brackets indicate hole states, using soft x-ray undulator radiation [1,2]. So far, the photoion yield spectroscopy and the resonant Auger electron spectroscopy were performed to characterize such doubly excited states in the excitation energy range between 900 and 912 eV at BL27SU of SPring-8 in Japan.

The present talk will mainly deal with the investigation of nonradiative decay properties of resonantly photoexcited $[1s2p](^{3,1}P)3p^2$ states of Ne atom. Partial ion yield spectra for the Ne^{2+} - Ne^{4+} ions were measured in the region of double excitation resonance by means of time-of-flight spectrometry [3]. The Ne^{3+} partial ion yield spectrum has been found to reveal resonant enhancement at the energy positions of doubly excited states which implies the most plausible decay channels leading to the third step Auger processes. Energy diagram of the excited and relaxed states of the neutral Ne atom as well as the Ne ions associated with the $[1s2p](^3P)3p^2$ state were calculated based on the multiconfiguration Dirac-Fock method in order to interpret the possible nonradiative decay channels. The low-energy electron spectrum originated from the second/third step Auger processes was preliminarily measured to show a rich structure induced at the $[1s2p](^3P)3p^2$ double excitation resonance.

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I-25

QUANTUM CALCULATIONS OF THE DIFFERENTIAL CROSS SECTION FOR ELECTRONS EJECTED IN AN ION ATOM COLLISION

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Because an ion is heavy, accurately describing the outcome when a fast ion collides with an atom treated in the independent particle model is simple. The task reduces to solving how a single quantum mechanical electron bound to some center is perturbed by the time dependent potential created as the ion follows a predetermined classical path. It has been commonly accepted for some twenty years that modern computers can directly solve such problems quite straightforwardly and theoretical focus had shifted to the breakdown of the independent particle model, i.e. correlation.

In fact, comparison between variant numerical quantum calculations and experiment have until recently been largely confined to total cross sections with a narrow and consequently possibly misleading focus on K-shell hole production. More convenient approximations have been mainly used for differential cross sections, notably the CTMC algorithm and the CDW approximation. The latter two methods can typically give errors of twenty percent or more in total cross sections but have been quite remarkably successful in reproducing the differential spectra of ejected ionized electrons.

A determined small cadre of theoreticians have found, and to their credit reported, convergence difficulties when seeking to describe quantum mechanically the same differential cross sections. In spite of these difficulties steady and rewarding progress has been made. For example, evidence is emerging of the importance of a purely quantum effect, i.e. Young interference, as the ejected electron scatters from the target and projectile centers of charge. The experimental confirmation of this result is tentative and much more work needs to be done.

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I-26

LASERS ON SELF-TERMINATING TRANSITIONS: PHYSICS AND APPLICATIONS

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The history of lasers on self-terminating transitions (STT), oscillating from the upper resonant level to the lower metastable one covers up to four decades. The number of obtained laser lines on STT in atomic and ionic spectra is not less than 44 (from ultraviolet 312,2 (Au) to infrared 6456,0 (Sr^+) nm). The parameters of the lasers are also impressive. A great number of unique properties (wide range of pulse recurrence frequencies, high pulse and average output power, large practical efficiency and gain of the active medium) being combined in the lasers of this kind have provided a constantly increasing broad sphere of scientific, industrial and medical applications. This increase consists both in deepening and broadening, involving the newer and newer aspects. On the other hand, the limits for improvement of lasers of such type can still be moved further. During the first period of intense development vast scientific research was performed, among them the practically complete studies of main processes and physical phenomena in the active media of these lasers; the lasing characteristics optimization; working out different techniques of obtaining metal vapors in the discharge, etc. The practical efficiency of the metal vapor lasers are ~ 1 %, the average lasing power ~ 100 W allowed to use them (and first of all the copper vapor laser (CVL)) for a large number of applications. The lasers of this type are produced by the industries of a number of countries.

The stage of rapid development in the end of the 80s was followed by a decrease in the research which, however, did not last long. In the recent years a renaissance in the interest in the STT lasers is observed, related to the achievement of physical efficiency of 9 % and, first of all, with the creation of so-called HyBrID CVL with the average power of ~ 200 W and practical efficiency of ~ 2 %. Another direction of the STT lasers development – the use of different additives to the active medium – have, to our opinion, the most promising perspectives. The wide range of additives (silver, zink, caesium, hydrogen, etc.) used for each type of STT laser, can essentially improve the kinetics of the excitation pulse and relaxation period. The mechanisms of their influence will be presented at the paper based on our experimental investigations.

Several specific applications of the STT lasers will be presented, among them the use of copper-vapor laser for mass-spectrometry of solid state surface, laser cleaning of the illuminators of space flying objects, remote sensing of metal layers in the upper atmosphere, etc.

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I-27

FERMI-SHUTTLE PROCESSES IN THE ELECTRON EMISSION BY ION IMPACT: LOW AND MEDIUM ENERGIES

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Ionization is one of the fundamental phenomena in collision physics. Differential spectra of ejected electrons provide detailed information about the collisions. Characteristic structures in these spectra can be associated with different collisions mechanisms. Large electron yields, compared to first-order theoretical predictions, have often been observed in the high-energy part of the electron spectra in ion-atom, ion-molecule and ion-solid collisions. Such fast electrons may play significant roles in many fields (astrophysics, ion-beam technologies) and hold also of considerable technological importance (plasma physics or analytical methods).

In this work we focus on the above high energy tails of the spectra in ion-atom collisions, where the electron velocity is higher than two times the projectile velocity (2V). In combined experimental and theoretical studies, we demonstrate that these parts of the spectra are correlated with a specific multiple scattering process, often referred to as Fermi-shuttle acceleration [1]. The energy gain of ejected electrons can be treated as a result of a ping-pong game, where the ball is the electron itself and the bats are the target and projectile cores.

The experiments have been performed in different laboratories, with ion impact energies in the 1 - 50 keV/u range. Theoretically, we applied a non-perturbative model, the classical trajectory Monte Carlo (CTMC) calculations [2,3]. A main advantage of the CTMC method is that many details of the classical collision scenario can be conveniently analyzed in its framework. The analysis of the CTMC trajectories, e.g., makes it possible to classify and identify multiple electron scattering events.

Both experiments and CTMC calculations have been performed for the same set of projectile-target combinations. A good general agreement has been found between experiment and theory in the studied cases. For the slowest collisions, the analysis of many CTMC events indicates the dominance of long (6-12-fold) Fermi-shuttle type scattering sequences in electron emission above 10 eV kinetic energy.

This work was supported by Hungarian OTKA Grants T046905, the grant "Bolyai" from the Hungarian Academy of Sciences, and the TéT Grant No. GR-11/03.

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I-28

The B-spline R-matrix method for electronic and photonic collisions

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The R-matrix method was successfully applied to different scattering problems last three decades, and there is a very elaborate suite of codes developed in Belfast (North Ireland) [1]. However, these codes have some serious restrictions on the representation of target wave functions that limits the accuracy of the low-energy scattering calculations. In this talk I present a new R-matrix code which implements two new ideas:

- using *B-spline* functions as universal basis set for continuum orbitals;
- allowing *non-orthogonal* orbitals for representation both bound and continuum one-electron radial functions.

B-splines [2] have some advantages in comparison to the numerical functions due to their excellent numerical properties and large flexibility in the choice of radial grid. The most important property for R-matrix calculations is the effective completeness of B-spline basis, so no Buttle correction required in this case.

All existing codes suppose that all one-electron orbitals are orthogonal. For bound orbitals, it means that many correlation effects (such as term-dependence or relaxation effects) can not be introduced directly. For continuum orbitals, the orthogonality means that we introduce the artificial restrictions on the total wavefunctions, and in order to compensate these restriction, the close-coupling expansion should contain some additional (N+1)-electron configurations that may lead to a pseudo-resonance structure.

The present implementation is based on the general programs [3] for angular integration with non-orthogonal orbitals that allows us to abandon the orthogonality constraints on the one-electron radial functions. It gives us the possibility of independent generation of different target states; and as a consequence, a much more accurate target description than before is possible. For example, it is possible the direct account for term dependence in one-electron orbitals. We do not have to use any additional (N+1)-electron bound terms in the close-coupling expansion. It provides us with more consistency in treatment of N-electron target and (N+1)-electron collision problem and reduces the problem of pseudo-resonance structure.

The present code has been successfully applied for different scattering problems and in some cases we get the considered improvement of cross sections in comparison to standard R-matrix calculations. Especially it concerns the cases where strong term-dependence of valence orbitals should be taken into account (see for example e + Ne results in [4]). The code is considered as being fully tested and was recently submitted in the CPC library. New recent results for the e + Fe^+ scattering and photodetachment of O^- will be presented as example of the further implementation of the code.

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I-29

AUGER ELECTRON - ION COINCIDENCE SPECTROMETRY AFTER ELECTRONIC EXCITATION OF L-SHELL IN ARGON

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The electron L–MM spectrum in argon is decomposed into contributions related to the specific final ionic charge states Ar^{2+} to Ar^{5+}. Because of the data available, the decay schemes related to different structures in non-coincidence Auger spectra could be verified and more accurately determined.

Argon was excited with short pulses of 1-keV electrons and the resulting final ionic charge states were detected by the time-of-flight spectrometer. Both spectrometers and the electron gun were coupled into the coincidence measuring loop running at frequency of 1 MHz. A short excitation pulse was generated in each cycle and the presence of an electron was checked. The ions were analysed only after the electron has been detected; if this was not the case, the ions were removed from the target. The final multi-hit distributions of ions detected by the spectrometer in the coincidence and non-coincidence measurement are described by the statistical model. A comparison is made with the previously published non-coincidence L–MM spectra recorded at various excitation modes, with the coincidence spectra of sharply defined initial states and finally, with theoretical predictions [1-4].

Acknowledgment. This work is partially supported by the bilateral grant BI-HU/04-05-013.

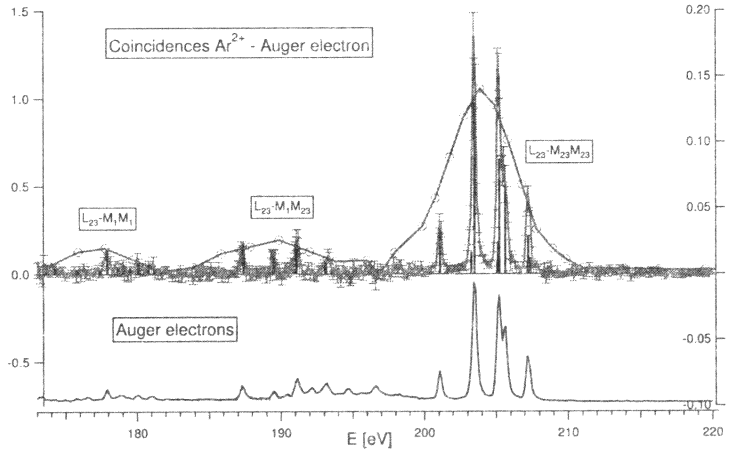

Figure 1: Ar^{2+} - Auger electron coincidence spectrum. Large circles represent data [4].

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POSTER CONTRIBUTIONS

P-1

X-RAY EMISSION FROM RADIATIVE RECOMBINATION OF BARE URANIUM IONS WITH ELECTRONS

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We report here the results of a state selective x-ray recombination experiment performed at the ESR storage ring with decelerated bare uranium ions of energy 23 MeV/amu [1] for relative electron energies 0-1000 meV. In this experiment the x-rays emitted from recombination of U^{92+} ions with electrons in the electron cooler were measured using two germanium detectors placed nearly at 0° and 180° with respect to the ion beam direction. The measurements were performed at cooling conditions and for six off-cooling electron cooler voltage settings. In this way, for electron energies below 200 meV the experiment was sensitive on the „enhancement" effect, while from the highest relative energy of about 1000 meV the transverse electron beam temperature was estimated. The experimental arrangement allowed us to measure simultaneously the photons emitted directly from radiative recombination to low n-states, namely K-RR, L-RR, as well as the Lyman and Balmer x-ray photons from subsequent deexcitation cascades following a recombination to high Rydberg states. From K-RR and L-RR intensities the recombination rates for n=1,2 states were obtained while the intensities of Lyman and Balmer transitions gave information on the recombination into a wide range of high n-states states. In this manner both the recombination to the low lying (n=1,2) and high n-states were simultaneously probed. The measured dependences of the recombination rate on the relative electron energies for different n-state regimes are compared with the theoretical calculations of the radiative recombination effect. A role of the recombination to high Rydberg states in context of the enhancement effect as well as the influence of the relativistic effects are discussed.

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P-2

Preliminary results on luminescence induced by thermal treatment and by N_2^+ ion bombardement on MWNT bundles

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In this paper we report preliminary studies on luminescence emission from bundles of multiwalled carbon nanotube (MWCNT). We performed measurements of luminescence emission induced both by heating (thermo-luminescence TL) and by ion bombardement (iono-luminescence IL). The MWCNT bundles are initially processed by Joule effect in the temperature range 600-2000 K for 15 hours. For increasing N_2 exposure we do not observe any N_2 absorbtion evidence on the sample as can be seen in both Auger and TL spectra. When the same sample is bombarded by N_2^+ ions at 2 keV, Auger analysis reveal N_2 presence even after thermal treatment at 1900 K. IL spectra, detected during ion bombardement, show a decrease in intensity as a function of time. This results are consistent with hypotesis of progressive sample metallization and are confirmed by the results obtained from Na deposition and Na^+ bombardement on MWCNT.

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P-3

ANGULAR DIFFERENTIAL IONIZATION CROSS SECTIONS FOR ANTIPROTON AND HELIUM COLLISIONS

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We present single and double ionization cross sections for antiproton and helium collisions in the impact energy range from 1 keV to 1 MeV. We compare the time-dependent two-electron coupled-channel (CC) calculations with other non-perturbative theories. Our approach permits to describe the ionization process of helium by charged particles impact [1]. We treat the collision of antiprotons with the helium target in the semiclassical approximation. Above 10 keV impact energy we use straight-line trajectories and below 10 keV we apply Coulomb hyperbolas to describe the motion of the antiproton. As basis set we use a highly-correlated Configuration Interaction (CI) wave function built up from Slater-like orbitals and regular Coulomb wave packets. To separate the excited, single- and double-ionized states we apply the Feshbach projection method.

Fig. 1. shows our CC result with Continuum Distorted Wave with Eikonal Initial State (CDW-EIS) [2] and Classical Trajectory Monte Carlo (CTMC) [3] calculations for 100 keV energy of antiprotons. At zero electron emission angle the anti-cusp can be seen clearly.

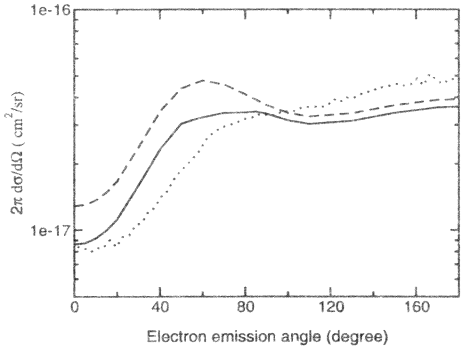

Figure 1. Angular differential ionization cross sections for electrons emitted in 100 keV antiproton and helium collisions. Solid line: coupled-channel method, dashed line: CDW-EIS, dotted line: CTMC.

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P-4

Mechanism for electronic excitation in the interaction of slow Na^+ with Al surfaces

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Electron emission is a fundamental consequence of the interaction of slow ions with solid surface and occurs at the expense either of the potential energy of incoming particles (potential electron emission) and of their kinetic energy (kinetic electron emission). Due to their low ionization potential, impact of alkali ions on metal surfaces is very well suited for studies of kinetic electron emission. Here, We report energy distributions and yields of electrons emitted in the interaction of slow Na^+ ions (150-4000 eV) on Al surfaces. Our measurements indicate the strong interplay between different emission mechanisms, such as Na-projectile and Al-target Auger electron emission, decay of bulk plasmons and electronic collision cascade. These results indicate that electron promotion occurring in binary collision between incoming projectiles and target atoms is the dominant primary excitation mechanism.

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P-5

VICINAGE EFFECTS IN CLUSTER IONIZATION BY ION IMPACT

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In a recent experiment, N. Stolterfoht and co-workers [1] observed the appearance of interference effects in the single ionization of randomly oriented H_2 molecules by the impact of heavy ions. The experimental data were reasonably adjusted by means of a simple model first derived by Debye [2] and independently by Ehrenfest [3] in 1915 for the diffraction of X-rays by molecules. However, recent experimental evidence [4] shows period doubling effects, which are usually associated to re-scattering events of the emitted electron by different centers. Here we show that, due to these multiple-scattering processes, a "vicinage" function appears superimposed to the Debye-Ehrenfest term. We demonstrate that its contribution is significant and cannot be neglected in any accurate evaluation of the electron momentum distribution.

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P-6

JOST FUNCTION DESCRIPTION OF ELASTIC AND FEW-BODY RESONANCES

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We discuss how the analysis of the zeros of the functions introduced by Res Jost in 1947 [1], acting individually or collectively, provides a comprehensive framework for describing resonances in single and multichannel collisions. In particular, we propose a generalization of Wigner threshold law [2] that copes with some deviations recently observed in opening reaction channels [3]. We also pay special attention to the appearance of zeros of the s-wave Jost function in the fourth quadrant of the complex momentum plane, as analysed by Nussenzveig in 1959 [4] but erroneously ruled out in following studies [5]. Finally, we discuss the possible experimental observation of these and others effects.

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P-7

SPECTROSCOPY OF AN OPTICAL EXCITED Ga DOPED SiO_2 SURFACE

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We have checked that when Ga vapour is kept in a cell of fused quartz (amorphous SiO_2), at a temperature of 900°C or above for one day or more, the effective density of Ga atoms is less than that corresponding to the saturated vapour pressure [1]. The loss of Ga atoms is due to the strong interaction between the Ga vapour and the SiO_2 walls by which Ga atoms are trapped inside the silica structure. The so "doped" silica gives rise to some typical fluorescence spectra following laser excitation. They start appearing at T=900°C and, once manifested, they persist even if the cell is cooled down and the fluorescence spectra are recorded at room temperature. No such spectra are detected in pure quartz when it is excited by the same radiation. Preliminary evidence of this effect has been reported [1] and here we show the outcome of its detailed spectroscopical analysis just begun. These spectra are independent on the shape of the cell, on the presence and the kind of buffer gas inside it. The experiment is performed by shining laser pulses at several different wavelengths starting with photons at 403.3 nm (24788.58 cm^{-1}), resonant with the fundamental Ga transition. Most of the peaks present in the spectrum around the resonant excitation, exhibit a typical Raman scattering aspect as, when the laser radiation is detuned from the resonance both to the red and to the blue of 185 cm^{-1} wave numbers, those peaks shift of the same amount so maintaining the same energy difference from the excitation. We think that the inclusions, inside the fused silica, of Ga atoms, produce structural changes responsible for the Raman scattering spectrum.

This hypothesis is confirmed by electron spin resonance (ESR) measurements done in SiO_2 samples heated up to 1050°C in He atmosphere either in absence or in presence of Ga vapour. Indeed, the detected ESR spectra evidence the presence of a signal centred around the value g=2 of the free electron peculiar to samples heated in atmosphere containing Ga.

The mechanism responsible for this permanent inclusion of Ga atoms inside the fused silica structure is not clear at the moment and further experiments based on temporal as well as frequency analysis of the fluorescence spectra following laser excitations at several largely different wavelengths are in progress.

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P-8

EMISSION AND ELECTRON/ION ANALYSIS OF THE ABLATED PLUME FROM $LiYF_4$ CRYSTALS DOPED WITH Tm^{3+} OR Nd^{3+} IONS.

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We report about the analysis of the plume ablated from YLF crystals doped with Tm (1% concentration) and with Nd (1.5% concentration), by laser pulses provided by the third harmonic of a Nd^{+}-YAG laser at 355 nm, pulse duration 13 ns, maximum pulse energy 130 mJ. The laser pulse is focused to a spot of 1mm diameter and the repetion rate is 10 Hz. The target is rotated so to reduce ablation of the same spot. The plume emission is spectroscopically analysed along its axis at different distances, d, from the target. A fibre transfers the emitted radiation, collected via a lens/iris combination above the view port on the topside of the ablation chamber, to the input slit of a 320 mm monochromator equipped with a 1200 grooves/mm grating and a frequency resolved spectrum is recorded via a photomultiplier and a boxcar averager system. The available spectral range is 300 – 700 nm. Most of the measurements are done at 6 J/cm^2 fluence, while the ablation threshold occurs below 3 J/ cm^2. The plume emission is very rich in features and shows the elemental lines belonging to all the components of the target either neutral or ionized and other features yet to be assigned. Most of these lines persist at d 1 cm with the exception of some transitions associated with neutral fluorine in the range 675-700 nm. The insertion of two electrodes perpendicular to the plume axis at d = 0, conveniently polarized, allows the detection of either electron or ion signals. These signals are time analysed via a 500 MHz digital oscilloscope. The electron signal gives information about the onset of the plume, while the delay of the ion signals in respect to the trigger given by the laser pulse, and their shapes provide some information on the dynamics of ablation and on the ion species ablated, respectively. Information about the plasma expansion can be obtained from the time resolved analysis of the single lines in the plume emission spectrum at different positions along the plume axis. Moreover the analysis of the intensities of the lines corresponding to each element can confirm, in the plume, the stoichiometric composition of the crystals. This analysis is just started and the results will be shown together with others obtained by changing some observation parameters such as the direct excitation of the constituents in the plume. This research is the subject of the PRIN '04 national project "Nanostructure photodeposition for non-linear optics", cofunded by the Italian MURST.

The crystals used in the experiment are grown and provided by the unit of the Scuola Normale Superiore (SNS) in Pisa, one of the partners in the project.

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P-9

PCI Effect in the Tl I 221.1 nm Line Excitation Function

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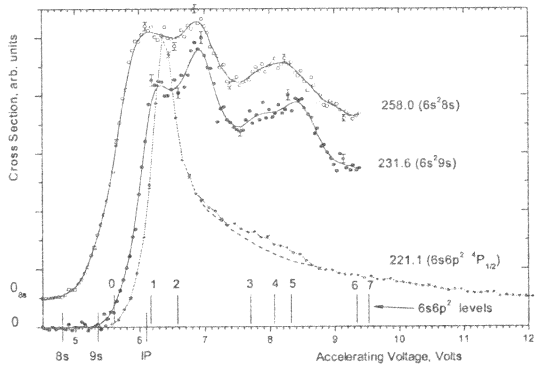
Recently a considerable post-collision interaction (PCI) contribution to the electron-impact excitation functions (EFs) of the Tl atom sharp series spectral lines [1, 2] in the autoionizing state (AIS) region of the $6s6p^2$ configuration [3] was found. The lowest $^4P_{1/2}$-state of the above configuration lies below the ionization potential. Its combination with the atomic ground state provides an intense 221.1 nm spectral line, the excitation of which was studied by us earlier [4]. Here we examine for the results of a thorough remeasuring this line EF, which, in our opinion, demonstrates the PCI effect on the $6s6p^2$ AIS.

Figure presents EF of the 221.1 nm line obtained. The EFs of the sharp series $6s^26p\ ^2P^o_{1/2}$ – $6s^2ns\ ^2S_{1/2}$ lines for n=8, 9 (258.0 and 231.6 nm) [1, 2] are depicted in the figure also. The vertical bars depict the positions of the excitation thresholds for the above lines (denoted by "8s", "9s"), the ionization potential (IP) and the levels of the $6s6p^2$-configuration (denoted by digits).

The FWHM of the main EF peak for the 221.1 nm line corresponds to the electron beam energy spread giving an evidence of the resonant nature of its excitation. In [4], the "narrowness" of this EF was related exclusively to the exchange character of excitation of its initial quartet $6s6p^2\ ^4P_{1/2}$-level ("0"). The main EF peak occurs close to the $6s6p^2$ AIS of the $^4P_{3/2}$-configuration ("1") and is shifted by ~0.12 eV with respect to the first peak of the 231.6 nm line (with the initial $6s^29s\ ^2S_{1/2}$-level) towards the higher energies The binding energies of initial levels for the 221.1 and 231.6 nm lines are ~0.501 and 0.7583 eV, respectively. Such specific observable shift could be due to PCI at the decay of the $6s6p^2\ ^4P_{3/2}$-AIS similarly to the 258.0 and 231.6 nm lines case [2].



The deviation from the monotonous EF decrease between 6.6 and 8.6 eV is evident. It could be related to the quartet $^4P_{5/2}$ ("2") and doublet $^2D_{3/2}$, $^2D_{5/2}$ and 60 $^2P_{1/2}$ + 35 $^2S_{1/2}$ ("3","4","5") AIS of the $6s6p^2$ configuration [3]. In this case the effect of the shape resonance of the $6s6p^2\ ^4P_{5/2}\varepsilon\ell$ ($\ell\geq1$) negative-ion state formed at the AIS term excitation and effectively decaying into $6s6p^2\ ^4P_{1/2} + \varepsilon_1\ell_1$ [2] is possible within the 6.6 eV to 7.6 eV energy region, while that in the 7.7 to 8.6 eV region could be due to the doublet levels-related PCI.

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P-10

Study of the interference effects in the ionization of H_2 by the use of two-center wavefunctions

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Due to the two-center character of the target molecule, interference effects occur in the photoionization of the molecular hydrogen [1]. In a previous paper the photoionization cross section have been calculated using a simplified description of the final state (plane waves)[2]. This approximation gives us a good description of the main features of interference effects, but it is gauge dependent (the angular distribution of the of the outgoing electrons depend on the used gauge and the cross section in length gauge is nearly four times higher than the cross section in velocity gauge [2]). Using a much more accurate description of final state (by two-center wavefunctions) this gauge dependence of angular distribution was reduced, but the cross section in length gauge is still higher. The photoionization cross section was calculated using the first order approximation of the time dependent perturbation theory. The two-center character of the final state was reproduced by different wavefunctions. The first type was the 2C wavefuntion [3], which is a plane wave multiplied by two Coulomb distorsion factors. The second one is a linear combination of two Coulomb functions. This wavefunction does not reproduce correctly the asymptotic behavior, but it describe well the two-center character of final state at the vicinity of the nuclei. Due to the complex structure of the final state wavefunctions the photoionization cross section was evaluated numerically. The partial-wave expantion of the final and initial wavefunctions was made and the partial photoionization cross sections have been studied. This partial-wave expantion alowed us a much more detailed study of the interference effects.

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P-11

NEAR THRESHOLD ELECTRON IMPACT IONIZATION CROSS SECTION FOR SULFUR ATOMS

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Up today electron-impact ionization is one of the most intensively investigated processes in atomic and molecular physics [1]. These experiments however, are associated with difficulties: high temperatures and densities are required to produce of atom beams, momochromatic intensive electron beams.

A crossed electron and atomic beams scattering geometry was employed to measure the ionization efficiency curve for sulfur atoms. Our electron spectrometer comprises two serially mounted hypocycloidal electron energy analyzers [1]. The whole spectrometer is immersed into the homogenous magnetic field. Great care was taken in selecting the value of the extracting potential at the electrode, mounted normally to the atomic beam direction. By careful choosing this potential as low as possible (~1.5 V), its influence on the motion of the monochromatized electrons in the collision region was minimized and the full collection of the formed ions was reached.

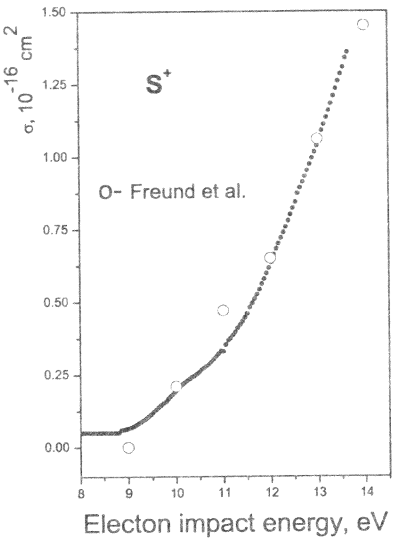

Fig.1

The atomic beam was produced using a compact effusion source made of the stainless steel with a microchannel exit to minimize the angular divergency of the beam. The temperature of the microchannel plate was taken about 50 K higher than that of the metal vapour in the heated reservoir. This atomic beam source enabled to produce an atomic beam with the concentration of two orders of magnitude higher than that in the case of a standard effusion source.

A typical value of the electron energy spread was 0.15 eV (FWHM) in the 0.1–15 eV energy range. The primary electron beam current was equal to 10^{-7} A. Such values of electron energy spread and beam current for the primary electron beam passing through the collision chamber were chosen to provide identical conditions for carrying out all the measurements. The energy scale was calibrated with the accuracy of ±0.05 eV.

In Fig.1 the measured ionization cross-section normalized to the results of Freund et al [1] is shown. The relative uncertainties in the cross section lie within 2%. The validity of the Wannier-law is tested. Four distinct resonance features are revealed in this curve at the energies above the ionization threshold. The obtained ionization cross section for sulfur atoms complement the available atomic data, allowing the resonance features to be resolved.

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P-12

Dynamic Interactions of Fast Ions with Multiwalled Carbon Nanotubes

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We use hydrodynamic model to describe dielectric response of a multiwalled carbon nanotube, consisting of up to several tens of concentric cylindrical shells, to an external point charge. In particular, we model the collective excitations of the nanotube's σ and π electrons by means of two separate fluids occupying each cylindrical shall of the nanotube, which are allowed to interact electrostatically with each other [1]. As a result, rich plasmon spectra are developed, with distinctly separated low-frequency group of quasi-acoustic plasmons corresponding to the π electron longitudinal oscillations. The low phase velocity of such quasi-acoustic plasmons can give rise to a drift instability in the presence of electron current through the nanotube.

The hydrodynamic model is further used to evaluate the stopping power, or the energy loss per unit path length, as well as the image potential, or the classical electrostatic self-energy, for ions moving parallel to the nanotube axis. It is found that both quantities are profoundly affected by the increasing number of shells, especially at higher ion speeds when the nanotube response is dominated by the high-frequency plasmons due to combined oscillations of both σ and π electrons. In particular, for ion channeling through carbon nanotubes at high speeds, the dynamical image force is found to efficiently deflect the ion trajectories towards the nanotube walls [2].

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P-13

ELECTRON EXCHANGE INFLUENCE on the ELECTRONIC ENERGY LOSS of IONS in SIMOX STRUCTURE

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The electronic energy loss of ions channelled in single crystal has long been a theoretical and experimental problem with application consequences. The loss in the subsurface region is mainly determined by initial ion beam charge. It is clear that the electron exchange between ion and the target is a continuous process during the ion motion in the crystal and thus modifying the energy loss. Another important feature of ion beam interaction with crystals is dependence of elementary processes on impact parameter with respect to scattering centres.

The simplest transmission experiments, which make use of channelling effect, require relatively thick crystals and thus high ion energy. At lower energy one can use RBS geometry with large angle scattering and single crystals formed in SIMOX structure. In the latter case the extraction of information about fundamental process of the energy transfer is more cumbersome [1].

The hypothesis on anomalies in stopping power [2] or back-scattering yield [3] due to pre-equilibrium charge state effect just after crossing the crystal surface were previously studied and rather not solved, as being behind the experimental resolution. Recently however, it was reported measurement on differences in the energy loss of He^{+} and He^{2+} ion beam channelled in Si single crystal (SIMOX) [4].

In this research report we analyse transmission experiments with single crystals and RBS measurements with SIMOX structure by means of Monte Carlo simulation code with explicit implementation of impact parameter dependence of the electron transfer and the electronic energy loss processes. It was shown that, although all the basic experimental characteristics of the ion channelling have been successively reproduced, effects related to the charge pre-equilibrium region turned out to be much smaller than these determined from experiment [4].

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P-14

ELECTRON SCATTERING ON SULFUR-CONTAINING MOLECULES

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During our systematic studies [1-3] we have found that the presence and location of particular atom in molecule considerably reflects in the shape and magnitude of total cross section (TCS) energy dependence. The effect is especially noticeable at low impact energies.

In this contribution we present (Fig. 1) our latest TCS measurements for electron scattering from sulfuryl chloride (SO_2Cl_2). Further, along with earlier TCS data for other molecules containing sulfur as a central atom, these results are used to demonstrate the importance of central atom in scattering processes. More results and discussion will be presented at the Conference.

Partial support by the MENiS and by the MNiI is acknowledged.

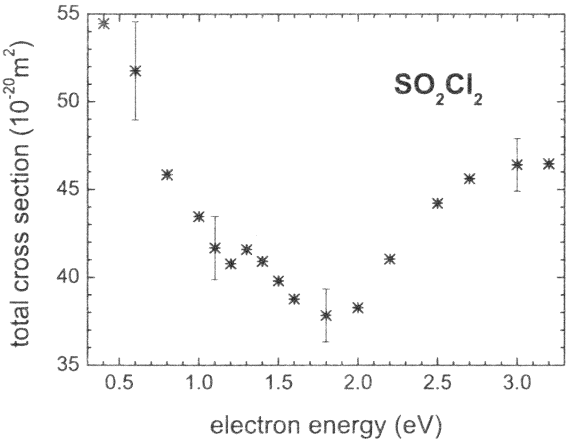

Figure 1: Absolute total cross section for electron scattering from sulfuryl chloride molecule (preliminary results).

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P-15

X-ray emission from collisions of O^{7+} with molecular and atomic gases in the 35 to 50 KeV range.

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The solar winds are mainly comprised of protons and helium ions; however, the energetic x rays emitted from ion-comet interactions originate from the smaller fraction of heavier highly charged solar-wind ions (e.g., C, N, O, Mg, Fe ions), which have large electron-capture cross sections. One of the goals of this work is to provide high-resolution spectroscopic information for modeling of soft x-ray emission observed from solar-wind ion interactions with cometary gases. Using the JPL ECR ion source [1] in conjunction with a grazing incidence XUV spectrometer, equipped with a CCD camera, x rays in the wavelength range from 2 to 40 nm have been measured in collisions of O^{7+} with CH_4, CO, He, H_2, and H_2O gases.

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P-16

Development of CNT/Si_3N_4 composites with improved mechanical and electrical properties

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Abstract

Silicon nitride based composites with different amount (1, 3 or 5 wt%) of carbon nanotubes have been prepared by using hot isostatic pressing. Composites with 1wt%, 5wt% or 10wt% carbon black and graphite have been manufactured, in comparison. Optimisation of the manufacturing processes has been performed, providing intact carbon nanotubes during high temperature sintering.

In the case of 1wt% or 3 wt% carbon nanotube addition the increase of gas pressure during sintering resulted in an increase of bending strength. It was found that microstructure features achieved by properly designed sintering parameters are the main responsible factors for the strength improvements. Scanning electron microscopy showed that carbon nanotubes have a good contact to the surface of silicon nitride grains (fig.1). The electrical properties of silicon nitride matrices with carbon addition may change essentially.

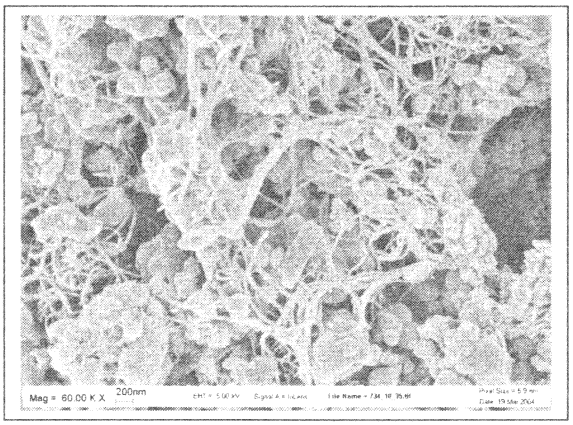

Figure 1. Fracture surfaces of CNT/Si_3N_4 composites: sintering at 1700°C, 2MPa, 0h (1% CNT)

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CO INNER-SHELL EXCITATION AND IONISATION STUDIED BY ELECTRON-ELECTRON COINCIDENCE EXPERIMENTS

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The CO inner shell excitation and ionization have been studied in a series of coincidence experiments. Energy loss - Auger electron coincidence experiments have been used to investigate the formation and decay of the CO ($1s^{-1}2\pi$ $^{1,3}\Pi$) inner shell excited states, while Auger electron-photoelectron and photoelectron-ion experiments have been performed to characterize the C 1s photoionization.

The multicoincidence-end station of the Gas Phase beamline at Elettra [1] has been used for both types of experiments. For the electron impact measurements it has been equipped with an electron gun which can be operated at different incident energies between 100 eV and a few keV. In this set-up both the inelastically scattered and Auger electrons are detected at 90° with respect to the direction of the incident beam. This scattering angle implies large momentum transfer, i.e. the kinematic conditions favoura non-dipole transitions, and makes them clearly visible. Then, via the energy loss-Auger electron coincidence experiments, the resonant Auger spectra due to the decay of both the singlet and triplet excited states have been determined.

In addition, the photoionisation of the C 1s core level has been studied via photoelectron-Auger experiments at about 318 eV photon energy. The angular distributions of the Auger electrons due to different CO^{2+} final states have been measured in coincidence with energy and angular selected photoelectrons. Finally the angular distribution of the photoelectrons has been measured in coincidence with ions emitted at 90° with respect to the polarization of the incident radiation. The combined results of these measurements are expected to provide valuable and new information on the dynamics of C1s photoionization.

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P-18

INTRINSIC AND EXTRINSIC CONTRIBUTIONS TO PLASMON EXCITATIONS

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In this work, we study in detail the process of excitation of bulk and surface plasmons during the emission of electrons in the proximity of a solid surface. We take into account the effects due to electron transport (extrinsic contribution) and to residual holes (intrinsic contribution) in the case of X- ray photoemission spectroscopy (XPS) and Auger electron spectroscopy (AES). We use the dielectric response of the metal and the specular reflection model for describing these processes. The results illustrate that, depending of the distance from the surface, to separate extrinsic and intrinsic contributions could be ambiguous due to interference phenomena in XPS and AES plasmon excitation. The results of the calculations are compared with experimental data as well as with the earlier works using the dielectric model [1,2].

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P-19

SOPPING POWER FORMULA FOR LOW AND INTERMEDIATE ENERGY POSITRONS

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Abstract:

A simple stopping power formula for positrons is presented. Analytical expressions for effective charge and effective mean excitation energies of target atoms in the modified Rohrlich and Carlson stopping power formula are employed. The Lenz-Jensen statistical atomic density model has been used for calculations of effective charge and effective mean excitation energies of target atoms. The calculated results of stopping power for positrons in some materials are compared with experimental data and a number of other calculations such as PENELOPE code results.

PACS: 34.50.Bw; 61.80 Fe:

Key Words: Stopping power, positrons, effective charge, effective mean excitation energy.

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P-20

PROGRESS IN ELECTRON-ION COLLISIONS STUDIES

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The detailed experimental high-resolution studies of inelastic processes have been carried out during the last decades in collisions of slow electrons with alkali [1], alkaline-earth [2], zinc [3], cadmium [4], thallium [5] and indium [6] metal ions by the VUV-spectroscopy method combined with the crossed beam technique.

The experimental setup comprises the following innovated elements: a high-temperature metal-vapour ion beam source; the spectral monochromators for the 40-600 nm region, a modulation system for the detection of extremely weak photon fluxes; a PC-based unit for controlling the experimental procedures and data processing.

The main attentation has been paid to: the role of resonances in the excitation of ions, elucidation of new regularities and phenomena in the dynamics of electron-ion scattering related to the excitation and decay of atomic autoionizing states (AIS), search for and study of the emission related to the radiative decay of AIS.

The following results have been obtained:

- the energy dependences of the electron-impact excitation cross-sections for the dipole-allowed, intercombination and non-dipole-allowed transitions;
- the resonance contribution to the electron-impact excitation cross-sections, energies and widths of the observed resonances;
- the wavelengths of the spectral lines corresponding to the radiative decay of quasimetastable atomic AIS with their tentative assignment;
- the role of relativistic, electron-correlation effects and configurational mixing in the probability redistribution for electron and radiative atomic AIS decay channels;
- the analysis of the excitation mechanisms for the spectral lines under study;
- the absolute cross-sections of electron-impact excitation and dielectronic recombination of singly-charged ions.

The obtained results show that the relativistic and correlation effects strongly influence the role of resonance processes and the ratio of the radiative and electronic AIS decay probabilities and that these effects become increasingly important for multi-electron atomic systems.

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Target element dependence in the elastic and inelastic energy loss of fast heavy ions

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Abstract:
The target atomic number dependence of elastic and inelastic stopping power has been investigated by using theoretical stopping power formulations from literature. The stopping powers for target elements with atomic numbers 3 to 92 are calculated on the basis of Montenegro et al. model and nuclear stopping powers is calculated from Wilson et al. formulation. Firstly, Z_2 dependence of the electronic stopping power is examined for light and heavy projectiles in these elements. We investigated Z_2 dependence of the nuclear stopping power also by comparing the stopping powers for all considered targets. A strong Z_2 oscillation in nuclear and electronic stopping power has been observed for light and heavy ions as a result of varying densities of neighboring elements. We have also determined the target materials which applies maximum total stopping force for some incident ions.

PACS: 34.50.Bw; 61.18.Bn:

Key Words: Stopping power, heavy ions, energy loss

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P-22

SINGLE AND DOUBLE K-SHELL IONIZATION CROSS SECTIONS OF SI

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In this work we study theoretically the electron emission following the ionization of Si($1s^2$). The reason for choosing the Si K shell is justified by the large number of experimental investigations of K X-ray spectra of Si induced by heavy and light ions. The main aim of these studies was to determine the double to single 1s ionization cross section ratios of Si using high-resolution X-ray spectroscopy [1].
We present single- and double ionization cross sections of silicon K-shell for proton impact within the framework of a three- [2] and four-body [3] Classical Trajectory Monte Carlo (CTMC) method. The calculations are based on the independent particle model. As projectiles we consider protons with energies between 0.25 and 4.5 MeV. Our results are compared with other theoretical calculations and experimental data.

This work was supported by the Slovenian Ministry of Education, Science and Sport of Slovenia through the research program *Low Energy Physics* (PO-0521-0106-02), the Hungarian Scientific Research Found OTKA Nos. T046095, T046454, the grant "Bolyai" from the Hungarian Academy of Sciences, and TéT Grant No. SLO-15/03.

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P-23

INFLUENCE of PHASE TRANSITION in NICKEL on ION CHANNELING in NI SINGLE CRYSTALS and on STOPPING in NI FOILS

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From the previous experimental results on transmission of ions through Ni foils and from theoretical analysis of the results we draw the conclusion about correlation between ferro-paramagnetic phase transition and the anomalous behaviour of the electronic energy loss end the energy loss straggling of ions in Ni at the Curie temperature T_c [1-2]. It seems that even tiny change of the electronic density of states (DOS) can have an influence on the interaction of energetic ions with foils. We expected similar effects during interaction of ions with magnetic single crystals.

We present experimental results on change of Rutherford angular yield (RBS) of protons back-scattered from subsurface regions of Ni and (for reference) Si single crystals as function of the crystals temperature.

Close to the room temperature the standard behaviour of channelling characteristics for both Ni and Si single crystals, like increase of the minimum yield χ_{min} and decrease of width at half-minimum $\psi_{1/2}$ with temperature for particular dips, were determined and analysed.

For Ni single crystal the anomalous behaviour of χ_{min} and $\psi_{1/2}$ at T_c was found and it was interpreted as due to the structural and ferro-paramagnetic phase transition at T_c. In the experiment the two concurrent processes: radiation damage - randomising the subsurface region and annealing of crystal – restoring and cleaning the crystal structure, were set to cancel each the other.

We implemented the interaction of ions with the field of magnetic domains in the Monte-Carlo code and the analysis of the RBS yield showed crucial role of classical magnetic domains in explanation of the effect.

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P-24

IONIZATION COEFFICIENTS IN GAS MIXTURES

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We have tested the application of the common *E/N* (Wieland approximation [1]) and the common mean energy (CME) combination of data for pure gases to obtain ionization coefficients for mixtures. Test calculations were made for Ar-CH_4, Ar-N_2, He-Xe and CH_4-N_2 mixtures. The Ar-CH_4 mixtures were found to be the most difficult combination of the selected gases for the application of the mixture law. The application of the technique for all other gases where we tried the same procedure gave much better results. The method was tested by using the ELENDIF code [2]. Fig. 1 shows $\alpha/N(E/N)$ for pure He, pure Xe and the mixture of these gases obtained by Boltzmann code, along with results obtained by Wieland approximation and CME procedure. The standard combination procedure gives poor results in general, due to the fact that the electron energy distribution is considerably different in mixtures and in individual gases at the same values of *E/N*. The CME method provides an extended region of reasonable usefulness, at least for the case when the ionization coefficients in pure gases do not differ by more than two orders of magnitude [3].

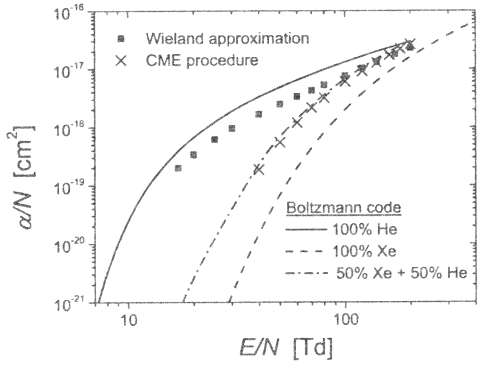

Figure 1: Calculated α/N vs. *E/N* for Xe, He and 50% Xe + 50% He mixture.

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ELECTRON IMPACT EXCITATION OF THE 6p7s $^3P_1$ STATE OF Pb ATOM

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In our previous paper [1] we reported preliminary results for relative differential cross section (DCS) for elastic electron scattering by atomic lead at 40 eV electron impact energy and the scattering angle range from 10° to 148° . We also performed inelastic DCSs measurements at the same target and here we present preliminary results on electron impact excitation of the 6p 7s $^3P_1$ state of Pb atom. The angular distribution of the scattered intensity in the range from 0° to 148° was determined at 40 eV electron impact energy also.The experiment was carried out using a crossed electron-atom beam technique in the electron spectrometer "ESMA", both described in more details elsewhere [1, 2].

An energy loss spectrum is shown in figure1. Obtained experimental results for relative inelastic DCS are presented in figure 2. Absolute DCS values will be determine through the normalization of relative DCS to the optical oscillator strength (OOS) utilizing the forward scattering function (FSF) for generalized oscillator strengths (GOS).

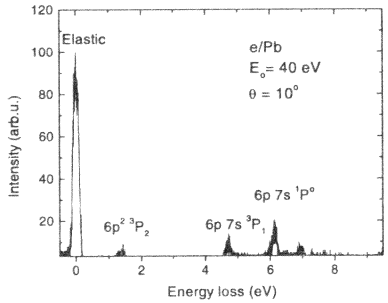

Figure 1: Energy loss spectrum of Pb atom

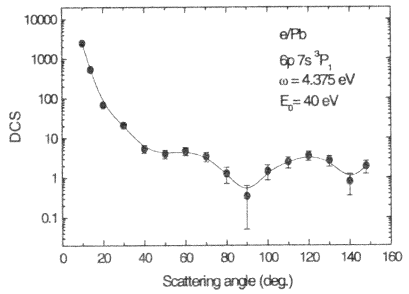

Figure 2: Relative DCSs for the 6s7p$^3P_1$ state

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ATOMIC EXCITATION AND IONIZATION FOLLOWING PHOTOIONIZATION — BEYOND THE SHAKE PROCESS —

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After inner-shell photoionization takes place, the electrons in the same atom experience sudden change in the central potential and can be excited to one of unoccupied bound states (shakeup) or ionized to the continuum (shakeoff) [1]. This process has been usually treated with the shake model and electron excitation probability is calculated in terms of imperfect overlap of electron wave functions between the initial and final states due to creation of an inner-shell vacancy.

However, the shake model is valid only for high-energy incident photons. When the velocity of the ejected photoelectron is slow, the presence of this electron causes additional atomic electron excitation. Recently we have developed a new model for atomic excitation accompanying inner-shell ionization, which takes into account the Coulomb interaction between the outgoing electron and atomic electrons as well as the change in the atomic potential [2]. The model is based on the time-dependent perturbation theory and the final expression for probability amplitude of electron transition is written as the sum of the overlap integral between the initial and final wave functions and the term due to the Coulomb scattering between two electrons. The first term corresponds the conventional shake process. It is interesting to note that the shake process is only monopole interaction, but higher-order multipole transitions are possible through the Coulomb interaction term.

This model is so general that it can be applied to any kinds of inner-shell ionization processes, such as photoionization, electron impact ionization and internal conversion of atomic nucleus. In the present work, we applied it to the case of the outer-shell electron excitation and ionization probabilities following K-shell ionization of Ne. The results indicate that contribution from the Coulomb interaction term is small, but very important for low-energy incident photons, because of strong enhancement of electron excitation probability due to the interference effect between the shake process and the monopole term of the Coulomb interaction. The dipole transition in the Coulomb interaction can explain the so-called conjugate shakeup process.

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P-27

A MONTE CARLO SIMULATION OF COLLISIONAL PROCESSES IN A TOWNSEND DISCHARGE IN NEON

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Abstract

In this work we have analyzed experimental transport data and in particular the spatial profiles of excitation coefficients for $2p_1$-$1s_2$ transition of neon. The spatial distribution of emission is normalized to give the excitation coefficients at the anode and thereby absolute spatial profile of excitation coefficient may be obtained. Electron excitation coefficients were determined from the measurements of the optical signal at the anode after correction for detector quantum efficiency. Measurements for neon were performed in a drift tube with planparalel electrodes. Swarm analysis is performed by comparing experimental and calculated transport coefficients. A null-collision Monte Carlo simulation code was employed, which involves accurate representation of non-equilibrium effects and complete sets of cross sections representing the transport of electrons, ions and fast neutrals. We perform the analysis of our data for neon by using Monte Carlo simulations with contribution of the electron reflection at the anode to the spatial distribution of the 585 nm line emission. Effect of the graphite anode is analysed for conditions of moderate to high values of reduced electric field. At moderate *E/N*, from 10 Td to 1000 Td, electron excitation dominates and it was possible to determine the electron ionization and excitation coefficients. At higher *E/N* the excitation growth towards the cathode is observed and attributed to fast neutral excitation. It was possible to determine the effective fast neutral excitation cross sections that fit the experimental emission profiles normalized to the excitation rates. It was necessary to make significant modifications to the available cross sections for excitation by fast neutrals in order to fit the experimental data. Those processes are of interest for sputtering devices and for fast neutral etching that would reduce charging damage in high aspect ratio integrated circuit processing.

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Photoionization of Eu^+ ions in the region of the 5p thresholds

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We have measured the relative photoionization cross sections of Eu^+ ($Z = 63$) ions in the region of 5p thresholds to compare with those of neutral Eu atoms. The motivation of the present study is to investigate the effect of the removal of the electron in the most outer-shell on the dilution of the (5p;5d) resonance. It is well known that the lanthanide photoabsorption spectra in the region of the 5p excitation are dominated by a broad asymmetric (5p;5d) ^1P resonance lying at an energy range between the $5p^5\ ^2P_{3/2}$ and $^2P_{1/2}$ limits [1]. For the heavier elements (Z = 66-70), strong discrete lines containing a large share of the 5p oscillator strength are observed for transitions to $^2P_{3/2}$ based levels. The detailed structure only for Yb ($Z = 70$) has been explained through the assignment of these discrete lines to the $5p^56s^2nd$ series because of its simplicity, where the electrons in the closed $4f^{14}$ configuration are expected to remain as spectators. Although the existence of unfilled 4f shells of other lanthanides (Tm, Er, Ho, Dy) results in some complexity, the broad similarity of photoabsorption spectra to that of Yb suggests that the 4f electrons retain their spectator role. For the light elements of the lanthanides, on the other hand, the dilution of the resonance into a large number of weaker transitions can be observed due to 6s-5d mixing because of their proximity, and such dilution is observed as pronounced feature in the 5p photoabsorption spectra of La ($Z = 57$) and Ba ($Z = 56$) [2]. Hartree-Fock calculations by Connerade and Tracy indicate that the 6s-5d degeneracy is most pronounced in La and Ba, and it tends to resolve itself gradually as one proceeds towards Yb. Thus if we could modulate the 6s-5d degeneracy somehow, we can expect to control the dilution of the resonance. It is considered that atomic and ionic Eu are good candidates for studying such phenomenon, because Eu is the unique element, in which both of the lowest energy level of atomic and ionic Eu have the core-like half-filled 4f shell, and it resides in the middle of the lanthanides. Such core-like feature results in the simplicity in comparison of the absorption spectra.

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PECULIARITIES OF THE RADIATIVE TRANSITION EXCITATION FROM THE INDIUM ION $5p^2\ ^3P_j$ LEVELS IN ELECTRON-ION COLLISIONS

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The detailed experimental studies of electron-impact excitation of the radiative transitions from the In^+ ion $5p^2\ ^3P_{0,1,2}$ levels to the $5s5p\ ^3P^o_1$ level have been carried out in the energy range from the threshold up to 30 eV at slow electron collisions with indium ions by a VUV-spectroscopy method combined with a crossed electron and ion beam technique:

$$e + In^+(4d^{10}5s^2)^1S_0 \rightarrow e_1 + In^{+*}(4d^{10}5p^2)^3P_{0,1,2} \rightarrow e_1 + In^{+*}(4d^{10}5s5p)^3P^o_1 + h\nu_n \quad (1)$$

The experimental setup [1] comprises the following elements: a high-temperature indium vapour ion source with a special ion-optical system, a 90° electrostatical capacitor for indium ion separation from atoms, a three-anode ribbon electron beam gun, a VUV spectral monochromator, a modulation system for the detection of extremely weak photon fluxes and a PC-based unit for controlling the experimental procedures and data processing.

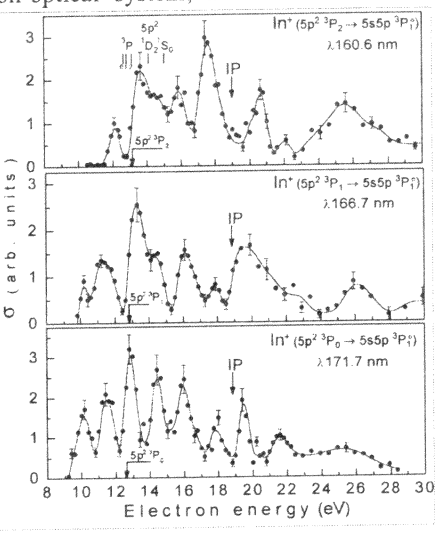

Figure 1. In^+ excitation functions

The energy dependences of the excitation cross sections for the spectral lines under study are presented in figure 1. The excitation functions reveal clearly resolved structure related to incident electron capture and formation of short-lived autoionizing states with subsequent decay both via electron and radiative channels. It has been found that the structure below the excitation tresholds are due to the radiative transitions between the $5p^2(^3P_{0,1,2})nl$ and $5s5p(^3P^o_1)nl$ states of indium atom in the process of dielectronic recombination, and they are the dielectronic satellites of spectral lines. The structure above the excitation thresholds results from the cumulative contribution of resonance processes, which dominate over the direct one, and is the manifestation of both correlation and relativistic effects.

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P-30

EXCITED BAND DENSITIES AND CASCADE PROCESSES OF INELASTIC ELECTRON-ELECTRON SCATTERING IN SEES AND TCS OF CRYSTALS

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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 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), spectra of target current (TCS), and low-energy electron transmission (LEET) spectra 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 present study deals with the development of the above-mentioned methods basing on the bulk energy-band structure (BES) of crystals. As before, (see, e.g. [1-4]) during the calculation of SEES, TCS and LEET spectra 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. The extrema in the SEES, TCS and LEET spectra reflect the energy position of the critical points (the band edges or boundaries and the points of extreme curvature of the dispersion branches) in the unoccupied BES. And there occurs a possibility for the experimental study of the electron dispersion in the region of energies much higher than the vacuum level (thus adding to the traditionally used data of the photoemission, inverse photoemission and optical spectroscopy). The method being developed enables one to distinguish between the volume effects in SEES, TCS and LEET spectra from the surface ones which are to be investigated separately [6,7].

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P-31

COINCIDENCE ELECTRON SPECTROMETER FOR STUDYING ELECTRON-ATOM COLLISIONS

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The energy- and angular distribution of electrons coming from electron-atom collisions are measured by distorted field cylindrical mirror electron spectrometers [1] in our laboratory. In the previous years the spectrometer system was supplemented by a coincidence equipment, in order to detect two of the electrons which are ejected simultaneously in a single collision event.

In our contribution we publish the details of our system with the block diagram and characteristics of the coincidence circuit. Due to the large accepted solid angle of the cylindrical mirror analysers the coincidence yield is still reasonable in the case of inner shell processes of low probability.

In our first measurements we are studying the Auger group ejected after the electronic inner shell ionization/excitation of argon. Previously we have studied the Auger group following the inner shell excitation of argon [2], but the coincidence technique makes possible a better separation from the ionization case. For example at 500 eV primary electron energy (the excess energy above the L ionisation potential is 251.5 eV) the $L_{2,3}$-$M_{2,3}M_{2,3}$ Auger spectrum is measured in coincidence with the 256(±2) eV electrons in order to study the Auger process following the inner shell excitation.

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P-32

An ION-BEM METHOD for ANALYSIS of the THERMAL EXPANSION of FOILS

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The measurements of thermal expansion coefficient α for metals has been a long standing problem [1] and anomalous behaviour of this simple parameter is still of interest [2].

In a previous paper [3] there were reported changes of characteristics of ion beam-foils interaction with the foil temperature.

In this work a method for measuring the thermal expansion for foils is proposed.

The method is based on analysis of proton beam spectra transmitted through the foil and on the assumption that the electronic stopping cross section per target atom remains independent of temperature.

We report on analysis of the energy lost by protons transmitted through foils as a function of temperature and as a function of incident ion energy. The aim was to extract information about the thermal expansion of Ta, Al and Ni foils.

It was shown that the foil expansion coefficient can differ significantly from that of the bulk and the hysteresis in $\alpha(T)$ is driven by structural transformation in the foil.

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P-33

INTERFERENCE EFFECTS IN THE PHOTOIONIZATION OF AR 3P

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The angular distribution of electrons ejected in atomic photoionization process gives detailed information on the structure of atoms, the dynamics of the process and the multielectron correlation effects. The angular distribution of 3p photoelectrons of argon was measured with linearly polarized synchrotron radiation in the 90-330 eV photon energy range in order to determine the dipole and nondipole parameters. The experiment was carried out at the beamline I411 on the third generation MAX-II storage ring in Max-Lab, Lund, Sweden. The emitted electrons were analyzed with ESA-22 electronspectrometer [1]. The photoelectrons were simultaneously detected at 20 different angles in the 15^0-345^0 angular region relative to the polarization vector in the polarization plane.

Strong interference was observed between the direct and indirect channels in the 3p shell photoionization of argon. Figure 1 compares the present experimental β parameters with the results of the R-matrix calculation of Gorczyca and Robicheaux [2] and our new multiconfiguration Dirac-Fock (MCDF) approximation in the 246-253 eV photon energy range. The present experimental dipole angular distribution parameters agree with theoretical values of both calculations. The difference between the dipole parameters β of Ar $3p_{1/2}$ and $3p_{3/2}$ subshells indicates the importance of the spin-orbit interaction in the photoionization.

This is the first experimental data for dipole and nondipole parameters to verify the interference between the direct and indirect photoionization.

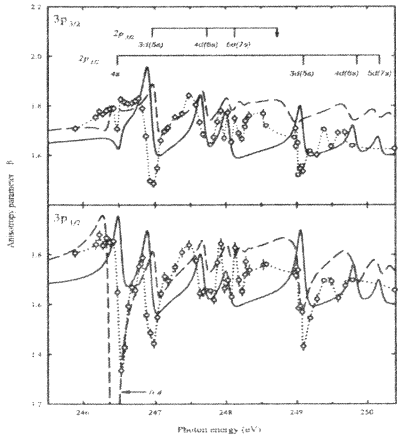

Figure 1: Comparison of the present experimental angular distribution β parameters (dots connected with dotted line) with the theoretical values of the R-matrix [1] (dashed line) and the MCDF (solid line) calculations. The $2p_{1/2, 3/2} \rightarrow ns/md$ resonance positions are shown in the figure as vertical bars whereas arrows indicate the corresponding threshold energies [3].

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P-34

GUIDING OF HIGHLY CHARGED IONS BY SiO_2 NANOCAPILLARIES

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The transmission of Highly Charged Ions (HCI) through nanocapillaries has attracted considerable attention during recent years [1, 2]. One of the motivations is that the interactions of HCI with the capillary walls can be used for probing their electrical properties.

We report effects that were observed when HCI are transmitted through highly ordered SiO_2 nano-capillaries with diameter of about 100 nm and aspect ratio close to 300 (Fig.1). The SiO_2 capillaries were fabricated [3] by photo-assisted electrochemical etching of n-type silicon and adopting silicon micromachining techniques, in collaboration with Microelectronics and Information Technology of KTH. The 7 keV Ne^{7+} ions were obtained from the 14 GHz Electron Cyclotron Resonance Ion Source (ECRIS) located at the Manne Siegbahn Laboratory, Stockholm. The nano-capillaries guide, by a self-organizing charge-up process, the Ne^{7+} ions so that nearly all of the transmitted ions still exist in their initial charge state, i.e. Ne^{7+}, as depicted in Fig.2. The guiding effect is also discerned in a shift of the centroids of the angular distributions for capillary tilts of a few degrees. The angular width of the transmitted beam through SiO_2 capillaries will be compared with those measured with PET capillaries.

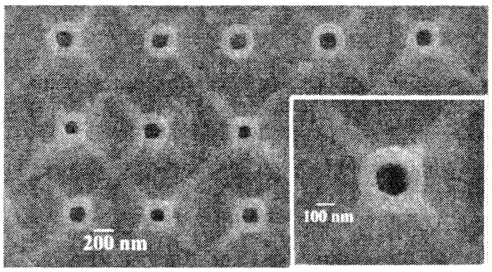

Figure1: Highly ordered SiO_2 nano-capillaries fabricated in a Si (100) wafer.

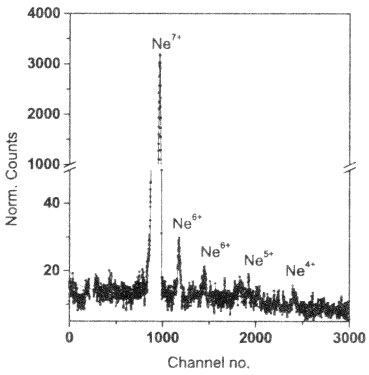

Figure 2: Charge state distribution of 7 keV Ne^{7+} transmitted through SiO_2 nano-capillaries.

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P-35

A TIME-OF-FLIGHT ELECTRON SPECTROMETER FOR THE STUDY OF ELECTRONS EMITTED IN THE ION BEAM DIRECTION IN ION - ATOM COLLISIONS

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We designed and constructed a new kind of time-of-flight electron spectrometer for measurements of the spectra of electrons emitted in forward direction in ion-atom collisions. The principle of operation of the spectrometer is shown in Fig. 1. The electrons ejected in a small angular range (typically $\pm 1^{\circ}$) around 0° from a gas jet target by a well-collimated ion beam (diameter: 0.5 mm) are reflected by an electrostatic mirror in backward angles. The electrostatic mirror is designed for the reflection of electrons in the energy range 5 20 eV. The angle between the normal of the mirror and the direction of the ion beam is 10°, so the angle of the backscattering is 160°. The backscattered electrons are detected by an array of channel electron multipliers (CEMs) mounted at a distance of about 30 cm from the mirror. The detector array consists of four CEMs allowing electron-electron coincidence measurements. The time of flight of the electrons is measured by detecting the electrons in coincidence with the charge-state analysed outgoing projectiles. The electrostatic mirror consists of eight electrodes. The optimal electrode potentials were determined by calculating the electron trajectories with help of the SIMION program for the electron energy range of interest. The spectrometer was tested by C^{+} on Ar collisions in the impact energy range between 100 and 300 keV.

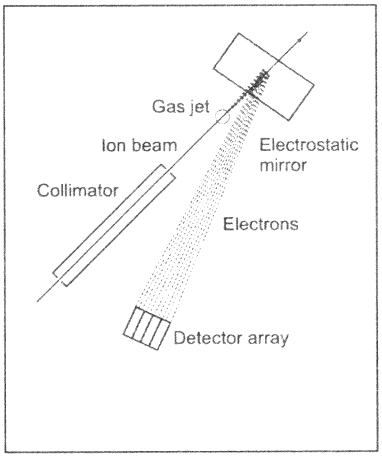

Figure 1: Scheme of the time-of flight electron spectrometer

The electrons were detected in coincidence with the outgoing C^{2+} ions. We could resolve the "Electron Loss to the Continuum" cusp (see e.g. [1]), and two narrower peaks located symmetrically on the low- and high-velocity wing of the cusp, the autoionization lines of the projectile. The time resolution of the spectrometer determined from the width of the autoionization lines is about 4 ns.

With this spectrometer in the future we would like to study the double ionization of He under triple coincidence conditions.

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P-36

VIBRATIONAL EXCITATION COEFFICIENTS FOR ELECTRONS IN HBr

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A set of cross sections for electrons in HBr was compiled and we have made calculations of all transport coefficients. The dominant feature in the inelastic energy losses, determining the properties of electron swarms are the vibrational excitation cross sections [1]. Those have very high and sharp peaks but their mean value is relatively high as well. In this paper we show the rate coefficients for electron excitation of vibrational levels in dc and rf swarms.

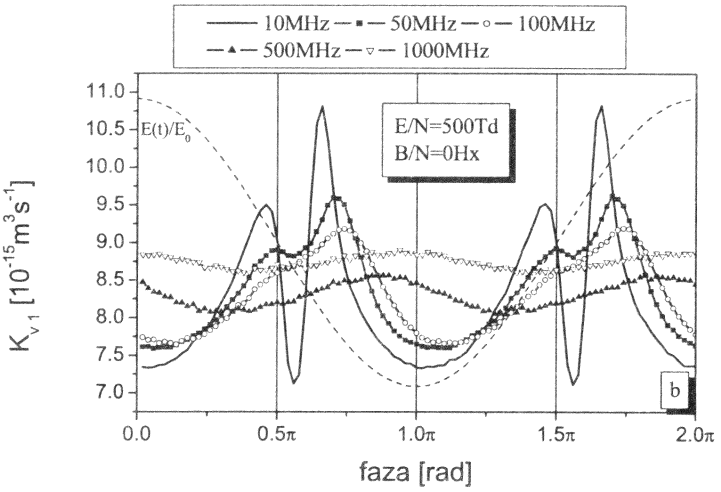

Figure 1: Dependence of excitation coefficient for v=1 level of HBr on phase for 500 T electric field and for different frequencies.

In Fig. 1 we show the time development of the vibrational excitation. At lower frequencies two peaked dependence is the result of the sharply peaked cross section and its overlap with the distribution function. The structure disappears at higher frequencies since electrons cannot relax their energy. Other features of electron transport in dc and rf fields will be discussed as well.

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P-37

PHOTO- AND THERMALLY STIMULATED RELAXATION PROCESSES IN PREIRRADIATED ATOMIC SOLIDS

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Rare–gas (Rg) atoms at low temperatures form the simplest weakly bound atomic insulators, which are easily modeled theoretically and this makes them especially well suited for investigation of relaxation processes. The electronic excitations in insulators induced by ionizing radiation initiate a sequence of relaxation reactions involving both atomic and electronic subsystems. The knowledge of the relaxation processes in preirradiated solids is an important issue for understanding of radiation effects, dynamics of carriers and surface reactions. The problem of interest is the topical problem of interconnection between atomic and electronic processes.

We present for the first time the results of real time correlation study of atomic and electronic relaxation processes including the recently found new relaxation channel – low-temperature sputtering from preirradiated atomic solids [1]. Films of pure and doped Rgs – Ne, Ar, Kr and Xe, were condensed on a cooled substrate with a concurrent irradiation by slow electrons. Relaxation processes were monitored using a combination of activation spectroscopy methods – photo- and thermally stimulated exoelectron emission (PSEE and TSEE), spectrally resolved thermally stimulated luminescence (TSL), with measurements of the neutral atom sputtering yields. A firm evidence of the recombination mechanism of the low-temperature sputtering from the surface of preirradiated films was obtained. The released from traps electrons recombine with self-trapped holes by the reaction $Rg_2^+ + e \rightarrow Rg_2^* \rightarrow Rg + Rg + h\nu + \Delta E$. The crowdion mechanism of the atom ejection from the surface is proposed. The parameters of crowdions (energy, effective mass and characteristic width) calculated for Rgs with a FCC lattice [2] are discussed in the context of the mechanism proposed.

Unusual relaxation channel – electronic relaxation promoted by atom-atom recombination reactions, was found. Atom-atom recombination followed by excited molecule formation resulted in electron detrapping via radiative optical transitions. The subsequent exoelectron emission and recombination of electrons with positively charged centers were detected.

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P-38

PLASMON EXCITATION IN NANOTUBES. COMPARISON WITH CAPILLARIES AND WIRES

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The present work is devoted to study the interaction between nonrelativistic charged particles and hollow cylindrical structures of nanoscopic dimensions, using classical and quantum mechanical formulations.

The dispersion relation is studied on the basis of a Drude model for the dielectric function, and the results are compared to the cases of wires and capillaries. This approach is used to calculate the induced field and stopping force on a moving particle in a semiclassical way, as well as to derive the average number of excited plasmons from a quantum mechanical point of view.

The formalism is illustrated with specific calculations, showing bulk and surface excitation processes, for different trajectories of the particle. In particular, we study the importance of resonance effects between the modes, already observed in wires (in our previous works). We provide integral expressions that may be used to calculate the excitation of the different modes and predict the conditions to obtain strong interference effects.

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P-39

Excitation 4^1P_1–n^1D_2 lines of Zn atoms by monoenergetic electrons

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Up today the excitation processes for the Zn atoms in the Zn, Cd, Hg group were weakly investigated.Below we present new experimental investigations for excitation of Zn atoms by monoenergetic electrons. The electron beam was formed by a hypocycloidal electron monohromator and crossed the coolision chamber. The excitation of atoms was carried out in the gas-filled cell. The optical excitation functions (OEF) were studied with the small step in energy (30 meV). At the incident current of 200 nA the energy spread of electrons was equal to 70 meV. The automated setup and the measuring method are described in [1].

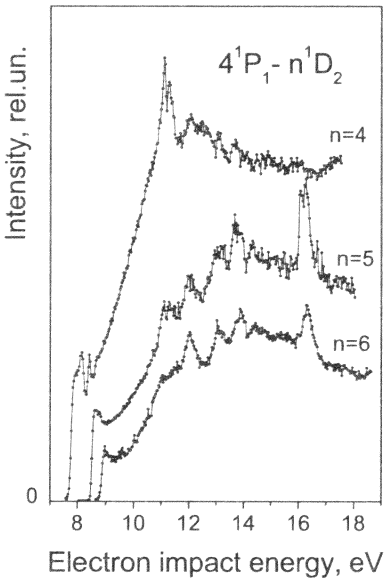

Fig. 1

OEF in the figure 1 reveal a clear structure below and after of the ionization threshold of the Zn atom (9.394 eV). The M-form feature near the threshold pays on itself an attention for OFV λ636.2 nm (n=4) at energy 8.33 eV. There are interesting also the features arising after the ionization threshold at energies 11.15 eV, 12.10 eV, 13.15 eV, 13.75 ev and 16.30 eV. Point out that its widths exceed the energy spread of electrons. Especially the feature at energy 16.30 eV is selected. As far as growth of the quantum number the contribution of these features to initial level population of the spectral line increases. At thementioned above energies there are a series of zinc atom autoionizing states, which can be accountable for the identification of these features on OEF .

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P-40

ELECTRON IMPACT EXCITATION OF THE n^1S_0-n^1P_1 REZONANCE SPECTRAL LINES OF Ca, Zn AND Cd ATOMS

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Up today the collision processes of electrons with the 2 group atoms were studied in many works by methods of electron- and photon- spectroscopy. Many interesting data on the effective elastic cross sections, excitation functions and ionization efficiency were obtained.However, reliable data on thenear-threshold electron-impact excitation of resonance lines are absent.

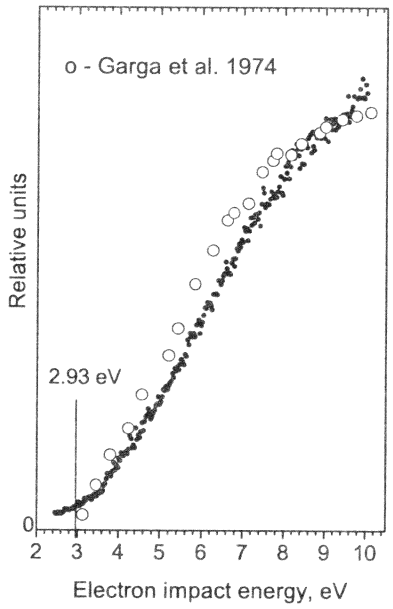

Fig. 1

Below we present experimental investigations of resonance spectral line optical excitation functions (OEF) for Ca, Zn and Cd atoms. The excitation of atoms was carried out in the gas-filled cell. The electron beam was formed by a hypocycloidal electron monohromator and
crossed the gas-cell in the coolision chamber. OEF were studied with the small step in energy (20-30 meV) by monoenergetic electrons in the beam equal to 50-80 meV. The automated setup and the measuring method are described in [1].

As an example in the Figure 1 the measured by us OEF of the Ca λ422.7 nm (4^1S_0-4^1P_1) resonance spectral line in comparison with measured earlier in [2] is presented. As it is visible, the common behavior of curves are similar. However, if OEF, measured in [2] has a smoth , the measured by us has a structure in the near-threshold energy region at energies 3,79 eV, 4,35 eV, 4.73 eV, 5,73 eV and 7.47 eV, respectively. The results on other atoms will be presented at the conference.

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P-41

DESIGN OF ELECTRON ENERGY ANALYSERS FOR ELECTRON IMPACT STUDIES

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We present the design of electron energy analyzers which are frequently needed electron optics systems in electron spectroscopy. By using the SIMION program, focusing characteristics are obtained for 180^0 hemispherical analyzers with five-element entrance optics considering fringing field effects, and compared with other types of analyzers, such as CMA and PPA, since these designs are the most suitable for use with both electrons and ions [1-2]. Transmission, energy and time resolution of the each energy analyzer are considered for non-relativistic electrons with design equations.

In addition, we present a way of optimizing the performance of some useful design, i.e., ideal field approximation, real apertures, Herzog, and Jost correction considering resolution improvement, as shown in Fig. 1. Results are shown for toroidal energy analyzers, in particular 127^0 cylindrical and 180^0 hemispherical analyzers. Focusing, energy resolution, and angular behavior of each type are investigated.

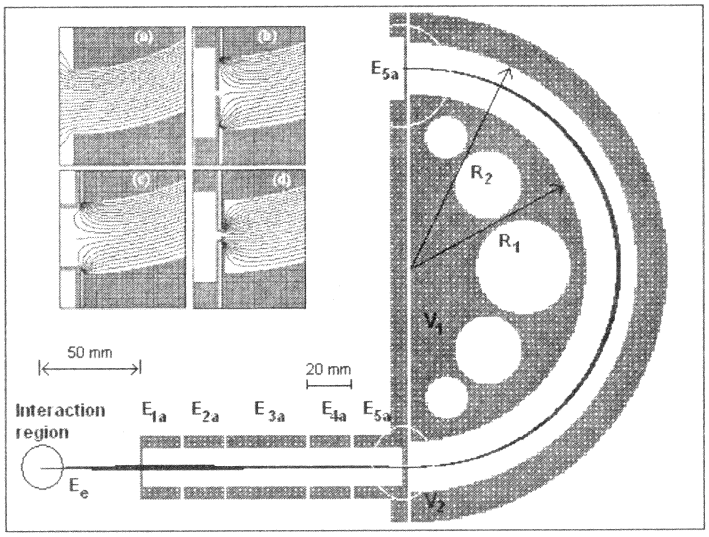

Figure 1. 180^0 hemispherical analyzer with entrance optics considering (a) ideal field approximation, (b) real aperture, (c) Herzog, and (d) Jost correction schemes.

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CHARACTERIZATION AND MODELING OF MULTI-ELEMENT ELECTROSTATIC LENS SYSTEMS

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Electrostatic cylinder lenses are widely used to control beams of charged particle with various energy and directions in several fields, especially in electron spectroscopy. In most applications, electrostatic lens system is operated to keep lens parameters constant over a wide range of voltage ratio of final to initial electron energy. Lenses used in this way are often referred to as 'zoom' lenses. So far, there have been several attempts to determine the zoom lens properties of multi-element electrostatic lenses. It is well known that a three-element lens can be used to aid the design of lenses having fixed image position, but the magnification is not constant [1]. However, the four element lenses can be operated with a constant magnification to produce an image at a specific position [2]. Electrostatic lens systems with more than four elements are generally used in experimental studies to maintain a truly zoom lens with constant magnification overall voltage ratios, additionally with afocal case [3].

In the current study, we investigated the zoom lens properties of the three, four and five element lens systems as a function of the lens voltages and their dimensions (see examples in Fig.1). Lens systems which consist of cylindrical electrodes, each spaced 0.1 diameter apart, was designed by using the SIMION 7.0 program. Three different lens configurations were studied to form an image at a specific position with constant magnification for use in experimental studies.

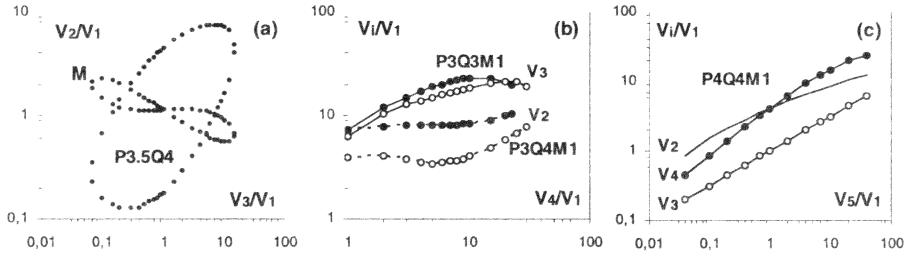

Figure 1. Zoom lens conditions of (a) three, (b) four and (c) five element lens systems having A/D=1 as a function of electron energy for a given object (P) and image (Q) distances with magnification (M) (This configuration will be denoted as P3Q3M1).

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Computational studies of hypocycloidal electron monochromator

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Charge particle selection to produce and analyze monochromatized particle beams has been used in various experimental studies of fundamental molecular processes since its first application in Ramsauer technique [1]. The trochoidal monochromator which employs crossed uniform electric and magnetic fields has been developed by Stamatovic and Schulz [2] and is widely used [3,4] to produce low energy electron beams with energy spread down to and below 20 meV [5]. In the original paper on the trochoidal monochromator [2] other monochromator geometries have been suggested including those with electric field produced by cylindrical electrodes where electrons follow hypocycloidal trajectories. This hypocycloidal monochromator has been recently applied in newly constructed electron spectrometers for surface studies [5,6].

In the present work we have performed computer calculations of the operation of an hypocycloidal electron monochromator using charge particle optics CPO-3D program [7]. Previously that monochromator and its optimization have been considered in [8]. Here we have carried out calculations of transmission of electrons in the monochromator, in the electric field which includes fringing fields at the boundary of the electrodes. We have also taken into account electrons which have transverse components of their velocities at the entrance to the monochromator. These calculations show that the energy resolution of the hypocycloidal monochromator is higher by about 20% (for 0.4 mm apertures) in comparison with trochoidal monochromator of equivalent dispersion.

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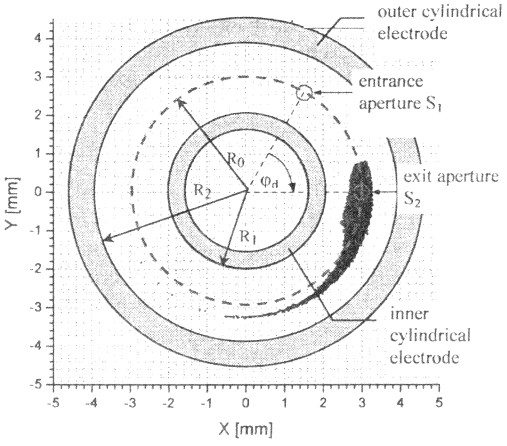

Figure 1: Dispersion of electrons with 0.1eV mean energy on the exit electrode of the monochromator with S_2 exit aperture.

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ION-PAIR PRODUCTION DUE TO ELECTRON-IMPACT DISSOCIATIVE IONIZATION OF SULFUR HEXAFLUORIDE MOLECULE

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Sulfur hexafluoride has received a considerable attention of researchers over last few decades because of its extreme "popularity" in various practical applications. This molecule possesses unique chemical structure that stipulates a diversity of processes accompanying its interactions with different particles ranging from controlled-energy electrons to high-energy photons, ions and neutrals. Data on electron-impact ionization of SF_6 are up to date rather scarce. Here we report on the results of the studies on the positive ion-pair production due to dissociative ionization of the SF_6 molecule by electron impact. The experiment was carried out by using the crossed-beam technique and the mass-spectrometric analysis of ions produced.

Rejoub *et al* [1] reported production of ion pairs as a result of electron-impact dissociative ionization of SF_6. We have observed the yield of all possible ionic fragments in this reaction, including the above ion pair production, and measured the energy dependences of relevant cross sections for the formation of the above ions. Figure 1 presents the energy dependences of the partial SF_3^+ and F^+ ion yield cross sections from the threshold up to 150 eV.

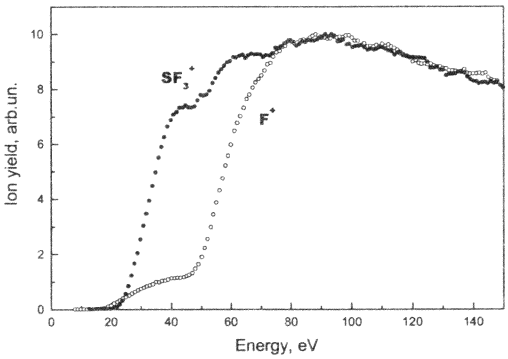

Figure 1. SF_3^+ and F^+ ion yield cross sections as the functions of incident electron energy

As is seen, the SF_3^+/SF_6 curve shows a pronounced structure with a distinct feature just above 40 eV. Feil *et al* [2] have attributed this structure to the Coulomb explosion of the metastable doubly-charged SF_4^{2+} ion with the threshold energy of about 43 eV:

$$e + SF_6 \rightarrow SF_4^{2+} + 3e \rightarrow SF_3^+ + F^+ + 2F + 3e$$

The same authors [2] have also reported the appearance energy for the SF_3^+ ions produced by the above reaction to be 45.5 eV. As our results show, we have confirmed the above assumption. In addition, the data on the F^+ ion yield (see figure 1) indicate the presence of a distinct rise of the cross section just in the same energy region, which, certainly, can be related to the contribution of the above reaction to the F^+ ion yield.

Thus, we have observed a clear correlation between the behavior of the structure in the partial SF_3^+ and F^+ ion yield cross sections due to dissociative ionization of the SF_6 molecule via the formation of the temporary SF_4^{2+} ion.

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P-45

Kinetic Electron Emission during Coulomb Explosion of Swift Molecular Ions in Grazing Scattering from Solid Surfaces

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We investigate how is kinetic electron emission from a solid surface influenced by the increasing inter-nuclear separation during Coulomb explosion of a fast, heavy diatomic molecule in the course of its grazing scattering from the surface under small angle of incidence. The electron stripping off the molecular projectile and subsequent charge evolution of the constituent ions are described by a semi-classical statistical model [1]. In order to study the dynamics of Coulomb explosion mediated by the surface, we use the dielectric formalism describing the dynamic polarization of the electron gas on the surface in the presence of two spatially correlated constituent ions. The scattering trajectories of these ions are calculated from the classical equations of motion, taking into account the repulsive forces due to surface atoms, the attractive dynamical image force on each ion, as well as the surface-mediated dynamical screening of the Coulomb repulsion between the constituent ions.

We further calculate the excitation spectra of electrons on the surface by means of the first-order, time-dependent perturbation theory, with the electron states obtained from a finite step-barrier potential, while the perturbation is represented by the potentials of the constituent ions dynamically screened by the surface dielectric response [2]. The spatial proximity of the constituent ions is found to give rise to significant interferences in the surface response, which directly affect the angle-resolved energy spectra of electrons emitted from the surface, obtained from integration along the ion scattering trajectories.

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P-46

THE STRUCTURAL PROPERTIES OF ALKALI ATOMS DOPED NOBLE GASS CLUSTERS

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Almost already after the discovery of Lennard-Jones interaction function in the beginning of XX^{th} century the study of noble gas clusters became some kind of benchmark for different as well structural, physical as algorithmical and numerical study.

Recently it has arisen an interest in analysing the properties of such the clusters doped with single or multiple alkali metal atoms. This is especially due to excimer-like character of electronic properties of such a structure. The second reason is the similarity of Mason-Schamp potential describing the metal - noble gas interaction and the Lennard-Jones function.

In our paper we present the structures of M_mN_{n-m} corresponding to the minimum total energy obtained using the evolutionary optimisation technique [1].

A special attention is pointed to the position of metal add-atom in the structure and the possible grouping of the larger number of metallic atoms.

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P-47

MANY-ELECTRON EFFECTS IN RADIATIVE ELECTRON CAPTURE BY HEAVY IONS

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Relativistic collisions of highly-charged, heavy ions with electrons and low-Z target atoms have been explored intensively during the recent years at the GSI facility in Darmstadt [1]. In such collisions, one of the major processes which leads to the loss of ions from the beam is the radiative electron capture (REC) into a bound state of the projectiles. Because of its practical importance, REC studies have been carried out for many elements and a wide range of projectile energies up to several hundreds MeV/u. Until now, however, most experiments have focused on the capture of electrons by *bare* projectile ions, including measurements on the total and angle-differential recombination cross sections as well as the polarization of emitted x-ray photons [2, 3]. Less emphasis, in contrast, was placed on the capture into high-Z, *few-electron* ions, partially also because no reliable many-electron (theory and) computations were available.

In this contribution, we apply the density matrix approach, based on Dirac's equation, to investigate the radiative electron capture into high-Z, *few-electron ions*, including different shell structures for their initial and final states. Special attention is paid to the total and angle-differential cross sections following REC into hydrogen-, helium- and lithium-like uranium ions [4]. From the comparison of the angular distributions of recombination x-ray photons as calculated within the effective one-electron model and Multi-Configuration Dirac-Fock (MCDF) approach, it is shown that many-electron effects become important for low-projectile energies.

Apart from the (total and angle-differential) REC cross sections, we have also applied the density matrix formalism to investigate the subsequent $K_{\alpha,\beta}$ photon emission following electron recombination into the excited states of (initially) hydrogen-like heavy ions.

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P-48

TARGET DEPENDENCE OF CHARGE EXCHANGE X-RAYS

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X-rays emitted in a series of cascade transitions after electron capture into high Rydberg states have been the center point of the interpretation of recent astrophysical observations [1]. Our group has carried a systematic laboratory investigation of K, L and M x-rays emitted by different highly charged ion projectiles colliding with various neutral targets [2].

Our present paper describes our finding that for Kr^{27+} projectiles there is a strong target dependence of the line intensity rations between the L and M x-rays. The result is somewhat surprising since these transitions occur after several preceding cascade steps. This points to a highly selective initial (n,l) distribution of the captured electrons for the different target gas atoms. For higher Kr charge states the difference between the L and M line ratios diminishes almost entirely.

The theoretical modeling of the initial capture process is based on our classical trajectory Monte-Carlo (CTMC) calculations.

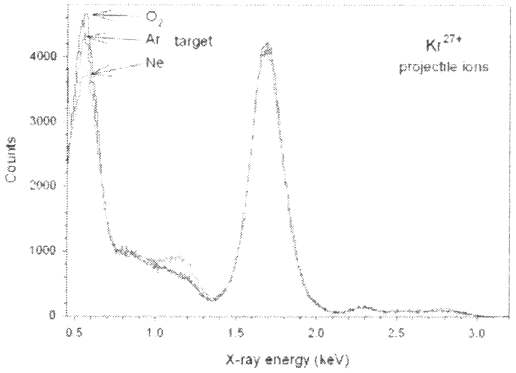

Figure 1: L and M x-rays of highly charged Kr^{27+} ions with different target gases used.

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Probing of a local electronic structure in small hydrogen bonding clusters using soft X-ray photoabsorption spectroscopy

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Inner-shell excitation of small hydrogen bonding clusters (methanol and ethanol) has been investigated by using partial ion yield method in the carbon and oxygen K-edge regions. The measurements were carried out at the beamline 27 at SPring-8. In recent reports, we indicated that the soft X-ray absorption (XA) spectroscopy of hydrogen bonding clusters is very sensitive to the change of electronic structure and useful to investigate the relationship between the electronic structure and geometrical structure of them [1]. In this study we applied the soft X-ray photoabsorption spectroscopy to investigate the hydrogen bonding properties of ethanol and methanol clusters.

Although the molecular structures and photoabsorption spectra of gas phase molecules are similar in methanol and ethanol, there are some pronounced differences between the XA spectra of their clusters. Especially, the difference can be seen at the O 1s to 3sa resonance excitation. The resonance excitation to the 3sa unoccupied orbital, which is one of the characteristic features in the oxygen K-edge region, was clearly seen in the total ion yield spectrum of both molecules. In the XA spectra of methanol cluster, the resonance peak was shifted to higher energies. However, this resonance feature was fully suppressed in the XA spectra of ethanol clusters. The difference in both spectra is discussed in terms of the change in the electronic structure around the O atom caused by the formation of hydrogen bonds in clusters.

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P-50

LASER OSCILLATION IN LEAD VAPOUR, OBTAINED BY LASER EVAPORATION

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A solid state YAG:Nd^+ laser with pulse energy up to 10 J, pulse length of 4 ms and repetition rate of 2 Hz was used for evaporation of metal targets. The targets, placed in the pumped out chamber with electrodes for transverse discharge in neon at several Torr pressure, were irradiated by focused laser beam.

Nonstationary metal vapour then may be excited by discharge pulses to search for new laser transitions in metal atom's spectra. The favorable thermo-physical and laser properties are stipulated the use of lead target for testing and setting up investigations to obtain the amplification on the well-known lead 722.9 nm self-terminating transition. It was established, that the amount of atoms, evaporated during one pulse is ~ 10^{18}.

The obtained metal vapor was excited by a train of current pulses with total number of 100 and with adjustable recurrence period of ~ 50 – 200 μs. The spherical resonator was used to establish the light amplification. The waveforms of emission pulses through the output mirror (1), the same with closed back mirror (2) and of evaporation laser pulse (3) are presented on Fig. 1. It is clearly shown that the intensity of the 722.9 nm spectral line more than twice is less when back mirror closed. Any other lead or neon close laying lines demonstrate so large intensity difference in 1 and 2 modes. So the amplification of this line in discharge is evidence.

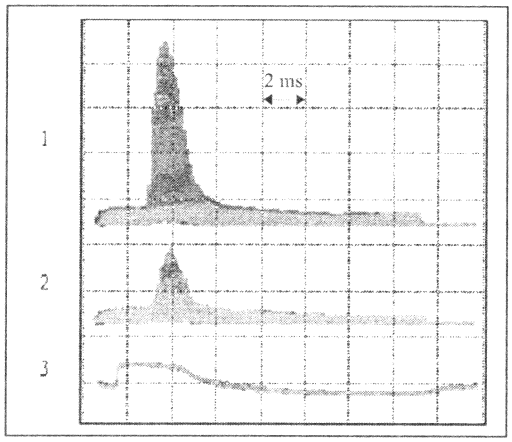

Fig. 1

Another targets as titanium, rhenium will be studied for new metal-vapour lasers

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ANGULAR DISTRIBUTION OF SCATTERED PROJECTILES FOLLOWING DOUBLE ELECTRON CAPTURE PROCESSES AT LOW ENERGY C^{4+} AND HELIUM COLLISIONS

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The recent availability of sources for slow highly charged ions (HCI), namely electron cyclotron resonance (ECR) and electron beam ion sources (EBIS) has led to a flurry of research activities, both experimental and theoretical, in the field of HCI-atom interactions. One of the interesting classes of these investigations is the study of multi-electron capture processes [1,2]. On the most fundamental level, its importance is derived from the applications in many fields, e.g. astrophysics, fusion research, atmospheric science, and plasma diagnostics. Angular differential cross section measurements provide also information from the interaction potential curves.

In this work a four-body classical trajectory Monte-Carlo (CTMC) method [3] is used to calculate the double electron capture probabilities in 470 eV C^{4+} and He collisions. The four particles have the corresponding masses and charges and the forces acting among the four bodies are taken to be pure Coulombic ones. The interaction between the two active electrons of the Helium atom is neglected. The impact parameter of the projectile and the orientation and velocity of the electrons moving around the target nucleus are randomly selected according to the Monte Carlo method. The binding energies of the electrons in the He atom are chosen conveniently 2 a.u. and 0.903 a.u., respectively. To distinguish between the various final states, the exit channels are tested at large distances from the collision center.

The angular distribution of scattered projectiles following double electron capture processes at low energy $C^{4+}$and helium collisions show an intense peak at 0° applying the 4-body CTMC method. This result is surprising at first sight because due to the slow projectile velocity we expected that the interaction time is plenty large enough creating large angle scattering for projectile. To solve this unexpected finding we calculated the contour plot of the double electron capture probabilities as a function of impact parameter b and scattering angle θ. According to our calculations, when the impact parameter is small (around 0°) the scattering angle is also small. At $b=0$ the scattering angle is 0°. We conclude that the dominant contribution of double electron transfer at the range of small impact parameters arise from the so called "knock-on" collisions, i.e. the C^{2+} ion remain almost rest after the collisions and the He^{2+} "scatter" into 0° (recoil effect).

The work was supported by the JSPS-HAS Cooperative Science Program, the Hungarian Scientific Research Found OTKA No. T046095, T046454, and the grant Bolyai from the Hungarian Academy of Sciences.

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P-52

THE ROLE OF PROJECTILE DOUBLE SCATTERING IN POSITRON-ATOM COLLISIONS

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The process of electron capture to the continuum (ECC) can be explained as a result of the special case of ionization, where the ionized target electron is strongly influenced by the outgoing projectile. The ECC peak appears at the energy where the electron velocity is almost the same as the projectile velocity. The ECC is well understood when the projectile is heavy particle. We have shown in our previous work [1] that the ECC electrons originate only from distance ionization, i.e. that part of the ionization channel where the distance between the electron and projectile is less than the distance between the electron and target nucleus. It was shown that the most important mechanism for ECC is the Coulomb focusing of ejected target electron in the direction of the projectile and the peak occur for positron impact as well in the triple-differential cross sections [2]. Since the mass of the positron and the electron is the same, the projectile energy is shared equally between the positron and electron after the ECC. Therefore the nominal value of the ECC peak in the electron/positron spectrum is $(E- E_b)/2$. Here E is the energy of the projectile and E_b is the binding energy of the electron in the target atom. Contrarily, the experimentally obtained positions of the ECC peak always appear at significantly lower/higher energies. To solve this puzzle model calculations within the frame work of classical trajectory Monte Carlo (CTMC) method are performed. The CTMC method has been successful in dealing with the ionization process in atomic collisions for light projectile impact as well.

In this work, the role of projectile double scattering in positron and hydrogen atom collisions is investigated. We present double differential cross sections of scattered positrons for the distance ionization channel at 50 eV impact energy using full and reduced CTMC method. The ECC peak, at this energy, is expected at E=18.2 eV. In spite of this fact for the case of full 3-body approximation the scattered positrons show ridge-like" structures, and the peak energy is shifted to the higher energy. But for the case, when the scattering of the positron on the target nucleus is neglected, the ECC peak is located at the nominal value. We conclude that the role of positron double scattering manifests itself in the energy shift of ECC peak [3].

The work was supported by the Hungarian Scientific Research Found OTKA Nos. T046095, T046454, the TéT Grant No. A-15/04, the grant Bolyai from the Hungarian Academy of Sciences.

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ENERGY LOSSES OF PROTONS TO HYDROGEN ATOMS

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Collisions among energetic particles are fundamental processes of nature having importance in many different areas of research and technology. Since the beginning of last century one of the exciting problems in collision theory is the calculation of the energy loss of ions passing through different stopping media. In recent decades both classical and quantum-mechanical theories have been used to calculate the stopping power of atoms, molecules and solids for various projectiles [1-3]. The main difficulty of calculations for atomic and molecular media is that many-body interactions have to be taken into account. Therefore, the success of various approaches to the calculation of stopping power depends in part on how far a given theory is capable of describing the many-body character of the collision.
The classical trajectory Monte Carlo (CTMC) method has been quite successful in dealing with energy loss processes in ion-atom collisions. The CTMC simulation is a non-perturbative method. One of its main advantages is that many-body interactions are exactly taken into account during the collision. This makes the CTMC method useful for the study of two- or more center effects. Moreover in the classical picture it is straightforward to switch on and off the interaction potentials between the individual particles and thereby to study the effects of particular interactions.
In this work the full and reduced three-body classical trajectory Monte Carlo (CTMC) theory are used to calculate energy losses of the projectile in proton-hydrogen atom collisions as a function of impact energy. The energies of the projectiles investigated were in the range of 10 and 1000 keV/amu. The total stopping power is presented along with partial contributions of the energy deposition among the channels of excitation, ionization and capture. Contributions of the projectile-electron and projectile-target nucleus interactions to the total stopping power are also investigated. Our results are compared with other theoretical calculations and experimental data. The present calculations verify that high order effects should be included for a proper description of electronic stopping power. Moreover we show that small impact parameter collisions are important; new reaction channels open and nucleon-nucleon interactions dominate in this collision range.

This work was partially supported by the National Natural Science Foundation of China (Grant No. 10025420 and 90206009), the Hungarian Scientific Research Found OTKA Nos. T038016, T046095, the grant "Bolyai" from the Hungarian Academy of Sciences, and TéT Grant No. CHN-3/2004.

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Stopping Power Calculations of Molecules for Swift Projectiles

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Abstract

The electronic stopping cross section of molecules is calculated by considering velocity dependent projectile and target electronic structure, and applying Bragg addition rule. The velocity dependencies are obtained from the Bohr adiabatic criterion using Thomas-Fermi atomic model for two separate screening functions. We derived first the electronic stopping cross section expression from Bethe approximation. The obtained results are compared with experiment and the other theoretical calculations.

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OPTIMISING THE PERFORMANCE OF ELECTRON GUN DESIGN FOLLOWING LENSES AND APERTURES

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The electron gun plays an important role for atomic and surface spectroscopy. Different types of electron gun has been designed for producing different electron beam energies [1-2]. In this study, we present the modeling and construction of seven-element electron gun with quadrapole deflector (see SIMION modeling and AutoCAD drawing in Fig. 1). The effects of cathode-anode distance and their voltages on the performance of electron gun are considered for directly-heated (with hairpin-filament, HC-type [3]) and indirectly-heated (IC-type [4]) cathode types of electron gun. Simulation was performed for cathode-anode distance from 0.5 to 8 mm with several acceleration voltages. Electron gun is operated in afocal, broad-beam and zoom mode for use in gun applications to achieve optimal beam geometry which may vary for different experimental purposes. This modeling proposed here may help to design new types of gun and applications using cylinder and aperture lenses in collision experiments.

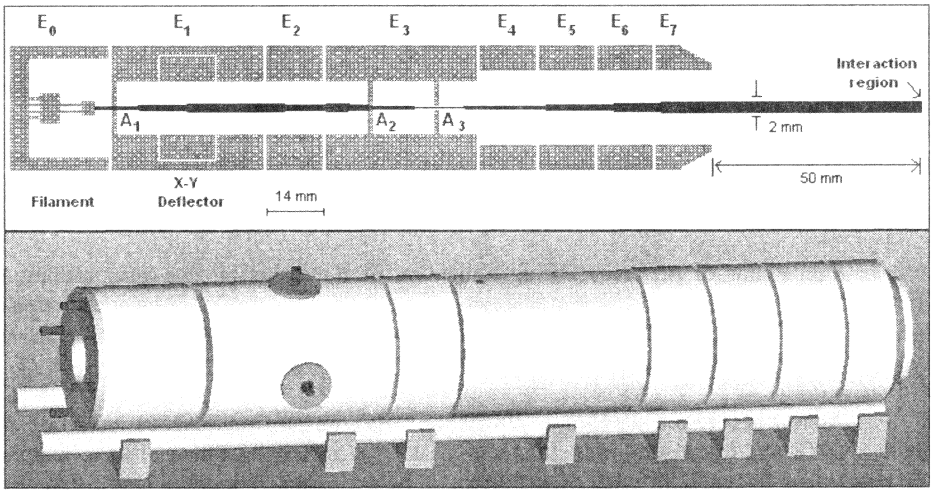

Figure 1. Seven-element electron gun in SIMION and AutoCAD program.

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P-56

LINEAR DICHROISM IN EXCITATION OF STRONG PERTURBED ATOMIC STATES

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We studied experimentally the two-photon excitation of $5d7s^3D_2$ state of *Ba* atom strongly perturbed in result of ac-Stark effect realisation. The perturbation of this state was fulfilled by influence of YAG-laser radiation. For excitation of this state we used the tunable dye- laser radiation. The investigations were performed by the resonant ionization spectroscopy method. We measured the Ba^+ ions yield caused by the ionization of *Ba* atoms through the two-photon resonance with perturbed $5d7s^3D_2$ state in cases when the electric vectors of both used radiations were parallel and orthogonal. The results of our investigations are presents in figure.

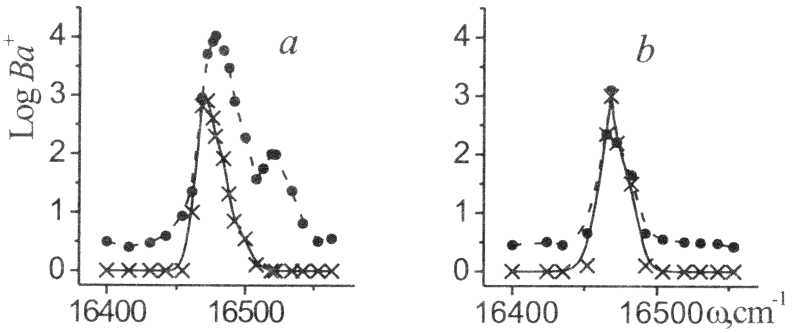

Fig. Yields of Ba^+ ions during ionization of *Ba* atoms by dye-laser radiation (crosses and solid lines) and by simultaneously action of dye- and YAG-laser radiations (circles and dashed lines) with parallel (a) and orthogonal (b) orientation of electric vectors of these radiations.

As follows from these figures the yield of Ba^+ ions at simultaneous influence of both (YAG- and dye-lasers) radiations with parallel orientation of their electric vectors is large than its yield in case of influence only dye-lasers radiation. Note, that the resonant structure at influence only of dye-lasers radiation is caused by ionization of *Ba* atoms trough resonant with unperturbed $5d7s^3D_2$ state. The resonant maximum in Ba^+ ions yield at 16520 cm^{-1} is caused by increasing of probability of perturbed $5d7s^3D_2$ state ionization in result of one-photon resonance with autoionising $5d4f\,[3/2]^o_1$ state. In case of orthogonal orientation of electric vectors the Ba^+ ions yield is the same as at influence only dye-lasers radiation. From these results follows that the excitation of perturbed state $5d7s^3D_2$ realised only in case, when the electric vectors of perturbed and excited radiations have the same orientations.

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THE SATURATION OF THE DOUBLY-CHARGED IONS FORMATION PROCESS UNDER REALISATION OF TWO-ELECTRON MECHANISM

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We present the results of investigations of functional dependence of two-charge ions (A^{2+}) yield (N^{2+}) under two-electron mechanism realisation on laser radiation intensity (F). Investigations were carried out for saturation regime. Fig. shows the result of measurements of Sr^{2+} ions yield produced upon ionisation of Sr atoms by Nd-glass laser radiation (9460 cm^{-1}) as the function on intensity of this radiation.

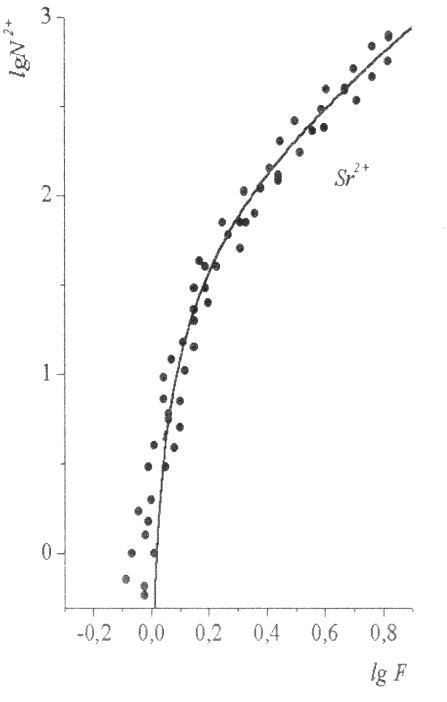
The previous investigations show that formation of A^{2+} ions formation under two-electron mechanism realisation is conditioned by excitation and following ionisation of strong perturbed states of neutral atoms. The perturbation of states is caused by realisation of ac-Stark effect. The realisation of this process begins under intensity F_0, which corresponds to condition: $\Delta E=\alpha F_0/4$ (ΔE-the change of states energy; α-the polarisability of this state). In saturation regime the A^{2+} ions yield is proportional to value V_o, in which the intensities F_0 are created.

For verify of this assumption we carried out the calculation of $V_o(F)$ function for the gaussian laser beams. For $V_o(F)$ function we obtained following analytical expression:

$$V_0 = C\left[\frac{1}{9}\left(\frac{F}{F_0}-1\right)^{\frac{3}{2}}+\frac{2}{3}\left(\frac{F}{F_0}-1\right)^{\frac{1}{2}}-\frac{2}{3}arctg\left[\left(\frac{F}{F_0}-1\right)^{\frac{1}{2}}\right]\right]$$

where $C=2\pi^2\rho^3/\lambda$ (r-minimal focusing radius; λ -laser radiation wavelength).

The results of calculations of $V_o(F)$ function are present in Fig. by solid curve. As one can see, for saturation regime the results of calculations have a good agreement with experimental results for Sr^{2+} ions yield. This agreement indicates that the process of Sr^{2+} ions formation under the two-electron mechanism realisation really is a threshold process - its realisation begins at some value of laser intensity F_0.



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P-58

QED THEORY OF LASER-ATOMS INTERACTION. MULTIPHOTON IONIZATION

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A quantum-electrodynamics (QED) theory is applied for studying interaction of atoms with an intense laser field without and in a presence of a DC electric field. Method bases on a description of atom in the field by the k- photon emission and absorption lines [1,2]. The lines are described by their QED moments of different orders, which are calculated within Gell-Mann & Low adiabatic formalism. We have studied the cases of single-, multi-mode, coherent, stochastic laser pulse shape. An account for stochastic fluctuations in a field effect is of a great importance. Results of the calculation for the multi-photon resonance and ionization profile in H, Na, Cs atoms are presented. Our method is compared with other (DFT et al) approaches [3]. It is also studied the phenomenon when an energy spectrum liberated in the high intensity multi-photon ionization exhibits succession of peaks separated by photon energy (above threshold ionization). Efficiency of method is demonstrated by QED perturbation theory calculations for the two-photon ionization cross-sections and photoelectron angular distribution for extended photon energy range (including above-threshold ionization) in Mg [1,3]. Comparison with the R-matrix calculation of Luc-Koenig et al [4] is given. There is considered a phenomenon of the Rydberg stabilization of the H atom in a strong laser field and estimated the rate of transition between the stabilized Rydberg state (n=40,m=2; E~10(8)V/cm) and ground state, when it's possible the radiation of photons with very high energy (short-wave laser amplification).

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P-59

DIAGNOSTICS OF ELEMENTARY PROCESSES IN A COLLISIONALLY PUMPED PLASMA AND SEARCH OF THE OPTIMAL PLASMA PARAMETERS FOR X-RAY LASING

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The X-ray laser problem has stimulated a great interest to development of theoretical methods for modelling the elementary processes in a collisionally pumped plasma. The shocking example is a scheme for accomplishing tabletop x-ray lasing in Li-like ion of Ne at 98 Å in an optically ionized plasma during recombination in the transient regime (Lawrence Livermore Nat. Lab.). The low temperature plasma sources show promise for producing lasing in the VUV and soft X-ray region. Two key theoretical problems must be solved in order to predict necessary plasma parameters needed for X-ray lasing: i). Highly accurate definition of the rate coefficients for plasma elementary processes that are responsible for the forming emission lines spectra; ii).Developing new exact kinetics calculation schemes for defining level populations, inversions, gain coefficients at definite plasma parameters. The most consistent approach to these problems is based on QED. Here the generalized energy approach in gauge invariant formulation [1] is used for consistent description of elementary processes in collisionally pumped laser plasma. It is developed an optimal scheme for calculation of the electron-collision strength and rate coefficients for the de-excitation (excitation) processes in the Ne-like multi charged ions plasma with estimating optimal plasma parameters for X-ray lasing. We consider Ne-like multicharged ions plasma. We applied our approach to estimate of electron collisional excitation cross-sections and strengths for Ne-and Ar-like ions. In table we present calculated and measured excitation cross-sections σ for Ne-like barium for two values of incident electron energy 5.69keV and 8.20 keV [2,3].

Level J	Measured Marrs etal [19]	Calculated Ivanov etal [5]	Calculated Zhang etal [20]	Calculated Reed [21]	Calculated Present paper
			E_{el}=5.69keV		
Sum (J=0)	2,50±0,35	2,48	2,58	2,60	2,51
$2p_{3/2}3d_{5/2}$ 1	3,98±0,56	3,20	3,44	3,56	3,25
$2p_{1/2}3d_{3/2}$ 1	2,12±0,30	1,78	2,42	2,00	1,84
			E_{el}=8.20keV		
Sum (J=0)	2,27±0,32	1,83	1,89	1,94	1,86
$2p_{3/2}3d_{5/2}$ 1	3,30±0,46	2,87	2,99	3,23	2,93
$2p_{1/2}3d_{3/2}$ 1	1,82±0,25	1,64	2,10	1,82	1,69

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P-60

ENERGY APPROACH TO QED THEORY OF CALCULATION OF POSITRON IMPACT IONIZATION OF MULTIELECTRON ATOMS

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Considered will be processes, which lead to single (outer shell) ionization of the multielectron atom. Positron impact can lead to ionization via two reaction channels usually called break up (of the atom into an electron and ion) and transfer (of one atomic electron to the projectile to form positronium. The most accurate positron ionization cross sections for example, for helium are presented in [1] and analysed in comparison with that for electron impact ionization. It should be noted that the features of particular interest are the merging of the cross sections above 600 eV when the first Born approximation is valid, the positron cross section exceeding the electron cross section at medium energies and a cross over of the cross section curves near threshold [1]. We suppose that a uniform theoretically comprehensive approach to the whole problem is needed. The most consistent approach to considered problems solving must base on QED. Here an energy approach in consistent gauge invariant formulation [2] has been used for consistent description of positron and electron collision (ionization) processes of the atom. In general form a scattered part for imaginary energy shift $Im\ \Delta E$ appears at first in the second order of the atomic perturbation theory in the form of integral over the scattered positron energy ε_{sc}: $\int d\varepsilon_{sc} G(\varepsilon_{iv}, \varepsilon_{ie}, \varepsilon_{in}, \varepsilon_{sc}) /(\varepsilon_{sc} - \varepsilon_{iv} - \varepsilon_{ie} - \varepsilon_{in} - i0)$ with $Im\Delta E = \pi G(\varepsilon_{iv}, \varepsilon_{ie}, \varepsilon_{in}, \varepsilon_{sc})$. Here ε_{in} *and* ε_{sc} are the incident and scattered energies respectively to the incident and scattered positron; G is a definite squired combination of the Coulomb and Breit inter particle interaction integrals [3]. We use further the optimized basis's of Dirac orbitals [2]. Preliminary results on positron impact ionization of helium are presented in table below and compared with results: A-Knudsen etal and B-Bielefeld (c.f.[1]).

Impact energy, EV	Measured A σ, (Å^2)	Measured B σ, (Å^2)	Calculated Present σ, (Å^2)
50	0,23	0,29	0,24
100	0,52	0,45	0,51
200	0,45	0,40	0,46

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P-61

THE BINOMIAL POTENTIAL OF ELECTRON-PROTON INTERACTION AND THE SOLUTION OF SOME PROBLEMS OF QUANTUM MECHANICS WITH ITS HELP

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In the given work some problems of the quantum mechanics are submitted as result of our incomplete representation about character of forces existing in interaction of electron with a proton. So if to present interaction of electron with a proton as the binomial potential:

$$V = -(e^2/r) + \Gamma/r^2$$

(1), where in the right part the first member represents a Coulomb's attraction of electron with a proton, and second - hypothetical pushing away of these particles, the simple and convincing answers can be given on many questions of the quantum mechanics. First of all, the answer to the most phenomenal question of the quantum mechanics is found: why in the theory of Schrödinger it is possible without sufficient representation about character of interaction of particles in system and without an explanation of oscillatory process to receive in the good consent with experiment discrete levels of energy. Further in work on the basis of potential (1) is shown the basic opportunity of the decision of a classical task of movement of electron in a field of a proton for atom of hydrogen, with an explanation of postulates of Bohr, a constant of Plank and other ratio, which could not be explained within the framework of the classical mechanics earlier. In the theory of Schrödinger with the help of potential (1) the opportunity has appeared to understand and to explain a number of its internal contradictions, including, for the first time in a task of atom of hydrogen it was possible to receive stable in time a wave package and to explain in classical interpretation the mechanism of birth of quantum. And in generally, potential (1) is submitted as a link between the classical and quantum theories. Thus, in the given work the attempt is undertaken to show, that potential of interaction of electron with a proton actually represents of two-members formula (1), instead of Coulomb's , as it is accepted now.

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UV-VUV BROADBAND EXCIMER-HALOGEN LAMP ON Ar-Kr-Xe-Br_2 MIXTURE

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In this report a results of investigation of excimer- halogen lamps radiation of low pressure in Ar-Kr-Xe-Br_2 and Kr-Xe-Br_2 mixtures with pumping the longitudinal glow discharge are present. The discharge was lit in a cylindrical quartz tube in length 10 cm. Internal diameter of a quartz tube made 14 mm. Radiation of plasma was registered with the help vacuum monochromator and photomultiplier FEU-142. The glow discharge was lit with the help of the high-voltage rectifier: Ich=1-50 mA, Uch=10 kW. Researches were carried out in a spectral range λ=130-300 nm.

At the low contents a bromine vapor in a mixture in a spectrum of radiation a spectral lines of atom of bromine (163.3 and 157.6 nm) were observed. The line 163.3 nm is analogue of a known line 206.2 nm atom of iodine which is widely used in iodine lamps of low pressure [1,2]. On bands of a molecule of bromine 289 nm, (185-170) nm, (210-185) nm etc., and also bromides bands of heavy inert gases the continuum with sharp border in the range of 165-300 nm was formed.

Optimization of an output of radiation of atoms of bromine, molecules of bromine and molecules XeBr and KrBr is given depending on pressure and partial structure of working mixtures.

In figure the results of optimization of contribution UV-VUV of radiation of a lamp depending on conditions of pumping are presented. For the glow discharge in Kr-Xe-Br_2 mixture a linear dependence of intensity of spectral line BrI and amplitudes of molecular bands from capacity which is entered in plasma was observed. Total capacity of radiation of a lamp on mixtures reached 5-7 W.

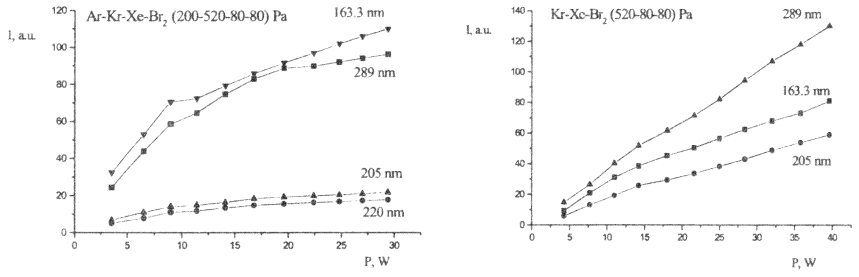

Figure 1. Dependence of relative intensity of spectral line BrI and amplitude of radiation of Br_2 band radiation of plasma of the glow discharge on Ar, Kr, Xe mixture with bromine vapors from capacity.

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K-,Fe-, Cu- PLASMA EMISSION SPECTRA IN LOW INDUCTIVE VACUUM SPARK. DIELECTRONIC SATELLITES LINES CALCULATION AND PLASMA DIAGNOSTICS

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Studying multi-charged ions plasma in a low inductive vacuum spark (LIVS) attracts a great interest because of importance for developing effective methods of plasma diagnostics [1]. We carried out analysis of experiments on studying the spectra satellite structure in the *K, Cu, Fe*-plasma in the LIVS. The results of calculation of the *K-,Fe-,Cu-* plasma *Li*-like satellite lines on the basis of the relativistic perturbation theory (PT) [2] and optimized Dirac-Fock (DF) method are presented and compared with experiment. Multi-numbered atomic calculations of the plasma elementary processes coefficients have shown that an adequate description of these processes can be only reached under using optimized basis's of wave functions. Hitherto this is one of the most fundamental problems. In ref. [2] it has been proposed a new fundamental approach to solving the cited problem. The optimized basis's of Dirac orbitals can be got from minimization principle for contribution of fourth QED PT diagrams to imaginary part of energy shift ImδE [2]. The minimization of functional ImδE_{ninv} leads to the integral differential equation system that can be solved using one of the standard numerical codes. In result we get the optimized basis of the Dirac relativistic orbitals. We have carried out a detailed comparison for probabilities and intensities of transitions, corresponding to the *Li*-like lines of dielectronic satellites to line $1s^{21}S_0$-$1s3p^1P_1$ of the LIVS Cu plasma radiation, calculated within our method (column D) and other theoretical approaches: PT on 1/Z (B), AUTOJOLS (C) (see table). It is carried out an estimate of the electron temperature (~2,56 keV) under electron density $10^{23}sm^{-3}$ in the LIVS, using relations between intensities of the dielectronic satellite lines and resonant lines of He-like ions.

Table. Experiment (A) and theoretical wavelengths (Å) and transition probabilities ($10^{13}s^{-1}$) for Li-like lines of the dielectron satellites in the Cu plasma in LIVS

Transitions	Transition probability			Wavelength			Wavelength
	B	C	D	B	C	D	A
$1s^22p^2P_{1/2}$ - $1s2p3p^2D_{3/2}$	58,8+1	55,7+1	56,5+1	1,2702	1,2700	1,2701	
$1s^22p^2P_{3/2}$- $1s2p3p^4D_{5/2}$	86,4+1	88,6+1	88,0+1	1,2702	1,2703	1,2702	1,2700±
$1s^22p^2P_{3/2}$- $1s2p3p^4S_{1/2}$	24,00	1,80	5,80	1,2713	1,2750	1,2731	0,0010
$1s^22p^2P_{3/2}$- $1s2p3p^4P_{3/2}$	14,10	12,0	13,1	1,2718	1,2719	1,2717	

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NEW CO-OPERATIVE LASER-ELECTRON NUCLEAR EFFECTS IN SPECTRA OF O-AND F-LIKE MULTICHARGED IONS IN PLASMA

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A great progress in development of laser technique and accelerators experiments resulted to a new class of problems in the plasma physics and diagnostics. It should be noted on a possibility of the using co-operative phenomena [1,2] due the interaction between photon, electron shells, nuclei nucleons for diagnostics. Attractive situation arises under transition from neutral atoms to multi charged ions due to the changing energy and geometric parameters. Possible new approach to the multi charged ion plasma diagnostics using the new laser-electron-nuclear effects is discussed. We consider a possibility of the experimental observation of set of the electron satellites in spectra of the electron-nuclear γ-transition of the nucleus in a multi charged ion-thermalized plasma. The nuclear transition in the isotope of Fe^{57} with energy 14,41 keV is considered for O-and F-like ions of Fe. The electron-nuclear lines in spectra of emission is calculated within QED energy approach [2] (see fig.1). It can be observed in the plasma of the O-and F-like ions and it is important that they are not overlapping by the Doppler broadening. One can suppose that K shell is significantly destroyed. Average kinetic energy for ions in such plasma $\sim E_i/10 \sim 1/20$c.u. (Coulomb units), where E_i is the 1s electron bond energy. The Doppler shift is $d\bullet\ \omega_D \approx aw/(10M)^{1/2}$; here aw is connected with γ quantum energy as: E[keV] $\approx 4Zaw$. If, say, aw=1, then $d\bullet\ \omega_D \approx 1/200\ (Z)^{1/2}$c.u. $\approx 0{,}15\ (Z)^{1/2}$ eV. For comparison let us give the values of the 1s,2s,2p-2p transition energies for one-electron ions with Z=10-50: $E(1s\text{-}2p_{3/2})=1{,}3\cdot 10^3\text{-}2{,}3\cdot 10^4$eV, $E(2s\text{-}2p_{3/2}) \approx E(2s\text{-}2p_{3/2}) = = 0{,}1\text{-}3{,}3\cdot 10^2$eV. Obviously the transition energies have an order of the Doppler shift. Calculated relative (to nuclear transition) intensities for the transitions: nl-n'l' (n=1-3, l=0-2) are~2-7(10^{-5}).

New consistent, quantum- mechanical approach to calculation of the electron-nuclear γ transition spectra (set of vibration-rotational satellites in molecule) of nucleus in molecule is proposed and based on the Dunham model potential approximation for potential curves of the diatomic molecules. Estimates are made for vibration-rotation-nuclear transition probabilities in a case of the emission and absorption spectrum of nucleus ^{127}I ($E^{(0)}_{\gamma}$= 203 keV) linked with molecule $H^{127}I$ [2].

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P-65

LASER PHOTOEXCITATION AND PHOTODISSOCIATION OF MOLECULES: OPTIMIZED SCHEMES

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Selective photo-ionization and photo-dissociation of molecules method is supposed to be very much perspective method for cleaning the semiconductor materials from molecular admixtures and other applications. In Los Alamos laboratory it was at first shown possibility of selective one-quantum dissociation of the admixtures molecules (PH_4 and other) by UV radiation of ArF excimer laser under action on molecules of SiH_4 . Laser cleaning of mono-silan represents a great interest for technology of obtaining a poor Si in the semiconductor industry. One of the important problem is carrying out the optimal schemes of laser photo-ionization and dissociation processes for molecules. Here we present a new multi-level optimized model for definition of the optimal form of laser pulse to reach the maximal effectiveness of laser action in process of laser photoionization (dissociation) of molecules. Model is based on differential equation of the Focker-Plank type in the partial derivatives for density of molecules with the vibration energy x on a chosen vibration level and operators, describing the RT relaxation and action of external radiation correspondingly [2]. As example, let us consider the conditions and parameters for optimal excitement for molecules of HCl (PH_3,CF_3Br, SiH_4 are also considered). In fig. we present the data of computer testing optimized model for HCl molecules (T=300K) and dependence (of number of particles) of the functional: $I(u)=\int f(x_1,t_1;x_2,t_2)h(x)dx$ in the energy interval $x\in[15,21]$ (in units of kT) upon x_1 and wavelength of laser radiation, corresponding to rotational transition x_1-x_2. Here $h(x)$ is some function., corresponding to required form of the final distribution $f(x,t,u)$, i.e. density of molecules with vibration energy x at moment $t \in [0,R]$. An important moment of calculation is connected with account for the real form of laser pulse [2]. Testing of model is carried out also for molecule PH_3 under laser UV radiation action on molecules of SiH_4. It is found the optimal set of physical parameters to provide an optimality of process.

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P-66

EMISSION DESCRIPTIONS OF PLAZMA OF TRANSVERSAL VOLUME DISCARGE IN PROPAN.

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Presently there is substantial progres in the development of the electro discharge chemical HF(V) and DF(V) lasers the radiation of which gets in the transparance window atmosphere.

One of the basic lacks of such lasers is the low resource of work in the gas-static mode. For better understanding of reasons which reduce the resource of work of these lasers it is necessary to conduct the special researches of molecule destruction of SF_6 propan and hydrogen in trasnsversal discharge.

In the report some experimental results breakbase of molecule of propan are presented in the transversal discharge of nanosecond duration, that is a part of the program of works on diagnostics of plasma discharge of chemical HF(V) lasers by the method of emission spectroscopy with temporal resolution.

The experiment was conducted on setting resolution the basic knot of which was a caprolon cylinder with the system of spherical aluminium electrodes and the system of preionization. Between them a transversal discharge lights up with the volume of (0,2–2)×12 cm^2. The radiation from discharge chamber was output on vacuum monohromator, and was registered in the wavelength range 100–300 nm. For the separation of monohromator from plasma the LiF window was used.

In the figure 1 typical spectogram of radiation of the mixture is presented He/C_6H_{12} (P HE – 100 torr, P C_6H_{12} – 3 torr, U=8 kB).

It is the wind band of continuons radiation on with a sharp channel in an ultraviolet region is observed on which the series of bands of fragments of molecule of propan is not claribied querlapped. What concernt to a band in region of λ=249 nm its identification on this moment is not found out. The similar spectra are received at other values of partial pressures and mixture molecule.

At present time they find dependence of brigthness of bands which were observed in the radiation spectrum of the discharge from propan pressure and the size. Of energycontribution.

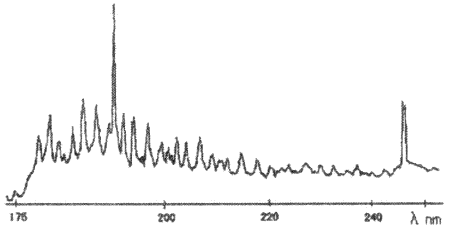

Figure 1. Typical spectogram of radiation of the mixture He/C_6H_{12}=100/3 torr.

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ELECTRON-IMPACT IONIZATION OF BARIUM ATOMS OUT OF THE TRIPLET METASTABLE STATES

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The process of ionization of barium atoms from the $6s5d^3D_{1,2,3}$-states has been studied using the crossed atomic and electron beam method. Atomic beam was formed by a thermo-effusion source and a system of collimating slits. Atoms were converted into the metastable states in an electric discharge with further separation of charged particles and atoms in short-lived excited states. Electron beam was produced by a five-electrode Pearce-type electron gun. The incident electron energy was varied from the threshold up to 20 eV at the electron energy spread not worse than 0.5 eV. Ions resulted from electron interaction with metastable atoms were collected by a special probe being a part of original detection system. Experiments were carried out at the working chamber vacuum of $\sim 10^{-7}$ Torr. The technical design of the experimental setup and the measurement technique are discussed in detail elsewhere (see, e.g., [1]). High reliability of results obtained using this experimental approach has been confirmed in our previous papers [1, 2].

As a result of the studies, we have obtained the absolute value of ionization cross section out of the triplet metastable states as well as the dependence of the above cross section on the incident electron energy. It has been found that the maximum cross section $Q^i_{max} = 3{,}2 \cdot 10^{-15}$ cm^2 is reached at the electron energy of $E_{max} = 6.6$ eV.

Present experimental results are compared to the theoretical calculations presented in [3]. It has been found that the theoretical data differ considerably from the experimental ones both by the maximum absolute value of ionization cross section and by the position of the maximum (see table).

Table. Effective ionization cross section for Ba atom out of the triplet metastable states

Q^i_{max}, 10^{-15} см^2		E_{max}, eV	
Present paper	Calculated [3]	Present paper	Calculated [3]
3.2	1.8	6.6	10

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INVESTIGATION OF THE SLOW-ELECTRONS INELASTIC INTERACTION WITH NUCLEIC ACID BASES MOLECULES

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The study of low energy electrons interaction with biomolecules is of particular interest not only for physics, but also in biomedical and ecological applications. Such investigations allows one to obtain the information unreachable by using other methods. In the present work we report on the results of spectral and mass-spectrometric studies of slow electrons collisions with nucleic acid bases molecules.

Investigation were carried out using crossed electron and molecular beam method. The experimental setup consists of such principal components as: molecular and electron beam sources, collision chamber, vacuum system, photon and ion detection systems. The molecular beam was obtained using special microchannel source, the electron beam – by means of five-electrode electron gun. The energy of the monoenergetic electron beam was varied in the 0,3–300 eV range. The molecules concentration was determined directly in experiment and was equal to $8 \cdot 10^{10}$ cm^{-3}. The electron beam current was about $2 \cdot 10^{-6}$A with an energy spread of $\Delta E_{1/2} \sim 0{,}3$ eV (FWHM). The electron gun was located in lengthwise magnetic field with induction $1{,}2 \cdot 10^{-2}$ Tl. The energy scale was calibrated using SF_6^- anions recorded in the same experimental conditions. The peculiarity of this experimental setup is the possibility of analysis not only radiation but also the positive and negative ions.

The emission spectra of the nucleic acid bases molecules (cytosine, thymine, adenine, uracile and guanine) excited by electron impact were obtained within the 200-600 nm range. This spectra have the compound structure, noticeably to differ from the photoexcitation ones. The excitation functions (the energy dependences of the excitation cross section) of biomolecules were measured in the electron energy range from the threshold up to 300 eV. Compound spectra are the results of various physical processes that take place simultaneously at the electron interaction with biomolecules. First of all, there are the direct excitation of singlet and triplet molecular levels and dissociative excitation too. The ionization function (for positive and negative ions) and threshold features are investigated. The absolute value of the cross sections positive and negative ions formation of the nucleic acid bases molecules was found in the direct experiment for the first time using our original technique. For example, the energy dependence of the effective cross sections for cytosine negative ions formation has the distinct resonance at 1.5 eV electron energy. Maximal ionization cross section is $4.2 \cdot 10^{-18}$ cm^2 and include the cross sections of the negative ion formation both for the whole molecule and its fragments. It is important, that probable damage of the nucleic acid molecules at low electron energy would have a place in consequence of the resonant, practically nonthreshold mechanism of the negative ions formation. The absolute value of the cross sections for positive cytosine ions is $7.8 \cdot 10^{-16}$ cm^2.

Thus, the physical processes (excitation, ionization, dissociative excitation and dissociative ionization) induced by low-energy (0,3-300 eV) electrons were investigated in the nucleic acid base molecules. Biophysical and radiological consequences of the inelastic processes caused by electron impact in biomolecules were analysed.

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OPTICAL CHARACTERISTICS OF A REPETITIVE VOLUME DISCHARGE IN A KRYPTON WITH FREON-12 MIXTURE

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In this work, we study the characteristics of a repetitive volume discharge in freon-12 and its mixtures with krypton.

The discharge operated in the an electrode system consisting of a spherical anode and a plane cathode with an interelectrode distance of 3 cm. Positive voltage was applied to the anode from a dc power supply with voltage 1 kV. Ballast resistance (20 kΩ) was used to limit the current and to stabilize the discharge. The mean discharge current was within 2 50 mA. A description of the experimental facility is given in [1].

The brightness of the UV radiation of plasma formed from pure freon-12 was 4 5 times lower than that of the discharge in the Kr/CF_2Cl_2 mixture. In the spectrum of the volumetric discharge in the Kr/CF_2Cl_2 mixture, the band of KrCl(B X) at 222 nm and the band of Cl_2^{**} at 200 nm were the brightest (Fig.1). The KrF(*B X*) emission band at 249 nm was also observed in the spectrum.

The study of the optical characteristics of the plasma of a short volumetric discharge in the Kr/CF_2Cl_2 mixture demonstrated that the glowing discharge exists in the repetitively pulsed mode (0.2-55 kHz) as a solitary domain. Shunting of the discharge gap with a pulse capacitor makes it possible to control the parameters of the current pulse and the discharge radiation pulse. To obtain the highest mean brightness of the UV radiation, mixtures with pressure ratio $P(Kr)/P(CF_2Cl_2)$=(400-600)/(80-120) Pa were optimal. The highest power in the radiation pulse was attained at a mean discharge current lower than 6 mA. On the basis of a discharge of this type, it is possible to develop a simple repetitively pulsed excimer-halogen lamp in which the active medium itself serves as a commutator.

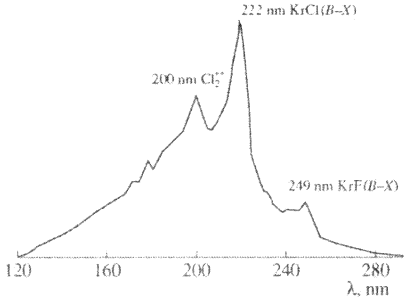

Fig.1. Plasma radiation spectra of a volumetric discharge in a mixture $P(Kr)/P(CF_2Cl_2)$=640/120 Pa.

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TWO-PHOTON EXCITATION OF ODD-PARITY STATES FROM THE GROUND STATE OF THE Ca ATOM

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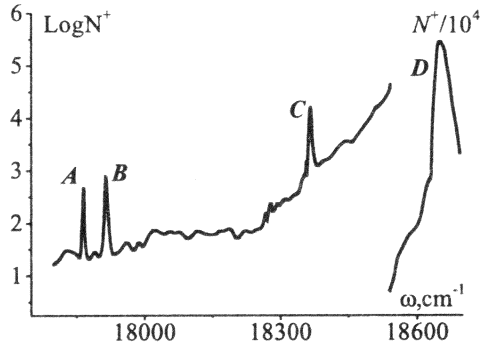
We studied experimentally the multiphoton transitions in the *Ca* atom induced by dye laser radiation (17800–18700cm^{-1}). The absorption of three photons of laser radiation is required to ionize Ca atoms. Absorption of two photons can excite the atoms to a number of states with different parity. The results obtained with the linearly polarized laser radiation are shown in the figure. One can see that, as the frequency varies from the resonance maximum to the interresonance intervals, the yield of Ca^+ ions changes significantly (by a factor of up to ~10^8).

It also follows from the figure that the dependence of the Ca^+ ion yield on the laser radiation frequency exhibits a distinct resonance structure with peaks of various amplitude. Analysis shows that only one of these maxima (labeled by the symbol *D* in the figure) can be identified according to the selection rules in the dipole approximation. This peak is associated with the two-photon transition from the ground $4s^{21}S_0$ state to the $4s4d^1D_1$ state. As for the other maxima (*A B C*) of the dependence $N^+(\omega)$, they cannot be associated, in the dipole approximation. At the same time, the frequencies of laser radiation corresponding to these maxima coincide with the frequencies of two-photon transitions forbidden in the dipole approximation by the parity selection rules: $4s^{21}S_0$ - $4s4p^3F_2^o$ (maximum *A*); $4s^{21}S_0$ - $5d4p^1D_2^o$ (*B*), and $4s^2\,^1S_0$ -$3d4p^1P_1^o$ (*C*). In these maxima, the yield of Ca^+ ions exceeds the yield in the interresonance intervals by two orders of magnitude. Note that the transitions corresponding to maxima *A B* and *C*, as well as the transition gives rise to maximum *D*, are two-photon transitions. However, unlike the transition associated with maximum *D*, each of the first three transitions consists of one virtual transition forbidden in the dipole approximation by the parity selection rules and another allowed transition.

Note that the single-photon transitions forbidden in the dipole approximation (the quadrupole transitions) have already been observed upon multiphoton ionization. As for the two-photon transitions forbidden in the dipole approximation, they have not yet been observed upon multiphoton ionization.



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CROSS SECTION CALCULATIONS FOR ELECTRON SCATTERING FROM SIMPLE BIOMOLECULES

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Ionising radiation damage to living cells is usually studied with Monte Carlo track structure codes. Recent experimental studies [1] have shown that low- and intermediate-energy electrons can induce significant damage to DNA via scattering processes. Thus the complete set of cross sections for electron collisions with DNA and its building blocks can be useful for further more detailed Monte Carlo analysis of ionising radiation damage to biomolecules. We present results of our recent calculations of impact ionisation and elastic cross sections for electron scattering from DNA and RNA bases [2] as well as simple sugar-phosphate analogues [3]. Also new results of our recent calculations for electron scattering from other simple biomolecular compounds will be presented and discussed. Differential and integral cross sections for elastic collisions between electrons and studied components have been calculated using independent atom method [4] with a static-polarization model potential. Cross sections for electron-impact ionisation of theses molecular targets have been derived using the binary-encounter-Bethe model [5].

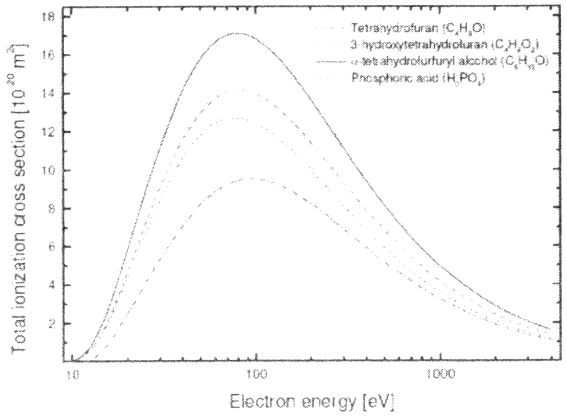

Figure 1. Electron impact ionisation cross section for simple sugar-phosphate analogues [3].

The work is a part of research programme sponsored by the Ministry of National Education and by the Ministry of Scientific Research and Information Technology.

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TOTAL CROSS SECTION MEASUREMENTS FOR ELECTRON COLLISIONS WITH NO_2 MOLECULES

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Comprehensive sets of cross section data for electron scattering with nitrogen oxides (NO_x) are of great importance when modelling of physico-chemical atmospheric processes.

In this work we present absolute total cross section for electron collisions with NO_2 molecules within 5-370 eV energy range. Measurements have been carried out using home build electrostatic electron spectrometer working in the linear transmission configuration [1]. In that system, monoenergetic (FWHM ~ 60 meV) electron beam produced with 127^0 dispersing element interacts with a sample gas within a scattering chamber; unscattered electrons are registered with the Faraday cup collector. The absolute total cross section at each electron impact energy is derived from the Bouguer-de Beer-Lambert attenuation formula using electron beam intensities in the presence and absence of the target in the scattering cell, target gas pressure and its temperature, as well as the length of the electron trajectory within interaction volume.

Present experimental total cross sections agree well according to the shape with data from earlier investigations [2,3] in the common energy range, however, some differences in the magnitude are observed. More results and detailed discussion will be presented at the Conference.

The work is a part of research programme sponsored by the Ministry of National Education (MENiS) and by the Ministry of Scientific Research and Information Technology (MNiI).

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AUTHOR INDEX

POST-DEADLINE ABSTRACTS

MEASUREMENT OF INNER SHELL IONIZATION CROSS SECTIONS BY LOW-ENERGY POSITRON IMPACT

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Threshold behavior of the cross sections for Cu K-shell and Ag, In and Sn L-shell ionization by positron impact has been studied by detecting the characteristic x-rays from thin film targets [1]. Development of an x-ray detector with thin Si(Li) crystals has enabled the measrements in this energy range from near threshold to tens of keV [2].

The determined values are plotted in figure 1 against the positron impact energy. They have been compared with the theoretical results calculated in the binary encounter formalism [3]. The values for the Cu K- and Ag L-shells have also been compared with the results in the plane wave Born approximation with Coulomb and relativistic corrections [4]. The measured cross sections for the Cu K-shell are in good agreement with the theories. The results for the Ag, In, and Sn L_3 shells are, however, smaller than the theoretical calculations. Discrepancies between experimental results and theoretical calculations are also observed for L x-ray production cross sections by electron impact [5].

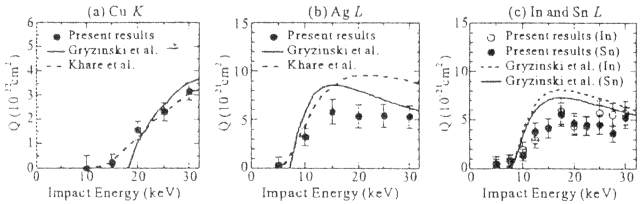

Figure 1: Inner shell ionization cross sections plotted against the positron impact energy. Theoretical results [3, 4] were also plotted.

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Multi Particle Effects in the Coulomb Continuum

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It has been shown that dynamical screening of Coulomb-interacting particles in the continuum is quite successful in describing ionization processes near threshold [1] if multi particle effects are important. This ansatz is extended from three to four interacting particles so that (e,3e) on helium can be described in the framework of Coulomb-waves without further approximations.

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